Polymer dynamics via cliques with applications to hard-sphere mixtures

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Abstract

Abstract polymer models are systems of weighted objects, called polymers, equipped with an incompatibility relation. An important quantity associated with such models is the partition function, which is the weighted sum over all sets of compatible polymers. Various approximation problems reduce to approximating the partition function of a polymer model. Central to the existence of such approximation algorithms are weight conditions of the respective polymer model. Such conditions are derived either via complex analysis or via probabilistic arguments. We follow the latter path and establish a new condition—the clique dynamics condition—, which is less restrictive than the ones in the literature. The clique dynamics condition implies rapid mixing of a Markov chain that utilizes cliques of incompatible polymers that naturally arise from the translation of algorithmic problems into polymer models. This leads to improved parameter ranges for several approximation algorithms, such as a factor of at least $2^{1/\alpha}$ for the hard-core model on bipartite $\alpha$-expanders.

Additionally, we apply our method to approximate the partition function of the multi-component hard-sphere model, a continuous model of spherical particles in the Euclidian space. To this end, we define a discretization that allows us to bound the rate of convergence to the continuous model. To the best of our knowledge, this is the first algorithmic application of polymer models to a continuous geometric problem and the first rigorous computational result for hard-sphere mixtures.

Keywords: Markov chain • partition function • Gibbs distribution • approximate counting • abstract polymer model
1 Introduction

Statistical physics models systems of interacting particles as probability distributions. This viewpoint explains a variety of real-world phenomena, including ferromagnetism [28], segregation [49], and real-world network generation [8]. A characteristic of such systems is that they undergo phase transitions depending on some external parameter. Such phase transitions have been recently linked with the tractability of computational tasks. These connections have lead to a two-way exchange: tools from statistical physics are used to explain computational phenomena, and tools from computer science are used to explain physical phenomena. An established technique for investigating phase transitions in statistical physics that involves translating the states of a spin system as perturbations from a ground state [16, Chapter 7] has been recently introduced to computer science as an algorithmic tool for computational tasks of spin systems [27].

To motivate the definition of the central mathematical object of this article, we give a high-level description of how to model a spin system in terms of perturbations from a ground state. Assume we want to study a spin system on a graph $G$. The states of the spin system are usually mappings $\sigma : V(G) \rightarrow Q$ from the vertices of $G$ to some finite set $Q$. Each such configuration $\sigma$ has a weight $w(\sigma) \in \mathbb{R}_{\geq 0}$ and the sum of the weights of all the configurations $Z = \sum_{\sigma} w(\sigma)$ is called the partition function. The probability distribution that characterizes our system gives $\mu(\sigma) = w(\sigma)/Z$, for each configuration $\sigma$. Let $\sigma_0$ be the ground state we use in this translation. Given a configuration $\sigma$, we identify the set of vertices $D \subseteq V(G)$ where, for each $v \in D$, we have $\sigma_0(v) \neq \sigma(v)$. Observe that we can uniquely identify this configuration by a set $\Gamma$ whose elements $y$ consist of a connected component of $G[D]$ together with the restriction of $\sigma$ on this component. Furthermore, we assign a weight $w_y$ to each $y \in \Gamma$, such that $\prod_{y \in \Gamma} w_y = w(\sigma)/w(\sigma_0)$. Thus, provided that all such sets of pairs $\Gamma$ contain no two pairs $y, y'$ that are incompatible, i.e., $\Gamma$ cannot be uniquely decoded to an assignment because for example $y$ and $y'$ map the same vertex to a different element in $Q$, there is a bijection between the configurations $\sigma$ and the sets $\Gamma$. Furthermore, the distribution $\mu$ is expressed as a distribution over the sets $\Gamma$, since it retains the property that the probability of $\Gamma$ is proportional to its weight. Such a construction suggests the following definition.

A polymer model $\mathcal{P} = (C, w, \star)$ is a tuple consisting of a non-empty, countable set $C$, a set $w = \{w_y\}_{y \in C}$ of positive real weights and a reflexive and symmetric relation $\star \subseteq C^2$. The elements $y \in C$ are called polymers. The relation $\star$ is called the incompatibility relation and, for $y, y' \in C$, we say that $y$ and $y'$ are incompatible if $y \star y'$, and that they are compatible otherwise. In addition, we call a finite subset $\Gamma \subseteq C$ a polymer family if and only if all polymers of $\Gamma$ are pairwise compatible. Given a polymer model $\mathcal{P}$, we let $\mathcal{F}(\mathcal{P})$ denote the set of all polymer families of $\mathcal{P}$. Note that $\mathcal{F}(\mathcal{P})$ is countable. The partition function of $\mathcal{P}$ is defined to be,

$$Z(\mathcal{P}) = \sum_{\Gamma \in \mathcal{F}(\mathcal{P})} \prod_{y \in \Gamma} w_y,$$

which we require to be finite. Further, the Gibbs distribution of $\mathcal{P}$ is the probability distribu-
tion $\mu^{(P)}$ over $\mathcal{F}^{(P)}$ such that, for all $\Gamma \in \mathcal{F}^{(P)}$,

$$
\mu^{(P)}(\Gamma) = \frac{\prod_{\gamma \in \Gamma} w_{\gamma}}{Z(P)} .
$$

(2)

A helpful interpretation for understanding the definition of a polymer model is the following. Ignoring the reflexivity of $\sim$, we view the pair $(C, \sim)$ as a graph, which we call the polymer graph. We observe that the families of $\mathcal{F}^{(P)}$ correspond to the independent sets of $(C, \sim)$. Thus, for the special case where $w_{\gamma} = \lambda \in \mathbb{R}$, for each $\gamma \in C$, the distribution $\mu$ is the hard-core model [48] on the polymer graph and $Z(P)$ is the independence polynomial [44].

In this article, we consider the following two computational tasks:

1. Approximately sampling from the Gibbs distribution of a polymer model, that is, return a random family $\Gamma$ from a distribution whose total variation distance from $\mu^{(P)}$ is at most $\epsilon$.

2. Returning an estimate $\tilde{Z}$, such that $(1 - \epsilon)Z(P) \leq \tilde{Z} \leq (1 + \epsilon)Z(P)$.

1.1 Known algorithmic results

There is an expanding list of results that utilize abstract polymer models to obtain efficient approximation and sampling algorithms for new parameter regimes for various spin systems on graphs. This line of research was initiated by Helmuth et al. [27], who used polymers to obtain polynomial-time approximation and sampling algorithms at a regime where the weight of the interactions of particles with an external field is low. Creative ways of translating a spin system into a polymer model utilize restrictions upon the input graph of a spin system in order to yield polynomial-time approximation algorithms for problems that are hard to approximate on general inputs. Such examples include spin systems on expander graphs [19, 30, 38], the hard-core model on unbalanced bipartite graphs [5], and the ferromagnetic Potts model on $d$-dimensional lattices [2]. Polymer models have also been used to approximate and sample edge spin systems (holant problems) at low temperatures [6].

Translating a spin system on a graph $G$ with $n$ vertices into an abstract polymer model commonly results in a polymer model that contains an exponential number of polymers in terms of $n$—as can be observed in our earlier discussion of such a translation. Therefore, the approximation and sampling algorithms we are interested in have runtime polynomial in $n$. There are two main algorithmic approaches for such algorithms.

(i) Cluster expansion This approach considers complex weights for the polymers and is based on the cluster expansion, an infinite series expansion of $\ln Z$. The essential element for polynomial-time computation is a theorem of Kotecký and Preiss [36, Theorem 1], a condition for establishing absolute convergence of the cluster expansion. By satisfying the Kotecký–Preiss condition, one can truncate the cluster expansion to its most significant terms and obtain an $\epsilon$-additive approximation for $\ln Z$. Computing the significant terms of the cluster expansion can be achieved by enumerating connected induced subgraphs of the polymer graph of size up to $\log |C|$. Using an algorithm of Patel and Regts [42], the enumeration takes polynomial time in terms of the input graph of the spin system. The $\epsilon$-additive approximation of $\ln Z$
immediately gives a multiplicative $\varepsilon$-approximation for $Z$. The runtime of this approach is commonly $O(n \log \Delta)$, where $\Delta$ is the maximum degree of the input graph $G$ for the spin system and $n = |V(G)|$. Approximating $Z$ together with the self-reducibility of the polymer model obtained gives a sampling algorithm for $\mu^{(P)}$, as shown by Helmuth et al. \cite{27}.

(ii) Markov chain Monte Carlo The first to use the Markov chain Monte Carlo method on polymers are Chen et al. \cite{7}. The idea of this method is to define a Markov chain with state space $\mathcal{F}^{(P)}$ and with stationary distribution $\mu^{(P)}$. The Markov chain requires the polymer model to have originated from a spin system on a graph $G$ with $n$ vertices. In each iteration, the chain samples a polymer $\gamma$ with probability proportional to its weight $w_\gamma$ and then adds or removes $\gamma$ from its state if possible. When the mixing condition \cite[Definition 1]{7} is satisfied, it is shown that the Markov chain converges to $\mu^{(P)}$ after $O(n \log n)$ many iterations. The mixing condition matches a convergence condition arising from an analysis by Fernández et al. \cite{14} of another stochastic process of polymers on lattices. An $\varepsilon$-approximate sampler for $\mu^{(P)}$ can be obtained by simulating the Markov chain. The computational challenge for this approach is to sample the polymer $\gamma$ in order to perform a transition of the Markov chain. As Chen et al. \cite{7} show, this can be done in expected constant time provided the sampling condition \cite[Definition 4]{7} is satisfied. This results in an $O(n \log n)$ algorithm for sampling from the Gibbs distribution of a spin system. Using simulated annealing, Chen et al. show that this sampler can be converted to a randomized approximation scheme (FPRAS) for $Z$ that runs in expected $O(n^2 \log n)$ time.

Comparison of the known conditions A number of conditions for the convergence of the cluster expansion has appeared in the literature, such as \cite{11,15,36}. The condition of Fernández and Procacci \cite{15} is the least restrictive among them, that is, the Kotecký–Preiss condition \cite{36} and others appearing in the literature imply the Fernández–Procacci condition. Thus, using the Fernández–Procacci condition, one could potentially obtain approximation algorithms for broader parameter ranges than the ones obtained by using the Kotecký–Preiss \cite{36} condition. However, the condition by Kotecký and Preiss \cite{36} is convenient to apply in polymer models of vertex spin systems and comes with implications on the rate of convergence of the cluster expansion used in algorithmic settings. When compared to cluster expansion conditions (restricted to non-negative real weights), the mixing condition of Chen et al. \cite{7} is less restrictive than the Kotecký–Preiss condition, however, it is incomparable with the condition of Fernández and Procacci \cite{15}. Note that the sampling condition \cite{7} the most restrictive of the aforementioned conditions.

1.2 Our results

We study a new Markov chain $(X_t)_{t \in \mathbb{N}}$ for abstract polymer models, whose stationary distribution is $\mu^{(P)}$. The dynamics of our Markov chain are based on a clique cover, that is, a set $\Lambda = \{A_i\}_{i \in [m]}$ with $\bigcup A = C$, such that the polymers in each clique $A_i$ are pairwise incompatible. Observe that when we consider families of compatible polymers in $A_i$, they contain at most one polymer. Our Markov chain at each step chooses uniformly at random a clique $A_i$ in $\Lambda$ and samples a family in $A_i$ according to the distribution $\mu_{|A_i}$ defined as follows. For $\gamma \in A_i$, we
have \( \mu_{|A_i}(\{y\}) = w_Y / Z_{|A_i} \) and, for the empty set, \( \mu_{|A_i}(\emptyset) = 1 / Z_{|A_i} \), where \( Z_{|A_i} = 1 + \sum_{y \in A_i} w_Y \).

If the family chosen is the empty family and \( X_t \) contains a polymer from \( A_i \), then the chain removes this polymer. If the family chosen contains a polymer, then, if possible, the chain adds this polymer to its state. For a detailed description of our chain, please refer to Definition 3.

Our chain applies to any abstract polymer model, since we can always use the trivial clique cover, where each clique contains exactly one polymer. However, clique covers with a much smaller number of cliques arise naturally from the translation of spin systems into a polymer model. For example, the translation we discussed earlier in the introduction yields a clique cover with \( n \) cliques, one for each vertex in the original graph \( G \). Since such cliques commonly have exponential size, our chain utilizes that a family of compatible polymers may contain at most one polymer from each \( A_i \). The chain in Chen et al. [7] also utilizes this fact, however, in a more restricted setting and with a different sampling distribution for each vertex-clique. An additional nice feature of our chain is that it coincides with the (spin) Glauber dynamics (cf. [13, insert/delete chain]) when considered with the trivial clique cover. This comes from the choice of sampling from \( \mu_{|A_i} \) for each clique chosen at each iteration.

Central to our mixing time analysis for this chain is the following condition.

\[ \text{◮ Condition 1 (clique dynamics). Let } \mathcal{P} = (C, w, *) \text{ be a polymer model, and let } f : C \rightarrow \mathbb{R}_{\geq 0}. \text{ We say that } \mathcal{P} \text{ satisfies the clique dynamics condition with } f \text{ if and only if, for all } y \in C, \text{ it holds that} \]

\[ \sum_{y' \in C : y' \neq y, y' \sim y} f(y') \frac{w_{y'}}{1 + w_{y'}} \leq f(y). \]

\[ \text{◭} \]

We show that when the clique dynamics condition is satisfied, the mixing time of our Markov chain is polynomial in the number of cliques in our clique cover and logarithmic to the choice of function \( f \) (Theorem 6). Note that our condition does not exclude polymer models with \( w_Y \geq 1 \) for some polymer \( y \). When restricted to the setting of Chen et al. [7], the clique dynamics condition is implied by the mixing condition and thus less restrictive. Involving the function \( f \) in our condition makes it easily comparable with the conditions for cluster expansion. As we discuss in Section 3.1, we show that the clique dynamics condition is more general than the Fernández–Procacci [15] condition for the cluster expansion—and consequently more general than the Kotecký–Preiss condition [36]. An interesting implication of our analysis is that cluster expansion conditions imply our condition for the mixing time of a Markov chain. To the best of our knowledge this is the first such connection. We conjecture that our condition can be further generalized, as tightness results indicated by hardness of approximation are restricted to the special case of the hard-core model [1, 17, 18, 45]. No such results are known for polymer models.

1.2.1 Methodology

To obtain the mixing time bound, we use coupling. The high-level idea of this technique is to define a potential \( \delta \) expressing distances between the states of the Markov chain \( Z_t \). If two (commonly correlated) copies \((X_t, Y_t)\) of the Markov chain \( Z_t \) after \( k \) transitions result in states such that \( \delta(X_k, Y_k) = 0 \) with high probability, then \( k \) bounds the mixing time of the Markov chain.
chain $Z_t$. One way of using this method, known as path coupling, is to define the metric on only adjacent pairs of states; in our setting, these are polymer families $\Gamma, \Gamma'$, where $\Gamma \cup \{\gamma\} = \Gamma'$ for some polymer $\gamma$. The metric $\delta$ is then extended to all pairs in the state space by considering a shortest path of adjacent pairs and summing their distances in terms of $\delta$. To obtain a bound on the mixing time then, we could apply a theorem of Dyer and Greenhill [12]. The theorem requires to show that the distance between $X_t$ and $Y_t$ when they are in adjacent states, reduces in expectation, i.e., $\delta(X_{t+1}, Y_{t+1} | X_t, Y_t) \leq \delta(X_t, Y_t)$. When the latter inequality is strict, the theorem implies a bound on the mixing time of the Markov chain $Z_t$ that is logarithmic in $D$—the diameter of the metric space defined by $\delta$. When the inequality is not strict, this results in a mixing time linear in $D$.

When interested in polymer models that come from a spin system on a graph $G$, the diameter $D$ of the metric chosen on the state space of $X_t$ can be exponential in $n$, as it depends on the choice of the function $f$ appearing in the clique dynamics condition. We show that if $\delta(X_{t+1}, Y_{t+1} | X_t, Y_t) < \delta(X_t, Y_t)$ for some appropriately chosen $\delta$, then it suffices to use the theorem of Dyer and Greenhill [12] to obtain the required mixing time bound. This is achieved if we assume that the inequality in clique dynamics condition is strict. However, the condition then becomes incomparable with the Fernández–Procacci [15] condition.

To make the conditions comparable, we revisit a theorem of Greenberg et al. [20] that gives a mixing time bound logarithmic in $D$ when $\delta(X_{t+1}, Y_{t+1} | X_t, Y_t) \leq \delta(X_t, Y_t)$. However, as we discuss in the appendix, the theorem is not applicable when one considers only adjacent pairs $(X_t, Y_t)$ with respect to $\delta$. The theorem does hold though when one performs the analysis over all pairs of states of the Markov chain, as we show in Section 3, which gives a mixing time bound that is polynomial in the number of cliques in the polymer model, assuming the clique dynamics condition.

### 1.2.2 Algorithms

Our main algorithmic result uses our Markov chain and the bound of its mixing time to approximately sample from $\mu$.

\textbf{Theorem 9.} Let $\mathcal{P} = (C, w, \star)$ be a computationally feasible polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$, and let $Z_{\text{max}} = \max_{i \in [m]} \{Z_{\mid \Lambda_i}\}$. Furthermore, assume that

(a) $Z_{\text{max}} \in \text{poly}(m)$,

(b) $\mathcal{P}$ satisfies the clique dynamics condition for a function $f$ such that, for all $\gamma \in C$, it holds that $e^{-\text{poly}(m)} \leq f(\gamma) \leq e^{\text{poly}(m)}$, and that,

(c) for all $i \in [m]$, we can sample from $\mu_{\mid \Lambda_i}$ in time $\text{poly}(m)$.

Then, for all $\varepsilon \in (0, 1]$, we can $\varepsilon$-approximately sample from $\mu$ in time $\text{poly}(m/\varepsilon)$.

Additionally, as we discuss in Section 4.2, we use self-reducibility on the clique cover and use the above theorem to obtain an $\varepsilon$-approximation algorithm for the partition function $Z$. 
Theorem 12. Let $\mathcal{P} = (C, w, +)$ be a computationally feasible polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$. Assume that $\mathcal{P}$ satisfies the conditions of Theorem 9.

Then, for all $\varepsilon \in (0, 1]$, there is a randomized $\varepsilon$-approximation of $Z$ computable in time $\text{poly}(m/\varepsilon)$.

Since it is common for spin systems on graphs with $n$ vertices to translate into polymer models with a clique cover of $n$ cliques, the above theorems imply polynomial-time algorithms for their respective problems. Assumption (a) is trivially satisfied for the applications we consider and, furthermore, assumption (b) allows for a broad range in the choice of the function $f$ appearing in the clique dynamics condition.

When we apply the above theorems to the spin systems previously studied in the literature, assumption (c) is not straightforward to satisfy, as the size of the cliques are commonly exponential in $n = |V(G)|$. Chen et al. [7] used the sampling condition in order to sample polymers in expected constant time. As we are interested in extending the parameter range while remaining in the realm of polynomial time computations, we do not need to use such a restrictive condition. For this purpose, we introduce the clique truncation condition.

Condition 24 (clique truncation). Let $\mathcal{P} = (C, w, +)$ be a polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$, and let $|\cdot|$ be a size function for $\mathcal{P}$. For all $i \in \{m\}$, we say that $\Lambda_i$ satisfies the clique truncation condition for a monotonically increasing, invertible function $g: \mathbb{R} \rightarrow \mathbb{R} > 0$ and a bound $B \in \mathbb{R} > 0$ if and only if

$$\sum_{\gamma \in \Lambda_i} g(|\gamma|)w_\gamma \leq B.$$

We show that when the clique truncation condition is satisfied, we can reduce the size of each clique to a polynomial in $n$ by removing low weight polymers from the polymer model. More precisely, Corollary 26 states that for an $\varepsilon$-approximation it is sufficient to consider only polymers $\gamma$ with $|\gamma| \leq g^{-1}(Bm/\varepsilon)$. This allows us to use the algorithm of Patel and Regts [42] to sample from the Gibbs distribution of each clique by enumerating all polymers in the clique. In all our calculations, the parameter range restrictions imposed by the clique truncation condition are weaker than the ones imposed by the clique dynamics condition. As illustrated in Table 1, this leads to improved parameter ranges for spin systems previously studied in literature (see Section 6.1 for a detailed discussion on the hard-core model on bipartite $\alpha$-expanders).

1.2.3 Application on the multi-component hard-sphere model

We apply our results to the multi-component hard-sphere model, an inherently geometric model that is central in the analysis of thermodynamics of liquids and liquid mixtures [4, 24]. It is a continuous model that studies the macroscopic behavior and distribution of spherical particles, assuming that the only interaction among the particles is the hard-core interaction, i.e., no two particles can occupy the same space. We are interested in the grand canonical ensemble of the hard-sphere model in a $d$-dimensional finite hypercube $V = [0, \ell]^d$. We consider $q$ polymers, assuming that the model satisfies the conditions of Theorem 9.

A similar idea was used for the hard-core model on bipartite expanders in the first arXiv version of Chen et al. [7].
Table 1: Improvement on the parameter ranges of our technique for problems with known approximation algorithms. Note that for a fair comparison we refined the calculations of the bounds in [30] in a similar fashion as in Section 6.1.

| Problem                                           | Previous range                          | New range                   |
|---------------------------------------------------|-----------------------------------------|-----------------------------|
| Hard-core model on bipartite $\alpha$-expanders   | $\lambda > (e^2\Delta^2)^{1/6}$ [30]  | $\lambda \geq (\frac{e}{0.8}\Delta^2)^{1/6}$ |
| $q$-state Potts model on $\alpha$-expanders       | $\beta > \frac{9/4+\ln(\Delta q)}{\alpha}$ [30] | $\beta \geq \frac{3/2+\ln(\Delta q)}{\alpha}$ |
| Hard-core model on unbalanced bipartite graphs    | $6\Delta L \Delta R \lambda_R \leq (1 + \lambda_L)^{\frac{\Delta q}{\alpha}}$ [5] | $3.3353\Delta L \Delta R \lambda_R \leq (1 + \lambda_L)^{\frac{\Delta q}{\alpha}}$ |
| Perfect matching polynomial                       | $z \leq \left(\sqrt{4.8572(\Delta - 1)}\right)^{-1}$ [6] | $z \leq \left(\sqrt{2.8399(\Delta - 1)}\right)^{-1}$ |

Different types of particles $Q = \{(r_1, p_1), \ldots, (r_q, p_q)\}$, represented as $d$-dimensional spheres of radius $r_i \in \mathbb{R}_{>0}$ and a chemical potential $p_i \in \mathbb{R}$. For each particle type $i \in [q]$, the centers of spherical particles are distributed according to a Poisson point process of intensity $e^{p_i}$ on $V$. The resulting distribution over all possible system states is characterized by the mixture of these point processes conditioned on the fact that the particles with radii corresponding to their particle type are non-overlapping. We are interested in approximating the grand canonical partition function of the multi-component hard-sphere model, which is the normalizing constant of the corresponding probability density over the states of the system (see Section 5 for a formal definition).

**Related work** Most rigorous algorithmic results for the hard-sphere model are restricted to the special case of a single component, i.e., one type of particle. Note that the one-component model has been used to obtain bounds for the optimal sphere packing density [9, 10, 23, 29, 43]. This model carries a historic weight, as in the seminal work of Metropolis et al. [39], the Monte Carlo method was introduced on a two-dimensional single-component hard-sphere model on 224 particles. Approximate-sampling Markov chain approaches have been mainly focused on the canonical ensemble of the model, that is, the distribution defined over a fixed number of spheres [25, 29, 33]. Considering the grand canonical ensemble, exact sampling algorithms have appeared in the literature for the two-dimensional model without asymptotic runtime guarantees [34, 35, 41]. Guo and Jerrum [22] have introduced an exact sampling algorithm for the grand canonical ensemble of the hard-sphere model on $d$-dimensions. The model they consider consists of a single type of particle of radius 1 and chemical potential $\ln(\lambda/\nu_d)$, where $\nu_d$ is the volume of the $d$-dimensional sphere of radius 1 and $\lambda \in \mathbb{R}_{\geq 0}$. The algorithm is based on rejection sampling with runtime in $O(\ell^d)$ using oracle access to a sampler from a continuous Poisson point process. The parameter regime for which their runtime guarantees apply is $\lambda < 2^{-(d+1)/2}$. Recently Helmuth et al. [26] considered the single-center dynamics, a continuous-state space Markov chain generalizing Glauber dynamics in order to study decay of
correlations for the model. Their results show that when $\lambda < 2^{-(d-1)}$, the single-center dynamics is rapidly mixing. Finally, we note that the hard-core model can be considered as discrete version of the mono-atomic grand canonical hard-sphere model. Although tight approximation results for the hard-core model exist, it is not known how these results on a discrete graph topology can be mapped to the original hard-sphere model in continuous space.

**Our results** We obtain an $\varepsilon$-approximation algorithm for the grand canonical partition function of the multi-component hard-sphere model (Theorem 19). We show that the runtime of our algorithm is polynomial in $\ell^d$, the number of particle types $q$, and $\varepsilon^{-1}$. To our knowledge, this is the first rigorous algorithmic result to consider multiple components.

To approximate the grand canonical partition function, we consider a discretization of the continuous model where the sphere centers are only allowed to be on grid points. We show that the partition function of the continuous model is closely approximated by the partition function of the discrete model with a sufficient number of points (Lemma 17). This is essentially achieved by giving a lower bound on the rate of convergence of the two functions in terms of the number of grid points considered. This shows that we can obtain an $\varepsilon$-approximation for the continuous model via an $\varepsilon$-approximation for the discrete model. Thus, we define a polymer model for the discrete hard sphere in terms of perturbations from the empty state. Our polymers simply consist of a center position on the grid together with a type of particle that occupies it. Two polymers are incompatible if and only if the particles overlap. This translation yields polymer cliques consisting of $d$-dimensional subgrids. The number of such subgrids only depends on $\ell$, the dimension, and the minimum particle radius of our system. Thus, the number of the polymer cliques in the cover is independent of the number of grid points chosen to approximate the continuous model. Consequently, the mixing time of our Markov chain is independent of the number of grid points. Note that for this application sampling form, the distribution of each clique does not require additional assumptions, such as the clique truncation condition. Finally, we convert the sampler for the polymer model to an $\varepsilon$-approximation for the partition function of the discrete model, which translates to an $\varepsilon$-approximation for the grand canonical partition function of the continuous model.

We note that our approximation algorithm does not require access to a continuous sampler. As we show in Section 5.3, when we apply our algorithm to the model with the chemical potential considered by Guo and Jerrum [22] and Helmuth et al. [26], the parameter range we get for one particle is $\lambda < 2^{-d}$, improving the bound in Guo and Jerrum [22]. The rapidly mixing bound of $\lambda < 2^{-(d-1)}$ from Helmuth et al. [26] is achieved via path coupling, using a refined potential that heavily abuses the symmetry of the single-particle model. This metric could be directly applied to the Glauber dynamics of the single-component discrete model (see [47]) and yield an approximation algorithm for this range. However, it is not obvious whether such a potential can be applied to the multi-component model or to polymer models. Finally, note that a discretization process in the spirit of ours might be applicable to establishing new bounds for the correlation decay of the hard sphere model using the correlation decay of the polymer model, as hinted in Helmuth et al. [26, Section 1.6].
1.3 Outline

The technical part of our article is structured as follows. We establish notation and introduce the tool for bounding the mixing time of our chain in Section 2. We define and analyze our Markov chain in Section 3. The algorithmic results are stated and proved in Section 4. We then apply our algorithms to the multi-component hard-sphere model in Section 5. In Section 6, we show how to efficiently sample polymers from their respective cliques, which we use to improve the parameter ranges of known algorithmic bounds on spin systems. Finally, in the appendix, we discuss why the theorem for bounding the mixing time of our chain in its original form does not apply.

2 Preliminaries

We denote the set of all natural numbers, including 0, by \( \mathbb{N} \) and the set of all real numbers by \( \mathbb{R} \). For an \( n \in \mathbb{N} \), let \([n]\) denote the interval \([1, n] \cap \mathbb{N}\). If the polymer model \( P \) is clear from context, we may drop the index and write \( F, Z, \) and \( \mu \) instead of \( F(P), Z(P), \) and \( \mu(P) \) respectively.

2.1 Restricted polymer models

We base the transitions of our Markov chain for a polymer model \((C, w, \ast)\) on restricted sets \( B \subseteq C \). We define the set of all polymer families restricted to \( B \) to be \( F|B = F \cap 2^B \). Further, we define the restricted partition function \( Z|B \) to be equation (1) but with \( F(P) \) replaced by \( F|B \). Similarly, we define the restricted Gibbs distribution \( \mu|B \) to be a probability distribution over \( F|B \), i.e., equation (2) but with \( Z(P) \) replaced by \( Z|B \). Our restrictions are special sets of polymers, which we define next.

By definition, for a polymer model, a polymer family \( \Gamma \) cannot contain incompatible polymers. Thus, when considering a subset \( B \subseteq C \) where all polymers are pairwise incompatible, at most one polymer of \( B \) is in \( \Gamma \). We call such a subset \( B \) a polymer clique.

Last, for an \( m \in \mathbb{N} \), we call a set \( \Lambda = \{ \Lambda_i \}_{i \in [m]} \) of polymer cliques a polymer clique cover if and only if \( \bigcup \Lambda = C \), and we call \( m \) the size of \( \Lambda \). Note that the elements of \( \Lambda \) need not be pairwise disjoint. Further note that, for each \( i \in [m] \), the partition function restricted to \( \Lambda_i \) simplifies to

\[
Z|\Lambda_i = \sum_{\gamma \in \Lambda_i} \prod_{\gamma' \in \gamma} w_{\gamma'} = 1 + \sum_{\gamma \in \Lambda_i} w_{\gamma},
\]

as the polymers of \( \Lambda_i \) are pairwise incompatible and thus each family of \( \Lambda_i \) (except \( \emptyset \)) contains a single polymer. Similarly, the Gibbs distribution restricted to \( \Lambda_i \) simplifies to \( \mu|\Lambda_i(\emptyset) = 1/Z|\Lambda_i = 1/(1 + \sum_{\gamma \in \Lambda_i} w_{\gamma}) \) and, for each \( \gamma' \in \Lambda_i \), to \( \mu|\Lambda_i(\{\gamma'\}) = w_{\gamma'}/Z|\Lambda_i = w_{\gamma'}/(1 + \sum_{\gamma \in \Lambda_i} w_{\gamma}) \).

2.2 Markov chains

For a Markov chain \( M \) with a unique stationary distribution \( D \) and an \( \varepsilon \in (0, 1] \), let \( \tau_M(\varepsilon) \) denote the mixing time of \( M \) (with error \( \varepsilon \)). That is, \( \tau_M(\varepsilon) \) denotes the first point in time \( t \in \mathbb{N} \)
such that the total-variation distance between $D$ and the distribution of $M$ at time $t$ is at most $\varepsilon$.

In order to bound the mixing time of our Markov chains, we use a theorem by Greenberg et al. [20, Theorem 3.3]. Unfortunately, the theorem is not correct in its original formulation. Therefore, we provide an alternative formulation, which we use. We give a full proof of this theorem in the appendix, where we also discuss why the original assumptions are insufficient.

**Theorem 2 (coupling with exponential potential).** Let $M$ be an ergodic Markov chain with state space $\Omega$ and with transition matrix $P$ such that, for all $x \in \Omega$, it holds that $P(x, x) > 0$. For $d, D \in \mathbb{R}_{>0}$, $d \leq D$, let $\delta : \Omega^2 \rightarrow \{0\} \cup [d, D]$ be such that $\delta(x, y) = 0$ if and only if $x = y$. Assume that there is a coupling between the transitions of two copies $(X_t)_{t \in \mathbb{N}}$ and $(Y_t)_{t \in \mathbb{N}}$ of $M$ such that, for all $t \in \mathbb{N}$ and all $x, y \in \Omega$, it holds that

$$E[\delta(X_{t+1}, Y_{t+1}) \mid X_t = x, Y_t = y] \leq \delta(x, y).$$

Furthermore, assume that there are $\kappa, \eta \in (0, 1)$ such that, for the same coupling and all $t \in \mathbb{N}$ and all $x, y \in \Omega$ with $x \neq y$, it holds that

$$\Pr[|\delta(X_{t+1}, Y_{t+1}) - \delta(x, y)| \geq \eta \delta(x, y) \mid X_t = x, Y_t = y] \geq \kappa.$$  

Then, for all $\varepsilon \in (0, 1]$, it holds that

$$\tau_M(\varepsilon) \leq \frac{(\ln(D/d) + 2 \ln(2))^2}{\ln(1 + \eta)^2 \kappa} \ln\left(\frac{1}{\varepsilon}\right).$$

If $\ln(D/d) \in \Omega(1)$, then this bound simplifies to

$$\tau_M(\varepsilon) \in O\left(\frac{(\ln(D/d))^2}{\ln(1 + \eta)^2 \kappa} \ln\left(\frac{1}{\varepsilon}\right)^3\right).$$

### 2.3 Approximate sampling and randomized approximation

We use the following formal notion of approximate sampling. Let $\nu$ be a probability distribution on a countable state space $\Omega$. For $\varepsilon \in (0, 1]$, we say that a distribution $\xi$ on $\Omega$ is an $\varepsilon$-approximation of $\nu$ if and only if $d_{TV}(\nu, \xi) \leq \varepsilon$, where $d_{TV}(\cdot, \cdot)$ denotes the total variation distance. Further, we say that we can $\varepsilon$-approximately sample from $\nu$ if and only if we can sample from any distribution $\xi$ such that $\xi$ is an $\varepsilon$-approximation of $\nu$.

We are also interested in approximating the partition function of polymer models, which we define as follows. For $x \in \mathbb{R}_{>0}$ and $\varepsilon \in (0, 1]$, we call a random variable $X$ a randomized $\varepsilon$-approximation for $x$ if and only if

$$\Pr[(1 - \varepsilon)x \leq X \leq (1 + \varepsilon)x] \geq \frac{3}{4}.$$ 

Note that if $x$ is the output to an algorithmic problem on some instance and independent samples of $X$ can be obtained in polynomial time in the instance size and $1/\varepsilon$, then this translates to the definition of an FPRAS.
3 Polymer dynamics

We analyze the following Markov chain for a polymer model with a polymer clique cover.

Definition 3 (polymer clique dynamics). Let \( \mathcal{P} \) be a polymer model, and let \( \Lambda \) be a polymer clique cover of \( \mathcal{P} \) with size \( m \). We define \( M(\mathcal{P}) \) to be a Markov chain with state space \( \mathcal{F} \). Let \( (X_t)_{t \in \mathbb{N}} \) denote a (random) sequence of states of \( M(\mathcal{P}) \), where \( X_0 \) is arbitrary. Then, for all \( t \in \mathbb{N} \), the transitions of \( M(\mathcal{P}) \) are as follows:

1. choose \( i \in [m] \) uniformly at random;
2. choose \( \Gamma \in \mathcal{F}_{[A_i]} \) according to \( \mu_{[A_i]} \);
3. if \( \Gamma = \emptyset \) then \( X_{t+1} = X_t \setminus A_i \);
4. else if \( X_t \cup \Gamma \) is a valid polymer family then \( X_{t+1} = X_t \cup \Gamma \);
5. else \( X_{t+1} = X_t \);

Given a polymer model \( \mathcal{P} = (C, w, +) \) and a polymer Markov chain \( M(\mathcal{P}) \), let \( P \) denote the transition matrix of \( M(\mathcal{P}) \). That is, for all \( \Gamma, \Gamma' \in \mathcal{F}(\mathcal{P}) \), the entry \( P(\Gamma, \Gamma') \) denotes the probability to transition from state \( \Gamma \) to state \( \Gamma' \) in a single step. Note that \( P \) is time-homogeneous and that, for all \( \Gamma, \Gamma' \in \mathcal{F}(\mathcal{P}) \) with \( P(\Gamma, \Gamma') > 0 \), it holds that the symmetric difference of \( \Gamma \) and \( \Gamma' \) has a cardinality of at most 1, since the polymer families of a polymer clique are all singletons. Further note that \( M(\mathcal{P}) \) has a positive self-loop probability, as the polymer families from a polymer clique are pairwise incompatible.

The transition probabilities of two neighboring states of \( M(\mathcal{P}) \) follow a simple pattern. In order to ease notation, for all \( y \in C \), let \( z_y = \sum_{i \in [m]}: y \in A_i \, \frac{1}{Z_{[A_i]}} \). For all \( \Gamma, \Gamma' \in \mathcal{F}(\mathcal{P}) \) such that there is a \( y \in C \), \( y \not\in \Gamma \) such that \( \Gamma' = \Gamma \cup \{ y \} \), it holds that

\[
P(\Gamma, \Gamma') = \frac{1}{m} \sum_{i \in [m]}: y \in A_i \, \mu_{[A_i]}(\{ y \}) = \frac{1}{m} \sum_{i \in [m]}: y \in A_i \, \frac{w_y}{Z_{[A_i]}} = \frac{w_y}{m} \quad \text{and that} \quad \sum_{i \in [m]}: y \in A_i \, \frac{1}{Z_{[A_i]}} \quad \text{all \( y \in C \)}
\]

\[
P(\Gamma', \Gamma) = \frac{1}{m} \sum_{i \in [m]}: y \in A_i \, \mu_{[A_i]}(\{ \emptyset \}) = \frac{1}{m} \sum_{i \in [m]}: y \in A_i \, \frac{1}{Z_{[A_i]}} = \frac{z_y}{m} > 0.
\]

We show that the polymer clique dynamics are suitable for sampling from the Gibbs distribution of a polymer model, since the limit distribution of the Markov chain converges to \( \mu \).

Lemma 4. Let \( \mathcal{P} \) be a polymer model. The polymer Markov chain \( M(\mathcal{P}) \) is ergodic with stationary distribution \( \mu(\mathcal{P}) \).

Proof. First, note that \( M(\mathcal{P}) \) is irreducible, as there is a positive probability to go from any polymer family \( \Gamma \in \mathcal{F} \) to the empty polymer family \( \emptyset \) in a finite number of steps by consecutively removing each polymer \( y \in \Gamma \). Similarly, there is a positive probability to go from \( \emptyset \) to any polymer family \( \Gamma' \in \mathcal{F} \) in a finite number of steps by consecutively adding all polymers \( y' \in \Gamma' \).

We proceed by proving that \( \mu(\mathcal{P}) \), which we abbreviate as \( \mu \), is a stationary distribution of \( M(\mathcal{P}) \). To this end, we show that \( M(\mathcal{P}) \) satisfies the detailed-balance condition with respect
to \( \mu \). That is, for all \( \Gamma, \Gamma' \in \mathcal{F} \), it holds that

\[
\mu(\Gamma) \cdot P(\Gamma, \Gamma') = \mu(\Gamma') \cdot P(\Gamma', \Gamma).
\]  

(6)

Note that it is sufficient to check equation (6) for all pairs of states with a symmetric difference of exactly one polymer.

Let \( \Gamma, \Gamma' \in \mathcal{F} \) and assume without loss of generality that \( \Gamma' = \Gamma \cup \{\gamma\} \) for some polymer \( \gamma \notin \Gamma \). Note that, by equation (5), \( P(\Gamma, \Gamma') = w_\gamma \cdot P(\Gamma', \Gamma) \). Further, by definition of the Gibbs distribution, we have \( \mu(\Gamma') = w_\gamma \cdot \mu(\Gamma) \). Thus, we get

\[
\mu(\Gamma) \cdot P(\Gamma, \Gamma') = \mu(\Gamma) \cdot w_\gamma \cdot P(\Gamma', \Gamma) = \mu(\Gamma') \cdot P(\Gamma', \Gamma),
\]

which shows that \( \mu \) is a stationary distribution of \( \mathcal{M}(\mathcal{P}) \).

Finally, we argue that \( \mathcal{M}(\mathcal{P}) \) is ergodic. Note that an irreducible Markov chain has a stationary distribution if and only if it is positive recurrent. In addition, every state of \( \mathcal{M}(\mathcal{P}) \) has a positive self-loop probability, which implies that the chain is aperiodic. This shows that \( \mathcal{M}(\mathcal{P}) \) is ergodic and concludes the proof. ■

Recall Condition 1 (clique dynamics) from the introduction. Assuming that the condition holds, we obtain the following bound on the mixing time of \( \mathcal{M}(\mathcal{P}) \).

**Lemma 5.** Let \( \mathcal{P} = (\mathcal{C}, w, \ast) \) be a polymer model satisfying the clique dynamics condition with function \( f \), and let \( \Lambda \) be a polymer clique cover of \( \mathcal{P} \) with size \( m \). Then, for all \( \varepsilon \in (0, 1] \), it holds that

\[
\tau_{\mathcal{M}(\mathcal{P})}(\varepsilon) \in O\left(\frac{m^3}{\min_{\gamma \in \mathcal{C}} \{z_\gamma\}} \ln\left(\frac{\max_{\gamma \in \mathcal{C}} \frac{f(\gamma)}{z_\gamma(1 + w_\gamma)}}{\min_{\gamma \in \mathcal{C}} \frac{f(\gamma)}{z_\gamma(1 + w_\gamma)}} \ln\left(\frac{1}{\varepsilon}\right)\right)\right).
\]

**Proof.** We aim to apply Theorem 2, which requires us to define a potential \( \delta \). We do so by utilizing the function \( \delta' : \mathcal{C} \rightarrow \mathbb{R}_{>0} \) with \( \gamma \mapsto f(\gamma)/(z_\gamma(1 + w_\gamma)) \). Let \( \oplus \) denote the symmetric set difference. For all \( \Gamma, \Gamma' \in \mathcal{F} \), we define

\[
\delta(\Gamma, \Gamma') = \sum_{\gamma \in \Gamma \oplus \Gamma'} \delta'(\gamma).
\]

Note that \( \delta(\Gamma, \Gamma') \) only depends on the symmetric difference of \( \Gamma \) and \( \Gamma' \) and that \( \delta(\Gamma, \Gamma') = 0 \) if and only if \( \Gamma \oplus \Gamma' = \emptyset \), which only is the case when \( \Gamma = \Gamma' \).

We continue by constructing a coupling between two copies of \( \mathcal{M}(\mathcal{P}) \), namely between \( (X_t)_{t \in \mathbb{N}} \) and \( (Y_t)_{t \in \mathbb{N}} \). We couple these chains such that, for each transition,

- both choose the same index \( i \in [m] \) and
- both draw the same polymer family \( \Gamma_i \in \mathcal{F}_{|\Lambda_i} \) from \( \mu_{|\Lambda_i} \).

This constitutes a valid coupling, as each chain transitions according to its desired marginal transition probabilities.
We now show for all $t \in \mathbb{N}$ and $\Gamma, \Gamma' \in \mathcal{F}$ that

$$E[\delta(X_{t+1}, Y_{t+1}) \mid X_t = \Gamma, Y_t = \Gamma'] \leq \delta(\Gamma, \Gamma').$$

Note that this trivially holds if $\Gamma = \Gamma'$, as the chains $X$ and $Y$ behave identically from then on. Thus, we are left with the case that $\Gamma \neq \Gamma'$, which implies that $|\Gamma \oplus \Gamma'| \geq 1$.

We introduce the following notation. For all $\gamma \in C$, let $N(\gamma) = \{\gamma' \in C \mid \gamma' \neq \gamma\}$ denote the neighborhood of $\gamma$. We extend this definition to arbitrary subsets of polymers $\mathcal{B} \subseteq C$ by $N(\mathcal{B}) = \bigcup_{\gamma \in \mathcal{B}} N(\gamma)$.

Let $\Delta = \Gamma \oplus \Gamma'$, and let $\gamma \in \Delta$. Assume without loss of generality that $\gamma \in \Gamma$. By equation (5), with probability $z_{\gamma}/m$, the chain $X$ removes $\gamma$ and the chain $Y$ remains in its state. Consequently, $\delta(X_{t+1}, Y_{t+1})$ decreases by $\delta'(\gamma)$. Similarly, if $\gamma \in \Gamma \setminus N(\Delta)$, with probability $w_{\gamma}z_{\gamma}/m$, the chain $Y$ adds $\gamma$ and the chain $X$ remains in its state. Again, $\delta(X_{t+1}, Y_{t+1})$ decreases by $\delta'(\gamma)$.

Let $\delta^-(\Gamma, \Gamma')$ denote the expected (conditional) decrease of $\delta$. By the observations above, we see that

$$\delta^-(\Gamma, \Gamma') = \sum_{\gamma \in \Delta} \delta'(\gamma)z_{\gamma} \frac{z_{\gamma}}{m} + \sum_{\gamma \in \Delta \setminus N(\Delta)} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma}}{m} = \sum_{\gamma \in \Delta} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma}}{m} + \sum_{\gamma \in \Delta \cap N(\Delta)} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma}}{m}.$$

Moreover, $\delta$ increases whenever a polymer $\gamma$ is added to only one of both chains. This only occurs if $\gamma \in N(\Delta) \setminus \Delta$ and has probability $w_{\gamma}z_{\gamma}/m$ for each such polymer. Similarly to the expected decrease, we denote the expected increase by $\delta^+(\Gamma, \Gamma')$. We bound

$$\delta^+(\Gamma, \Gamma') \leq \sum_{\gamma \in N(\Delta) \setminus \Delta} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma}}{m} \leq \sum_{\gamma \in \Delta} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma}}{m} - \sum_{\gamma \in \Delta \cap N(\Delta)} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma}}{m}.$$

Together, we obtain

$$E[\delta(X_{t+1}, Y_{t+1}) \mid X_t = \Gamma, Y_t = \Gamma'] = \delta(\Gamma, \Gamma') + \delta^+(\Gamma, \Gamma') - \delta^-(\Gamma, \Gamma')$$

$$\leq \delta(\Gamma, \Gamma') + \sum_{\gamma \in \Delta} \sum_{\gamma' \in N(\gamma)} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma'}}{m} - \sum_{\gamma \in \Delta} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma'}}{m} \frac{1 + w_{\gamma}}{m}$$

$$= \delta(\Gamma, \Gamma') + \sum_{\gamma \in \Delta} \left( \sum_{\gamma' \in N(\gamma)} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma'}}{m} - \delta'(\gamma)w_{\gamma} \frac{z_{\gamma'}}{m} \frac{1 + w_{\gamma}}{m} \right).$$

We proceed by showing that, for each $\gamma \in \Delta$, the respective summand in the sum above is at most zero. By the definition of $\delta'$, we get

$$\sum_{\gamma' \in N(\gamma)} \delta'(\gamma)w_{\gamma} \frac{z_{\gamma'}}{m} - \delta'(\gamma)w_{\gamma} \frac{z_{\gamma'}}{m} \frac{1 + w_{\gamma}}{m} = \frac{1}{m} \left( \sum_{\gamma' \in N(\gamma)} f(\gamma') \frac{w_{\gamma}}{1 + w_{\gamma'}} - f(\gamma) \right).$$
By the definition of $N(y)$ and since $\mathcal{P}$ satisfies the clique dynamics condition, we bound

$$\frac{1}{m} \left( \sum_{y' \in N(y)} f(y') \frac{w_{y'}}{1 + w_{y'}} - f(y) \right) = \frac{1}{m} \left( \sum_{y' \in C: y' \neq y} f(y') \frac{w_{y'}}{1 + w_{y'}} - f(y) \right) \leq 0.$$ 

Consequently, we get that

$$\mathbb{E}[\delta(X_{t+1}, Y_{t+1}) | X_t = \Gamma, Y_t = \Gamma'] \leq \delta(\Gamma, \Gamma').$$

We now show that there are values $\eta, \kappa \in (0, 1)$ such that, for all $t \in \mathbb{N}$ and all $\Gamma, \Gamma' \in \mathcal{F}$ with $\Gamma \neq \Gamma'$, it holds that

$$\Pr[|\delta(X_{t+1}, Y_{t+1}) - \delta(\Gamma, \Gamma')| \geq \eta \delta(\Gamma, \Gamma') | X_t = \Gamma, Y_t = \Gamma'] \geq \kappa. \quad (7)$$

Note that every polymer family in $\mathcal{F}$ has at most $m$ polymers because it can have at most one polymer from each polymer clique. Thus, for $\Lambda = \Gamma \oplus \Gamma'$, we bound $|\Lambda| \leq 2m$. Consequently, there is at least one polymer $y \in \Delta$ such that $\delta'(y) \geq \delta(\Gamma, \Gamma')/(2m)$. Assume without loss of generality that $y \in \Gamma$. With probability $z_y/m$, chain $X$ deletes $y$ and chain $Y$ remains in its state, resulting in $|\delta(X_{t+1}, Y_{t+1}) - \delta(\Gamma, \Gamma')| \geq \delta'(y) \geq \delta(\Gamma, \Gamma')/(2m)$, Thus, equation (7) is true for $\eta = 1/(2m)$ and $\kappa = z_y/m \geq (\min_{y \in C} \{z_y\})/m$.

It remains is to determine $d, D \in \mathbb{R}_{\geq 0}$ such that, for all $\Gamma, \Gamma' \in \mathcal{F}$ with $\Gamma \neq \Gamma'$, it holds that $\delta(\Gamma, \Gamma') \in [d, D]$. Let $\Delta = \Gamma \oplus \Gamma'$, noting again that $|\Lambda| \leq 2m$. We choose

$$d \geq \min\{\delta'(y)\} = \min_{y \in C} \left\{ \frac{f(y)}{z_y(1 + w_y)} \right\} \quad \text{and}$$

$$D \leq 2m \max_{y \in C} \{\delta'(y)\} = 2m \max_{y \in C} \left\{ \frac{f(y)}{z_y(1 + w_y)} \right\}.$$ 

Applying Theorem 2 and observing that $\ln(1 + \frac{1}{2m})^2 \geq \frac{1}{4m}$ concludes the proof.

Last, we combine Lemmas 4 and 5 and obtain the main result of this section.

**Theorem 6.** Let $\mathcal{P} = (C, w, \ast)$ be a polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$, and let $Z_{\max} = \max_{\iota \in [m]} \{Z_{\Lambda_{\iota}}\}$. Further, assume that $\mathcal{P}$ satisfies the clique dynamics condition with function $f$, and let $f_{\max} = \max_{y \in C} \{f(y)\}$ and $f_{\min} = \min_{y \in C} \{f(y)\}$.

Then the Markov chain $M(\mathcal{P})$ has the unique stationary distribution $\mu^{(\mathcal{P})}$ and, for all $\epsilon \in (0, 1]$, it holds that

$$\tau_{M(\mathcal{P})}(\epsilon) \in \mathcal{O}\left( m^3 Z_{\max} \ln\left( m^2 Z_{\max}^2 \frac{f_{\max}}{f_{\min}} \right) \frac{1}{\ln \left( \frac{1}{\epsilon} \right)} \right).$$

**Proof.** By Lemma 4, it follows that $M(\mathcal{P})$ has the unique stationary distribution $\mu^{(\mathcal{P})}$. The bound on the mixing time follows from Lemma 5 and by observing that, for all $y \in C$, it holds
that

\[ \frac{1}{Z_{\text{max}}} \leq z_y \leq m \text{ and } 1 \leq 1 + w_y \leq Z_{\text{max}}. \]

Note that, if a polymer model \( \mathcal{P} \) satisfies, for all \( y \in C \) and some \( f : C \to \mathbb{R}_{>0} \), that

\[ \sum_{y' \in C : y' + y} f(y')w_{y'} \leq f(y), \]

then it satisfies the clique dynamics condition for the same function \( f \). Although the condition above is slightly more restrictive than the clique dynamics condition, it is more convenient to use for algorithmic applications. It can be seen as a weaker and more general version of the mixing condition by Chen et al. [7].

### 3.1 Comparison to conditions for cluster expansion

In order to set our clique dynamics condition in the context of existing conditions for absolute convergence of the cluster expansion, we compare it to the condition of Fernández and Procacci [15]. We choose it for comparison because it is, to the best of our knowledge, the least restrictive condition for absolute convergence of the cluster expansion of abstract polymer models. As Fernández and Procacci [15] show, their condition is an improvement over other known conditions, including the Dobrushin condition [11] and the Kotecký–Preiss condition [36].

**Definition 7 (Fernández and Procacci [15]).** Let \( \mathcal{P} = (C, w, \sim) \) be a polymer model, and let \( N(y) = \{y' \in C \mid y' \sim y\} \). We say that \( \mathcal{P} \) satisfies the Fernández–Procacci condition if and only if there is a function \( f : C \to \mathbb{R}_{>0} \) such that, for all \( y \in C \), it holds that

\[ \sum_{\Gamma \in \mathcal{F}(\mathcal{P}) \mid N(\gamma)} \prod_{y' \in \Gamma} f(y')w_{y'} \leq f(\gamma). \]

Note that we state the condition slightly differently from the version of the original authors to ease comparison. The original form is recovered by setting \( f : y \mapsto f'(y)/w_y \) for some function \( f' : C \to \mathbb{R}_{>0} \). Further, the original version allows \( f \) (or \( f' \) respectively) to take the value 0. However, note that if \( f(\gamma) = 0 \) for any \( \gamma \in C \), then the condition is trivially void because \( \emptyset \in \mathcal{F}(\mathcal{P}) \), which lower bounds the left hand side of the inequality by 1.

The following statement shows how our clique dynamics condition relates to the Fernández–Procacci condition as given in Definition 7.

**Proposition 8.** If a polymer model \( \mathcal{P} = (C, w, \sim) \) satisfies the Fernández–Procacci condition for a function \( f \), then it also satisfies the clique dynamics condition for the same function.

**Proof.** Note that \( \emptyset \in \mathcal{F}(\mathcal{P}) \mid N(y) \) and, for all \( y' \in C \) with \( y' \sim y \), it holds that \( \{y'\} \in \mathcal{F}(\mathcal{P}) \mid N(\gamma) \). Thus,

\[ \sum_{y' \in C : y' + y} f(y')w_{y'} < 1 + \sum_{y' \in C : y' + y} f(y')w_{y'} \leq \sum_{\Gamma \in \mathcal{F}(\mathcal{P}) \mid N(y)} \prod_{y' \in \Gamma} f(y')w_{y'} \leq f(y). \]
As discussed above, this implies that $\mathcal{P}$ satisfies the clique dynamics condition.

Note that Proposition 8 implies that if a polymer model satisfies the Fernández–Procacci condition for a function $f$, then Theorem 6 bounds the mixing time of the polymer Markov chain for any given clique cover. Further, Proposition 8 and its implied mixing time bounds for the polymer Markov chain carry over to all convergence conditions that are more restrictive than the Fernández–Procacci condition, such as the Dobrushin condition and the Kotecký–Preiss condition.

4 Algorithmic results

We now discuss how the polymer Markov chain $M$ of a polymer model $\mathcal{P}$ with a clique cover of size $m$ is used to approximate $Z(\mathcal{P})$ in a randomized fashion. To this end, $M$ is turned into an approximate sampler for $\mathcal{P}$ (Theorem 9). Then this sampler is applied in an algorithmic framework (Algorithm 1) that yields an $\varepsilon$-approximation of $Z(\mathcal{P})$ (Theorem 12). Under certain assumptions, such as that the restricted partition function of each polymer clique is in $\text{poly}(m)$, the approximation is computable in time $\text{poly}(m/\varepsilon)$.

In order to discuss the computation time of operations on a polymer model rigorously, we need to make assumptions about the operations we consider and their computational cost. To this end, we say that a polymer model $\mathcal{P} = (C, w, +)$ with a polymer clique cover $\Lambda$ of size $m$ is computationally feasible if and only if all of the following operations can be performed in time $\text{poly}(m)$:

1. for all $i \in [m]$, we can draw $\Lambda_i$ uniformly at random,
2. for all $i \in [m]$ and all $\gamma \in C$, we can check whether $\gamma \in \Lambda_i$,
3. for all $\gamma, \gamma' \in C$, we can check whether $\gamma \neq \gamma'$,
4. for all $\gamma \in C$, we can compute $w_\gamma$.

In addition to the more complex operations above, we further assume that, for all $\gamma \in C$ and all $\Gamma \in \mathcal{F}$, we can compute $\Gamma \setminus \{\gamma\}$ and $\Gamma \cup \{\gamma\}$, and we can decide whether $\Gamma = \emptyset$ in time $\text{poly}(m)$.

Please note that we do not use assumption (4) in this section and it could thus be dropped from the definition. However, as we require it for our results in Section 6.1, where we consider algorithmic applications of polymer models, we include it here.

4.1 Sampling from the Gibbs distribution

We show under what assumptions one can approximately sample from the Gibbs distribution of a computationally feasible polymer model in time polynomial in the size of the clique cover.

Theorem 9. Let $\mathcal{P} = (C, w, +)$ be a computationally feasible polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$, and let $Z_{\max} = \max_{i \in [m]} \{Z_{\Lambda_i}\}$. Further, assume that

(a) $Z_{\max} \in \text{poly}(m)$,
(b) $P$ satisfies the clique dynamics condition for a function $f$ such that, for all $\gamma \in C$, it holds that $e^{-\text{poly}(m)} \leq f(\gamma) \leq e^{\text{poly}(m)}$, and that,

c) for all $i \in [m]$, we can sample from $\mu_{|A_i}$ in time $\text{poly}(m)$.

Then, for all $\epsilon \in (0, 1]$, we can $\epsilon$-approximately sample from $\mu$ in time $\text{poly}(m/\epsilon)$.

**Proof.** In order to sample from $\mu$, we utilize the polymer Markov chain $M(P)$ based on $A$. By Theorem 6, it holds that

$$
\tau_{M(P)}(\epsilon) \in O\left(m^3 Z_{\text{max}} \ln \left(\frac{m^2 Z_{\text{max}}^2}{f_{\text{max}} f_{\text{min}}} \right)^2 \ln \left(\frac{1}{\epsilon} \right)\right).
$$

Due to assumptions (a) and (b), it holds that $\tau_{M(P)}(\epsilon) \in \text{poly}(m/\epsilon)$. It remains to show that each step of $M(P)$, as laid out in Definition 3, can be computed in time $\text{poly}(m)$. To this end, let $X_t$ denote the current state of $\text{poly}(m)$.

Because of assumptions (1) and (c), for all $i \in [m]$, we can draw $A_i$ uniformly at random and can sample $\Gamma \in F_A$ according to $\mu_{|A_i}$ in time $\text{poly}(m)$. This covers lines 1 and 2.

Regarding Line 3, note that we can check whether $\Gamma = \emptyset$ in time $\text{poly}(m)$. Assume that $\Gamma = \emptyset$, and note that $|X_t| \leq m \in \text{poly}(m)$, as $X_t$ contains at most one polymer per polymer clique. In order to compute $X_t \setminus A_i$, it suffices to iterate over every $\gamma \in \Gamma$ and check if $\gamma \in A_i$, which can be done in time $\text{poly}(m)$, by assumption (2). Once we found $\gamma \in A_i$, we remove it in time $\text{poly}(m)$.

Regarding Line 4, assume now that $\Gamma = \{\gamma\}$ for some $\gamma \in A_i$. In order to decide if $X_t \cup \Gamma$ is a valid polymer family, it is sufficient to iterate over all $\gamma' \in X_t$ and check whether any of them is incompatible to $\gamma$. By assumption (3) this can be done in time $\text{poly}(m)$, which concludes the proof.

By making a slightly stronger assumption about the polymer model, assumptions (a) and (b) of Theorem 9 are easily satisfied.

**Observation 10.** Recall from Section 3 that if $P$ satisfies, for all $\gamma \in C$, the slightly more restrictive condition

$$
\sum_{\gamma' \in C: \gamma' \neq \gamma} f(\gamma') w_{\gamma' \gamma} \leq f(\gamma),
$$

then the clique dynamics condition is satisfied for the same function $f$. Thus, if equation (8) holds for an appropriate function $f$, assumption (b) also holds. Further, by setting $\gamma$ to be the polymer in $A_i$ that minimizes $f$, equation (8) implies that $Z_{|A_i} \leq 2$, meaning that assumption (a) is trivially satisfied.

4.2 Approximation of the partition function

By now, we mainly discussed conditions for approximately sampling from the Gibbs distribution. We now discuss to turn this into a randomized approximation for the partition function. To this end, we apply self-reducibility [32]. However, note that the obvious way for applying
Algorithm 1: Randomized approximation of the partition function of a polymer model

**Input:** polymer model \( \mathcal{P} = (C, w, \star) \), polymer clique cover of \( \mathcal{P} \) with size \( m \), number of samples \( s \in \mathbb{N}_{>0} \), sampling error \( \epsilon_s \in (0, 1] \)

**Output:** \( \epsilon \)-approximation of \( Z(\mathcal{P}) \) according to Lemma 11

1. for \( i \in [m] \) do
2.   for \( j \in [s] \) do
3.     \( \Gamma^{(j)} \leftarrow \epsilon_s \)-approximate sample from \( \mu_{|K_i|} \);
4.     \( \hat{\sigma}_i \leftarrow \frac{1}{s} \sum_{j=1}^{s} \mathbb{1}\{\Gamma^{(j)} \in \mathcal{T}_{|K_{i-1}|}\} \);
5.     \( \hat{\sigma} \leftarrow \prod_{i \in [m]} \hat{\sigma}_i \);
6. return \( 1/\hat{\sigma} \);

self-reducibility, namely based on single polymers, might take \(|\mathcal{C}| \) reduction steps. This is not feasible in many algorithmic applications of polymer models.

To circumvent this problem, we propose a self-reducibility argument based on polymer cliques. By doing so, the number of reductions is bounded by the size of the clique cover that is used, thus adding no major overhead to the runtime of our proposed approximate sampling scheme. Besides this idea of applying self-reducibility based on cliques, most of our arguments are analogous to known applications, like in [31, Chapter 3].

We proceed by formalizing clique-based self-reducibility. Let \( \mathcal{P} = (C, w, \star) \) be a polymer model, and let \( \Lambda \) be a polymer clique cover of \( \mathcal{P} \) with size \( m \). We define a sequence of subsets of polymers \( (K_i)_{0 \leq i \leq m} \) with \( K_0 = \emptyset \) and, for \( i \in [m] \), with \( K_i = K_{i-1} \cup A_i \).

Further, for all \( i \in [m] \), let \( \sigma_i = Z_{|K_{i-1}|}/Z_{|K_i|} \). Note that \( Z_{|K_0|} = 1 \) and \( Z_{|K_m|} = Z \). It holds that

\[
Z = \prod_{i \in [m]} \frac{Z_{|K_i|}}{Z_{|K_{i-1}|}} = \left( \prod_{i \in [m]} \sigma_i \right)^{-1}.
\]

Hence, when approximating \( Z \), it is sufficient to focus, for all \( i \in [m] \), on approximating \( \sigma_i \).

For all \( i \in [m] \), a similar relation holds with respect to the probability that a random \( \Gamma \in \mathcal{T}_{|K_i|} \) is already in \( \mathcal{T}_{|K_{i-1}|} \). More formally, let \( i \in [m] \), and let \( \Gamma \sim \mu_{|K_i|} \). Note that

\[
\mathbb{E}\left[ \mathbb{1}\{\Gamma \in \mathcal{T}_{|K_{i-1}|}\} \right] = \sum_{\Gamma \in \mathcal{T}_{|K_i|}} \mu_{|K_i|}(\Gamma) \cdot \mathbb{1}\{\Gamma \in \mathcal{T}_{|K_{i-1}|}\} = \sum_{\Gamma \in \mathcal{T}_{|K_{i-1}|}} \mu_{|K_i|}(\Gamma) = \frac{Z_{|K_{i-1}|}}{Z_{|K_i|}} = \sigma_i, \tag{9}
\]

We use these observations in order to obtain a randomized approximation of \( Z \) (Algorithm 1) by iteratively, for all \( i \in [m] \), approximating \( \sigma_i \) by sampling from \( \mu_{|K_i|} \).

The following result bounds, for all \( \epsilon \in (0, 1] \), the number of samples \( s \) and the sampling error \( \epsilon_s \) that are required by Algorithm 1 to obtain an \( \epsilon \)-approximation of \( Z \).

**Lemma 11.** Let \( \mathcal{P} = (C, w, \star) \) be a polymer model, let \( \Lambda \) be a polymer clique cover of \( \mathcal{P} \) with size \( m \), let \( Z_{\max} = \max_{i \in [m]} \{Z_{|A_i|}\} \), and let \( \epsilon \in (0, 1] \). Consider Algorithm 1 for \( \mathcal{P} \) with \( s = 1 + 125Z_{\max}m/\epsilon^2 \) and \( \epsilon_s = \epsilon / (5Z_{\max}m) \).

Then Algorithm 1 returns a randomized \( \epsilon \)-approximation of \( Z \).
Proof. Let \( i \in [m] \). We start by bounding \( \sigma_i \). Note that \( Z_{K_i} \geq Z_{K_i - 1} \) and \( Z_{K_i} \leq Z_{K_{i - 1}}Z_{A_i} \). Thus, \( 1/Z_{\max} \leq \sigma_i \leq 1 \).

The remaining proof is split into two parts. First, we bound \( E[\hat{\sigma}] \) with respect to \( 1/Z \). Second, we bound the absolute difference of \( \hat{\sigma} \) and \( E[\hat{\sigma}] \). Combining both errors concludes the proof.

Bounding \( E[\hat{\sigma}] \). Note that, for all \( i \in [m] \), it holds that \( \sigma_i - \varepsilon_s \leq \hat{\sigma}_i \leq \sigma_i + \varepsilon_s \), since \( \hat{\sigma}_i \) is the mean of \( \varepsilon_s \)-approximate samples. By the bounds on \( \sigma_i \) and our choice of \( \varepsilon_s \), we get

\[
\left( 1 - \frac{\varepsilon}{5m} \right) \sigma_i \leq E[\hat{\sigma}_i] \leq \left( 1 + \frac{\varepsilon}{5m} \right) \sigma_i.
\]

Recall that \( 1/Z = \prod_{i \in [m]} \sigma_i \). Further, since \( \{\hat{\sigma}_i\}_{i \in [m]} \) are mutually independent, we have \( E[\hat{\sigma}] = \prod_{i \in [m]} E[\hat{\sigma}_i] \). Consequently, since, for all \( x \in [0,1] \) and all \( k \in \mathbb{N}_{>0} \), it holds that

\[
e^{-x/k} \leq 1 - x/(k+1) \quad [31, \text{Chapter 3}],
\]

we obtain

\[
e^{-\varepsilon/4} \frac{1}{Z} \leq \left( 1 - \frac{\varepsilon}{5m} \right)^m \frac{1}{Z} \leq E[\hat{\sigma}] \leq \left( 1 + \frac{\varepsilon}{5m} \right)^m \frac{1}{Z} \leq e^{\varepsilon/4} \frac{1}{Z}, \tag{10}
\]

Bounding the absolute difference of \( \hat{\sigma} \) and \( E[\hat{\sigma}] \). By Chebyshev’s inequality, we get

\[
\Pr\left[ |\hat{\sigma} - E[\hat{\sigma}]| \geq \frac{\varepsilon}{5} E[\hat{\sigma}] \right] \leq \frac{25 \Var[\hat{\sigma}]}{\varepsilon^2 \left( E[\hat{\sigma}]^2 \right)^2} = \frac{25 \left( E[\hat{\sigma}]^2 \right)^2}{\varepsilon^2 \left( E[\hat{\sigma}]^2 \right)^2} - 1.
\]

Again, by the mutual independence of \( \{\hat{\sigma}_i\}_{i \in [m]} \), we have \( E[\hat{\sigma}]^2 = \prod_{i \in [m]} E[\hat{\sigma}_i]^2 \) and \( E[\hat{\sigma}^2] = \prod_{i \in [m]} E[\hat{\sigma}_i]^2 \). Thus,

\[
\Pr\left[ |\hat{\sigma} - E[\hat{\sigma}]| \geq \frac{\varepsilon}{5} E[\hat{\sigma}] \right] \leq \frac{25}{\varepsilon^2 \left( \prod_{i \in [m]} \frac{E[\hat{\sigma}_i]^2}{E[\hat{\sigma}_i]^2} \right)^2} = \frac{25}{\varepsilon^2 \left( \prod_{i \in [m]} \left( 1 + \frac{\Var[\hat{\sigma}_i]}{E[\hat{\sigma}_i]^2} \right) \right)^2} - 1.
\]

For bounding the variance of \( \hat{\sigma}_i \), recall that \( \hat{\sigma}_i = \frac{1}{s} \sum_{j \in [s]} \mathbb{1}\{I^{(j)} \in \mathcal{T}_{K_i-1}\} \), where \( \{I^{(j)}\}_{j \in [s]} \) are independently drawn from an \( \varepsilon_s \)-approximation of \( \mu_{|K_i|} \). By equation (9), we have

\[
\Var[\hat{\sigma}_i] = \frac{1}{s^2} \sum_{j \in [s]} \Var\left[ \mathbb{1}\{I^{(j)} \in \mathcal{T}_{K_i-1}\} \right] = \frac{1}{s} E[\hat{\sigma}_i](1 - E[\hat{\sigma}_i]).
\]

Noting that \( E[\hat{\sigma}_i] \geq (1 - \varepsilon/(5m)) \sigma_i \geq 4/(5Z_{\max}) \), we bound

\[
\frac{\Var[\hat{\sigma}_i]}{E[\hat{\sigma}_i]^2} = \frac{1}{s E[\hat{\sigma}_i]} - \frac{1}{s} \leq \frac{5Z_{\max}}{4s}.
\]

Hence, using that, for all \( x \in [0,1] \) and all \( k \in \mathbb{N}_{>0} \), it holds that \( e^{x/(k+1)} \leq 1 + x/k \), we obtain

\[
\Pr\left[ |\hat{\sigma} - E[\hat{\sigma}]| \geq \frac{\varepsilon}{5} E[\hat{\sigma}] \right] \leq \frac{25}{\varepsilon^2 \left( 1 + \frac{5Z_{\max}}{4s} \right)^4 - 1} \leq \frac{25}{\varepsilon^2 \left( e^{5Z_{\max}m/(4s)} \right)^4 - 1} \leq \frac{25 \, 5Z_{\max} m}{\varepsilon^2 \, 4s - 1}.
\]

Due to our choice of \( s \), and using the same approach as in bounding equation (10), with proba-
bility at least $3/4$, it holds that
\[ e^{-\varepsilon/4}E[\hat{\sigma}] \leq \left(1 - \frac{\varepsilon}{2}\right)E[\hat{\sigma}] \leq \hat{\sigma} \leq \left(1 + \frac{\varepsilon}{2}\right)E[\hat{\sigma}] \leq e^{\varepsilon/4}E[\hat{\sigma}]. \]  
(11)

Combining the results. Combining equations (10) and (11) yields that
\[ (1 - \varepsilon)Z \leq e^{-\varepsilon/2}Z \leq \frac{1}{\hat{\sigma}} \leq e^{\varepsilon/2}Z \leq (1 + \varepsilon)Z \]

with probability at least $3/4$, which concludes the proof.

Based on Algorithm 1 and Lemma 11, we now state our main theorem on the approximation of the partition function of an abstract polymer model.

\textbf{Theorem 12.} Let $\mathcal{P} = (C, w, +)$ be a computationally feasible polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$. Assume that $\mathcal{P}$ satisfies the conditions of Theorem 9. Then, for all $\varepsilon \in (0, 1]$, there is a randomized $\varepsilon$-approximation of $Z$ computable in time $\text{poly}(m/\varepsilon)$.

\textit{Proof.} The statement follows from Lemma 11, choosing the parameters of Algorithm 1 accordingly. Note that Theorem 9 both assume that $Z_{\text{max}} \in \text{poly}(m)$. This implies that $s \in \text{poly}(m/\varepsilon)$ and that we can sample $\varepsilon_s$-approximately from $\mu$ in time $\text{poly}(m/\varepsilon)$. Note that, for all $i \in [m]$, the same holds for $\mu_{|K_i}$, as this only requires the Markov chain to ignore some of the polymer cliques in each step.

\section{5 Multi-component hard-sphere mixtures}

We study the grand canonical ensemble of the hard-sphere model in a $d$-dimensional finite hypercube $V = [0, \ell]^d$ of side length $\ell \in \mathbb{R}_{\geq 1}$. In this model, particles are represented as $d$-dimensional balls; let $v_d$ denote the volume of a $d$-dimensional unit ball. We consider a mixture of $q \in \mathbb{N}_{>0}$ different types of particles $Q = \{(r_i, p_i)\}_{i \in [q]}$, each characterized by a radius $r_i \in \mathbb{R}_{>0}$ and a contribution to the chemical potential $p_i \in \mathbb{R}$. In what follows, we assume for the maximum radius $r_{\text{max}} = \max_{i \in [q]}\{r_i\}$ that $r_{\text{max}} \in \mathcal{O}(\ell)$, which means that the largest observed particles are asymptotically not larger than the considered spatial region $V$. Moreover, we assume that particles of the same type are indistinguishable, which is usually the case for the systems considered in statistical physics. That is, all placements of non-overlapping particles in $V$ that are similar up to swapping two particles of the same type are considered as one and the same configuration.

As we briefly discussed in Section 1.2.3, a probabilistic interpretation of this model is that, for each particle type $i \in [q]$, the centers of particles are distributed according to a Poisson point process of intensity $e^{p_i}$ on $V$. The distribution of states in the ensemble is characterized by the mixture of these point processes conditioned on the particles not overlapping.

In this probabilistic sense, the grand canonical partition function is the normalizing constant of the corresponding probability density over all states of the system. For a given space $V$ and
a set of \( q \) particle types \( Q \), it is formally defined as

\[
Z(V, Q) = 1 + \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \cdots + k_q = k} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) \int_{V^k} D_{r(1), \ldots, r(k)}(x^{(1)}, \ldots, x^{(k)}) \, d\nu^{d \times k},
\]

where

- \( k_i \) represents the number of particles of type \( i \),
- \( \sum_{k_1 + \cdots + k_q = k} \) denotes the sum over all \( (k_i)_{i \in [q]} \in \mathbb{N}^q \) such that \( \sum_{i \in [q]} k_i = k \),
- for each \( i \in [q] \), the factor \( \frac{1}{(k_i)!} \) cancels the effect of double-counting placements that are equal up to swapping particles of type \( i \),
- \( r(i) \) assigns particle \( i \) its radius, i.e., \( r(i) = r_j \) for \( j \in [q] \) such that \( \sum_{a < j} k_a < i \leq \sum_{a \leq j} k_a \),
- \( D_{r(1), \ldots, r(k)} : \mathbb{R}^{d \times k} \to \{0, 1\} \) is 1 if and only if the particles with radii \( r(1), \ldots, r(k) \) and centers \( (x^{(1)}, \ldots, x^{(k)}) \in \mathbb{R}^{d \times k} \) are non-overlapping, and
- \( \nu^{d \times k} \) is the Lebesgue measure on \( \mathbb{R}^{d \times k} \).

Readers who are familiar with this model from physics might notice that we omitted the influence of the inverse temperature and the Boltzmann constant. We did this in order to simplify notation. However, note that this can be included by scaling the chemical potentials appropriately. A physicist’s version of this definition can, for example, be found in [50].

In the following section, we propose a discrete version of the hard-sphere model and prove sufficient conditions for approximating its partition function via a polymer representation (Lemma 15). Then, we show how the continuous model is mapped to the discrete model, and we bound the speed of convergence with respect to the resolution of the discretization (Lemma 17). Based on that, we obtain rigorous computational results for the continuous model (Theorem 19) and demonstrate their application to a common form of chemical potential (Proposition 20).

### 5.1 Discrete hard-sphere model and polymer representation

We discretize the hard-sphere model in the following sense: instead of allowing particles to take arbitrary position in a continuous \( d \)-dimensional cube \( V \), we restrict their centers to be at discrete grid points of a finite \( d \)-dimensional square lattice.

Formally, the discrete hard-sphere model in \( d \) dimensions is defined by a finite integer lattice \( G = [0, n]^d \cap \mathbb{N}^d \) for \( n \in \mathbb{N}_{>0} \) and a set of \( q \) particle types \( Q = \{(r_i, p_i)\}_{i \in [q]} \), again each characterized by a radius \( r_i \in \mathbb{R}_{>0} \) and a chemical potential \( p_i \in \mathbb{R} \). As before, particles of the same type are assumed to be indistinguishable.

Analogously to the continuous model, the grand canonical partition function of the discrete
The hard-sphere model is defined by

$$Z(G, Q) = 1 + \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1, \ldots, k_q} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) \sum_{x^{(1)}, \ldots, x^{(k)}} D_{r(1), \ldots, r(k)}(x^{(1)}, \ldots, x^{(k)}),$$

where

- $k_i$ is the number of particles of type $i \in [q]$.
- $\sum_{k_1, \ldots, k_q}$ denotes the sum over all $(k_i)_{i \in [q]} \in \mathbb{N}^q$ such that $\sum_{i \in [q]} k_i = k$, and
- $r(i)$ and $D_{r(1), \ldots, r(k)} : \mathbb{R}^{d \times k} \rightarrow \{0, 1\}$ are defined as in the continuous case.

We continue by showing how we use polymer models to approximate the grand canonical partition function of the discrete hard-sphere model. For this, we use the following definition of a polymer representation.

**Definition 13 (polymer representation of the discrete hard-sphere model).** Given an instance of the discrete hard-sphere model $(G, Q)$, we define its polymer representation to be the polymer model $\mathcal{P} = (C, w, \ast)$ such that

- each polymer $y \in C$ is defined by a tuple $(x_y, r_y, p_y)$ with $x_y \in G$ and $(r_y, p_y) \in Q$, and each such combination results in a polymer,
- two polymers $y, y' \in C$ are incompatible if and only if $d(x_y, x_{y'}) < r_y + r_{y'}$, and,
- for each polymer $y \in C$, we set $w_y = e^{p_y}$.

Further, we might say that a polymer $y \in C$ with $y = (x_y, r_y, p_y)$ is of type $i \in [q]$ if $(r_y, p_y) = (r_i, p_i)$, and at position $x \in G$ if $x_y = x$.

The following lemma justifies using this polymer representation to approximate the grand canonical partition function of the discrete hard-sphere model.

**Lemma 14.** For an instance of the discrete hard-sphere model $(G, Q)$ and its polymer representation $\mathcal{P} = (C, w, \ast)$ as in Definition 13, it holds that $Z(\mathcal{P}) = Z(G, Q)$.

**Proof:** Since 0 contributes 1 to $Z(\mathcal{P})$ it is sufficient to show

$$\sum_{|\Gamma| \geq 1} \prod_{y \in \Gamma} w_y = \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \cdots + k_q} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) \sum_{x^{(1)}, \ldots, x^{(k)}} D_{r(1), \ldots, r(k)}(x^{(1)}, \ldots, x^{(k)}).$$

We start by rewriting the left-hand side in terms of the power set of the set of polymers:

$$\sum_{|\Gamma| \geq 1} \prod_{y \in \Gamma} w_y = \sum_{|\Gamma| \geq 1} \prod_{y \in \Gamma} w_y \prod_{y, y' \in \Gamma} (1 - \mathbb{1}\{y \neq y'\}) = \sum_{k \in \mathbb{N}_{>0}} \sum_{|\Gamma| = k} \prod_{y \in \Gamma} w_y \prod_{y, y' \in \Gamma} (1 - \mathbb{1}\{y \neq y'\}).$$
Let $B_i \subseteq C$ for $i \in [q]$ be the set of polymers of type $i$. Note that the sets $B_i$ form a partition of $C$. Thus, we have

$$\sum_{k \in \mathbb{N}_{>0}} \sum_{p_i \in \mathbb{Z}} \prod_{y \in \Gamma} w_y \prod_{y, y' \in \Gamma \atop y \neq y'} (1 - \mathbb{1} \{y \neq y'\})$$

$$= \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \ldots + k_q = k} \sum_{p_i \in \mathbb{Z}} \prod_{y \in \Gamma} w_y \prod_{y, y' \in \Gamma \atop y \neq y'} (1 - \mathbb{1} \{y \neq y'\}).$$

We rewrite equation (12) as

$$\sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \ldots + k_q = k} \prod_{i \in [q]} e^{k_i p_i} \left( \sum_{x^{(K+1)}, \ldots, x^{(K+k_1)}} \frac{1}{k_1!} \right) \ldots \sum_{x^{(K+1)}, \ldots, x^{(K+k_q)}} \frac{1}{k_q!} \prod_{i, j \in [q]} \prod_{i < j} \prod_{k_i + 1 \leq a \leq K_i + k_i} \prod_{k_j + 1 \leq b \leq K_j + k_j} \mathbb{1} \left\{ d(x^{(a)}, x^{(b)}) \geq r_i + r_j \right\}.$$  \hspace{1cm} (13)

Last, using that

$$\prod_{i, j \in [q]} \prod_{i < j} \prod_{k_i + 1 \leq a \leq K_i + k_i} \prod_{k_j + 1 \leq b \leq K_j + k_j} \mathbb{1} \left\{ d(x^{(a)}, x^{(b)}) \geq r_i + r_j \right\} = D_{r(1), \ldots, r(k)}(x^{(1)}, \ldots, x^{(k)}),$$

we conclude the proof by simplifying equation (13) to

$$\sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \ldots + k_q = k} \prod_{i \in [q]} e^{k_i p_i} \left( \sum_{x^{(K+1)}, \ldots, x^{(K+k_1)}} \frac{1}{k_1!} \right) \ldots \sum_{x^{(K+1)}, \ldots, x^{(K+k_q)}} \frac{1}{k_q!} D_{r(1), \ldots, r(k)}(x^{(1)}, \ldots, x^{(k)})$$

$$= \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \ldots + k_q = k} \prod_{i \in [q]} e^{k_i p_i} \left( \prod_{i \in [q]} \frac{1}{k_i!} \right) \sum_{x^{(1)}, \ldots, x^{(k)}} D_{r(1), \ldots, r(k)}(x^{(1)}, \ldots, x^{(k)}).$$
Using this equality, we obtain conditions for an efficient approximation of the grand canonical partition function of the discrete hard-sphere model by investigating the computational properties of its polymer representation. Our result is presented in the following lemma.

**Lemma 15.** Given an instance of the $d$-dimensional discrete hard-sphere model $(G, Q)$ with $G = [0, n]^d \cap \mathbb{N}^d$ and $q$ particle types $Q = \{(r_i, p_i)\}_{i \in [q]}$, let $r_{\min} = \min_{i \in [q]} \{r_i\}$, and let $b_d(r)$ be an upper bound on the number of integer points in a $d$-dimensional sphere of radius $r \in \mathbb{R}_{>0}$, centered at the origin. Assume that, for all $i \in [q]$, there is an $h_i \in \mathbb{R}_{>0}$ with

$$\exp\left(-\left(\frac{n}{r_{\min}}\right)^d\right) \leq h_i \leq \exp\left(\left(\frac{n}{r_{\min}}\right)^d\right)$$

such that, for all $j \in [q]$, it holds that

$$\sum_{i \in [q]} b_d(r_i + r_j) e^{h_i} \leq 1. \tag{14}$$

Then, for each $\varepsilon \in (0, 1]$, there is a randomized $\varepsilon$-approximation of $Z(G, Q)$ computable in time

$$\text{poly}\left(\frac{n \sqrt{d}}{2 r_{\min}} \right)^d \frac{q + d \ln(n)}{\varepsilon}.$$  

\begin{proof}
By Lemma 14, it is sufficient to approximate the partition function $Z(\mathcal{P})$ of the polymer representation $\mathcal{P} = (C, w, +)$ of $(G, Q)$. We show that, by Theorem 9, we can sample efficiently from $\mu(\mathcal{P})$. Applying Theorem 12 afterward concludes the proof.

We start by fixing a polymer clique cover $\Lambda$ of $\mathcal{P}$ and bounding its size. To this end, for a tuple $(i_1, \ldots, i_d) \in \mathbb{N}^d$, let

$$H_{i_1, \ldots, i_d} = \{ (x_1, \ldots, x_d) \in G \mid \forall j \in [d]: i_j \left[ \frac{2}{\sqrt{d}} r_{\min} \right] \leq x_j < (i_j + 1) \left[ \frac{2}{\sqrt{d}} r_{\min} \right] \}.$$ 

In other words, we divide $G$ into subcubes with side length at most $2 r_{\min}/\sqrt{d}$. Note that each pair of polymers $\gamma, \gamma' \in C$ with $x_\gamma, x_{\gamma'} \in H_{i_1, \ldots, i_d}$ is incompatible, as $d(x_\gamma, x_{\gamma'}) < 2 r_{\min}$. We identify each polymer clique by a tuple $(i_1, \ldots, i_d) \in \mathbb{N}^d$ and set

$$\Lambda_{i_1, \ldots, i_d} = \{ \gamma \in C \mid x_\gamma \in H_{i_1, \ldots, i_d} \}.$$ 

This results in $|\Lambda| = O((n \sqrt{d}/r_{\min})^d)$ polymer cliques, from which we can draw one uniformly at random by choosing $d$ uniform integers, each of size $O(n \sqrt{d}/r_{\min})$. Further, note that checking whether a polymer $\gamma \in C$ is in a certain polymer clique can be done by checking whether $x_\gamma$ is in the corresponding region of the grid; and checking $\gamma + \gamma'$ is equivalent to comparing their Euclidean distance to the sum of their radii.

We now show that $\mathcal{P}$ satisfies the clique dynamics condition for an appropriate function $f$. To simplify this step, we use Observation 10. For each $\gamma \in C$ of type $i \in [q]$, we set $f(\gamma) = h_i$. Note that if a polymer $\gamma' \in C$ of type $i$ is incompatible to $\gamma$, then $d(x_{\gamma'}, x_{\gamma}) < r_{\gamma'} + r_{\gamma}$.
The number of such pairs is bounded from above by \( b_d(r_i + r_j) \). Thus, for each \( \gamma \in C \), it holds that
\[
\sum_{y' \in C : y' + \gamma} w_{y'} f(y') \leq \sum_{i \in [q]} b_d(r_i + r_j) e^{\rho_i} h_i.
\]

Without loss of generality, let \( \gamma \) be of type \( j \in [q] \). By equation (14),
\[
\sum_{i \in [q]} b_d(r_i + r_j) e^{\rho_i} h_i \leq h_j.
\]

Because \( r_y = r_j \) and \( f(y) = h_j \), Observation 10 implies that assumptions (a) and (b) of Theorem 9 are satisfied.

It remains to show that we can sample from the Gibbs distribution of each polymer clique efficiently. For each \( i \in \mathbb{N}^d \), let \( H_i \) denote the region of the grid that corresponds to \( \Lambda_i \). For all \( y \in \Lambda_i \) of type \( j \in [q] \), it holds that
\[
\mu|_{\Lambda_i}(\{y\}) = \frac{w_y}{Z|_{\Lambda_i}} = \frac{e^{\rho_j}}{Z|_{\Lambda_i}} \text{ with } Z|_{\Lambda_i} = 1 + \sum_{y \in \Lambda_i} w_y = 1 + |H_i| \sum_{j \in [q]} e^{\rho_j},
\]
where \( |H_i| \) denotes the number of grid points in \( H_i \). Note that \( |H_i| \) can be calculated exactly in time \( O(d \ln(n)) \) knowing \( r_{\text{min}}, n \), and \( d \). Thus, we can compute \( Z|_{\Lambda_i} \) in time \( O(q + d \ln(n)) \). We sample from \( \mu|_{\Lambda_i} \) as follows:

1. sample \( x \in H_i \) uniformly at random,
2. sample \( j \in [q] \) with probability proportional to \( e^{\rho_j} \), and
3. return \( \emptyset \) with probability \( \frac{1}{Z|_{\Lambda_i}} \) and \( \{y\} \) with \( y = (x, r_j, p_j) \) otherwise.

Note that step 1. needs time \( O(d \ln(n)) \) by drawing \( d \) integers uniformly from the range that corresponds to \( H_i \). In step 2., we enumerate in time \( O(q) \). Further, we return \( \emptyset \) with probability \( 1/Z|_{\Lambda_i} \) and, for each \( y \in \Lambda_i \) of type \( j \in [q] \), we return the \( \{y\} \) with probability
\[
\frac{Z|_{\Lambda_i} - 1}{Z|_{\Lambda_i}} \cdot \frac{1}{|H_i|} \cdot \frac{e^{\rho_j}}{\sum_{j \in [q]} e^{\rho_j}} = \frac{Z|_{\Lambda_i} - 1}{Z|_{\Lambda_i}} \cdot \frac{e^{\rho_j}}{Z|_{\Lambda_i} - 1} = \frac{e^{\rho_j}}{Z|_{\Lambda_i}},
\]
which results in the desired distribution \( \mu|_{\Lambda_i} \).

Note that the problem of getting an upper bound \( b_d(r) \) on the number of integer points in a hypersphere is sometimes also referred to as the Gauss circle problem in \( d \) dimensions. Tight asymptotic upper bounds on this remain an open mathematical problem. An overview on known bounds are, for example, reported by Strömbergsson and Södergren \[46\]. In general, \( b_d(r) = 2^d r^d \) works as a crude bound if \( r \geq 2^{-d} \). However, depending on the radius \( r \) and the number of dimensions \( d \), more sophisticated bounds are applicable.
5.2 Discretization method and results on the continuous model

We now show how our results on the discrete hard-sphere model relate to the continuous version. In order to do so, we start by defining a transformation from the continuous to the discrete model for a given resolution.

**Definition 16 (discretization of the continuous hard-sphere model).** Let \((V, Q)\) be an instance of the \(d\)-dimensional continuous hard-sphere model with \(V = [0, \ell)^d\) and \(q\) particle types \(Q = \{(r_i, p_i)\}_{i \in \{q\}}\). Further, let \(\rho \in \mathbb{R}_{>0}\) be such that \(\rho \ell \in \mathbb{N}_{>0}\). The **discretization of \((V, Q)\) with resolution \(\rho\)** is a \(d\)-dimensional discrete hard-sphere model \((G^{(\rho)}, Q^{(\rho)})\) with

- \(G^{(\rho)} = [0, \rho \ell]^d \cap \mathbb{N}^d\)
- \(Q^{(\rho)} = \{(r_i^{(\rho)}, p_i^{(\rho)})\}_{i \in \{q\}}\), where \(r_i^{(\rho)} = \rho r_i\) and \(p_i^{(\rho)} = p_i - d \ln(\rho)\).

The following lemma shows that, for sufficiently large resolutions \(\rho\), the discretization can be seen as an approximation of the continuous hard-sphere model in terms of the grand canonical partition function.

**Lemma 17.** Let \((V, Q)\) be a continuous hard-sphere model with \(V = [0, \ell)^d\) and \(q\) particle types \(Q = \{(r_i, p_i)\}_{i \in \{q\}}\), let \(r_{\min} = \min_{i \in \{q\}}(r_i)\), and let \(p_{\max} = \max_{i \in \{q\}}(p_i)\). For every resolution \(\rho \geq 2\sqrt{d}\), it holds that

\[
Z(V, Q) \geq \left(1 - \frac{1}{\rho} \exp\left(\Theta\left(\frac{\sqrt{d}}{2r_{\min}} d \ln(l) + q e^{p_{\max}}\right)\right)\right) \cdot Z(G^{(\rho)}, Q^{(\rho)})
\]

\[
Z(V, Q) \leq \left(1 + \frac{1}{\rho} \exp\left(\Theta\left(\frac{\sqrt{d}}{2r_{\min}} d \ln(l) + q e^{p_{\max}}\right)\right)\right) \cdot Z(G^{(\rho)}, Q^{(\rho)}).
\]

**Proof.** We prove the lemma by bounding the additive error \(|Z(V, Q) - Z(G^{(\rho)}, Q^{(\rho)})|\). Because \(Z(V, Q) \geq 1\), this directly results in the desired multiplicative bound.

In order to obtain an additive bound, we start by transforming \(Z(G^{(\rho)}, Q^{(\rho)})\) to a form that is more similar to the form of \(Z(V, Q)\). Note that, for each \(k \in \mathbb{N}_{>0}\) and \((k_1, \ldots, k_q) \in \mathbb{N}^q\) with \(k_1 + \cdots + k_q = k\), it holds that

\[
\prod_{i \in \{q\}} \frac{e^{k_i p_i^{(\rho)}}}{k_i!} = \left(\frac{1}{\rho}\right)^{d-k} \prod_{i \in \{q\}} \frac{e^{k_i p_i}}{k_i!}.
\]

Let \(\phi^{(\rho)}: G^{(\rho)} \to V\) with \((x_1, \ldots, x_d) \mapsto \phi^{(\rho)}(x) = (x_1/\rho, \ldots, x_d/\rho)\). Note that, for all \(x^{(i)}, x^{(j)} \in G^{(\rho)}\) with assigned radii \(r^{(\rho)}(i) = \rho r(i)\) and \(r^{(\rho)}(j) = \rho r(j)\), it holds that

\[
d\left(x^{(i)}, x^{(j)}\right) \geq r^{(\rho)}(i) + r^{(\rho)}(j) \iff d\left(\phi^{(\rho)}(x^{(i)}), \phi^{(\rho)}(x^{(j)})\right) \geq r(i) + r(j).
\]
Thus, we see that

\[
Z(G^{(\rho)}, Q^{(\rho)}) = 1 + \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \cdots + k_q = k} \frac{\prod_{i \in [q]} e^{k_i p_i}}{k_i!} \sum_{(x^{(1)}, \ldots, x^{(k)}) \in (G^{(\rho)})^k} D_{r^{(\rho)(1)}, \ldots, r^{(\rho)(k)}}(x^{(1)}, \ldots, x^{(k)})
\]

\[
= 1 + \sum_{k \in \mathbb{N}_{>0}} \sum_{k_1 + \cdots + k_q = k} \frac{\prod_{i \in [q]} e^{k_i p_i}}{k_i!} \sum_{(x^{(1)}, \ldots, x^{(k)}) \in (G^{(\rho)})^k} \left(\frac{1}{\rho}\right)^{d_k} D_{r^{(\rho)(1)}, \ldots, r^{(\rho)(k)}}(\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})).
\]

(15)

We continue by rewriting

\[
\sum_{(x^{(1)}, \ldots, x^{(k)}) \in (G^{(\rho)})^k} \left(\frac{1}{\rho}\right)^{d_k} D_{r^{(\rho)(1)}, \ldots, r^{(\rho)(k)}}(\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)}))
\]

for any fixed \( k \in \mathbb{N}_{>0} \) and \( k_1 + \cdots + k_q = k \) as an integral over \( V^k \). Let \( \varphi^{(\rho)}(G^{(\rho)}) \subseteq V \) denote the image of \( \varphi^{(\rho)} \), and let \( \Phi^{(\rho)} : V \to \varphi^{(\rho)}(G^{(\rho)}) \) with

\[
(x_1, \ldots, x_d) \mapsto \left(\frac{\lfloor \rho x_1 \rfloor}{\rho}, \ldots, \frac{\lfloor \rho x_d \rfloor}{\rho}\right).
\]

Further, for all \( k \in \mathbb{N}_{>0} \) and all \( (x^{(1)}, \ldots, x^{(k)}) \in \left(\varphi^{(\rho)}(G^{(\rho)})\right)^k \), let

\[
W^{(\rho)}_{x^{(1)}, \ldots, x^{(k)}} = \left\{(y^{(1)}, \ldots, y^{(k)}) \in V^k \mid \forall i \in [k] : \varphi^{(\rho)}(y^{(i)}) = x^{(i)}\right\}
\]

\[
= \left(\varphi^{(\rho)}\right)^{-1}(x^{(1)}) \times \cdots \times \left(\varphi^{(\rho)}\right)^{-1}(x^{(k)}).
\]

Note that the sets \( W^{(\rho)}_{x^{(1)}, \ldots, x^{(k)}} \) partition \( V^k \) into \((d \times k)\)-dimensional hypercubes of side length \( 1/\rho \).

Thus, for all \( (x^{(1)}, \ldots, x^{(k)}) \in \left(\varphi^{(\rho)}(G^{(\rho)})\right)^k \), it holds that

\[
\nu^{d \times k}(W^{(\rho)}_{x^{(1)}, \ldots, x^{(k)}}) = \left(\frac{1}{\rho}\right)^{d_k}.
\]
By this and by the definition of a Lebesgue integral for elementary functions, we obtain

\[
\sum_{(x^{(1)}, \ldots, x^{(k)}) \in (G^{(\rho)})^k} \left( \frac{1}{\rho} \right) D_{r(1), \ldots, r(k)} (\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)}))
\]

\[
= \sum_{(x^{(1)}, \ldots, x^{(k)}) \in (G^{(\rho)})^k} \nu^{d \times k} \left( \frac{W^{(\rho)}(x^{(1)}, \ldots, x^{(k)})}{\varphi^{(\rho)}(x^{(1)}, \ldots, x^{(k)})} \right) D_{r(1), \ldots, r(k)} (x^{(1)}, \ldots, x^{(k)})
\]

\[
= \sum_{(x^{(1)}, \ldots, x^{(k)}) \in (G^{(\rho)})^k} \nu^{d \times k} \left( \frac{W^{(\rho)}(x^{(1)}, \ldots, x^{(k)})}{\varphi^{(\rho)}(x^{(1)}, \ldots, x^{(k)})} \right) \cdot D_{r(1), \ldots, r(k)} (x^{(1)}, \ldots, x^{(k)})
\]

\[
= \int_{V^k} D_{r(1), \ldots, r(k)} (\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})) \, d\nu^{d \times k}.
\]

Substituting this expression back into equation (15) yields

\[
Z(G^{(\rho)}, Q^{(\rho)}) = 1 + \sum_{k \in \mathbb{N}_{>0}} \sum_{\ell \in [q]} \left( \prod_{\ell = k} \left( \frac{\ell + 1}{\ell} \right)^{k_{k_{\ell}}} \right) \int_{V^k} D_{r(1), \ldots, r(k)} (\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})) \, d\nu^{d \times k}.
\]

We now express \( |Z(V, Q) - Z(G^{(\rho)}, Q^{(\rho)})| \) in terms of the absolute difference of the integrals for all \( k \in \mathbb{N}_{>0} \) and all \( k_1, \ldots, k_q \). Note that the integrals only depend on the resulting assignment of \( r(1), \ldots, r(k) \). We fix any set of radii \( r(1), \ldots, r(k) \) and write \( D \) for \( D_{r(1), \ldots, r(k)} \) to simplify notation. We aim for a bound on

\[
\left| \int_{V^k} D(x^{(1)}, \ldots, x^{(k)}) \, d\nu^{d \times k} - \int_{V^k} D(\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})) \, d\nu^{d \times k} \right|
\]

\[
\leq \int_{V^k} \left| D(x^{(1)}, \ldots, x^{(k)}) - D(\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})) \right| \, d\nu^{d \times k}.
\]

Let \( N^{(\rho)} \subseteq V^k \) be such that for all \( (x^{(1)}, \ldots, x^{(k)}) \in N^{(\rho)} \) it holds that \( D(x^{(1)}, \ldots, x^{(k)}) \neq D(\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})) \). Note that \( N^{(\rho)} \) actually also depends on the assigned radii. As \( D \) is an indicator function, it holds that

\[
\int_{V^k} \left| D(x^{(1)}, \ldots, x^{(k)}) - D(\varphi^{(\rho)}(x^{(1)}), \ldots, \varphi^{(\rho)}(x^{(k)})) \right| \, d\nu^{d \times k} = \nu^{d \times k}(N^{(\rho)}).
\]

We construct a superset of \( N^{(\rho)} \), of which we calculate the Lebesgue measure. First, note that \( N^{(\rho)} = \emptyset \) for \( k = 1 \), as in this case \( D(x^{(1)}) = D(\varphi^{(\rho)}(x^{(1)})) = 1 \) for all \( x^{(1)} \in V \). Further, let \( K = (\ell \sqrt{d}/(2r_{\min}))^d \). Note that, for all \( k > K \), it holds that at least two particles have distance less than \( 2r_{\min} \), meaning that such a configuration has always overlapping particles.
and $N^{(\rho)} = \emptyset$. We are left with considering $2 \leq k \leq K$.

We observe that, for all $(x^{(1)}, \ldots, x^{(k)}) \in V^k$ such that

$$D(x^{(1)}, \ldots, x^{(k)}) \neq D(\Phi^{(\rho)}(x^{(1)}), \ldots, \Phi^{(\rho)}(x^{(k)})),$$

there is be a pair of points $x^{(i)}, x^{(j)}$ for $i, j \in [k]$ such that $i \neq j$ and

$$d(x^{(i)}, x^{(j)}) < r(i) + r(j) \leq d(\Phi^{(\rho)}(x^{(i)}), \Phi^{(\rho)}(x^{(j)})) \quad \text{or}$$

$$d(x^{(i)}, x^{(j)}) \geq r(i) + r(j) > d(\Phi^{(\rho)}(x^{(i)}), \Phi^{(\rho)}(x^{(j)})).$$

As, for every point $x^{(i)} \in V$, it holds that

$$d\left(x^{(i)}, \Phi^{(\rho)}(x^{(i)})\right) \leq \frac{\sqrt{d}}{\rho},$$

there is a pair of points $x^{(i)}, x^{(j)}$ for $i, j \in [k]$ such that $i \neq j$ and

$$\left|r(i) + r(j) - d\left(x^{(i)}, x^{(j)}\right)\right| \leq 2\frac{\sqrt{d}}{\rho}.$$

For all $i, j \in [k]$ with $i \neq j$ let $S^{(\rho)}_{i,j} \subseteq V^k$ be the set of points $(x^{(1)}, \ldots, x^{(k)}) \in V^k$ such that this is the case. Then

$$v^{d \times k}(N^{(\rho)}) \leq v^{d \times k}\left(\bigcup_{1 \leq i < j \leq k} S^{(\rho)}_{i,j}\right) \leq \sum_{1 \leq i < j \leq k} v^{d \times k}(S^{(\rho)}_{i,j}).$$

By Fubini’s theorem, noting that $S^{(\rho)}_{i,j}$ only depends on $i$ and $j$, we get

$$v^{d \times k}(S^{(\rho)}_{i,j}) = \int_{V^k} \mathbb{1}\left\{\left|r(i) + r(j) - d(x^{(i)}, x^{(j)})\right| \leq 2\frac{\sqrt{d}}{\rho}\right\} d\nu^{d \times k}$$

$$= \ell^{d(k-2)} \int_{V^2} \mathbb{1}\left\{\left|r(i) + r(j) - d(x^{(i)}, x^{(j)})\right| \leq 2\frac{\sqrt{d}}{\rho}\right\} d\nu^{d \times 2}$$

$$\leq \ell^{d(k-1)} \cdot v_d \cdot \left(\left(r(i) + r(j) + 2\frac{\sqrt{d}}{\rho}\right)^d - \left(r(i) + r(j) - 2\frac{\sqrt{d}}{\rho}\right)^d\right),$$

By the assumption $\rho \geq 2\sqrt{d}$ and the binomial theorem, we further bound

$$\left(r(i) + r(j) + 2\frac{\sqrt{d}}{\rho}\right)^d - \left(r(i) + r(j) - 2\frac{\sqrt{d}}{\rho}\right)^d \leq \sum_{i=0}^{d} 2 \cdot \mathbb{1}\{i \text{ is odd}\} \binom{d}{i} (r(i) + r(j))^{d-i} \left(2\frac{\sqrt{d}}{\rho}\right)^i.$$
where \( r \) is odd. By the Taylor expansion of \( e^x \), we obtain
\[
\frac{2\sqrt{d}}{\rho} \sum_{i=1}^{d} 2 \cdot \mathbb{1} \{ i \text{ is odd} \} \left( \frac{d}{i} \right) (r(i) + r(j))^{d-i} \left( 2\sqrt{d} \right)^{i-1}
\]
\[
\leq \frac{2\sqrt{d}}{\rho} \sum_{i=1}^{d} 2 \cdot \mathbb{1} \{ i \text{ is odd} \} \left( \frac{d}{i} \right) (r(i) + r(j))^{d-i} \left( \sqrt{d} \right)^{i-1}
\]
\[
\leq \frac{2\sqrt{d}}{\rho} (r(i) + r(j) + 1)^d.
\]

Using this bound for \( \nu^{d \times k} \left( S_{k+} \right) \), we obtain
\[
\nu^{d \times k} \left( N^{(\rho)} \right) \leq 2v_d \cdot \ell^{d(k-1)} \frac{2\sqrt{d}}{\rho} \sum_{1 \leq i < j \leq k} (r(i) + r(j) + 1)^d
\]
\[
\leq 2v_d \cdot \ell^{d(k-1)} \frac{2\sqrt{d}}{\rho} \cdot k^2 \cdot (2r_{\text{max}} + 1)^d,
\]

where \( r_{\text{max}} = \max_{i \in [q]} \{ r_i \} \). Thus, we get
\[
\left| Z(V, Q) - Z(G^{(\rho)}, Q^{(\rho)}) \right| \leq \sum_{k=2}^{K} \sum_{k_1 + \cdots + k_q \in [q] \setminus \{N\}} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) \nu^{d \times k} \left( N^{(\rho)} \right) \lesssim \sum_{k=2}^{K} \sum_{k_1 + \cdots + k_q \in [q] \setminus \{N\}} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) \cdot 4v_d \cdot \ell^{d(k-1)} \cdot \sqrt{d} \cdot k^2 \cdot (2r_{\text{max}} + 1)^d.
\]

We simplify the bound further by bounding
\[
\frac{1}{\rho} \sum_{k=2}^{K} \sum_{k_1 + \cdots + k_q \in [q] \setminus \{N\}} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) \cdot 4v_d \cdot \ell^{d(k-1)} \cdot \sqrt{d} \cdot k^2 \cdot (2r_{\text{max}} + 1)^d
\]
\[
\leq \frac{1}{\rho} \cdot 4v_d \cdot \ell^{d(K-1)} \cdot \sqrt{d} \cdot K^2 \cdot (2r_{\text{max}} + 1)^d \sum_{k=2}^{K} \sum_{k_1 + \cdots + k_q \in [q] \setminus \{N\}} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right).
\]

Applying the multinomial theorem, we obtain
\[
\sum_{k=2}^{K} \sum_{k_1 + \cdots + k_q \in [q] \setminus \{N\}} \left( \prod_{i \in [q]} \frac{e^{k_i p_i}}{k_i!} \right) = \sum_{k=2}^{K} \frac{1}{k!} (e^{p_1} + \cdots + e^{p_q})^k \leq e^q e^{p_{\text{max}}},
\]

where the last inequality follows from the Taylor expansion of \( e^x \) at 0.
Overall, we bound

\[
|Z(V, Q) - Z(G^{(\rho)}, Q^{(\rho)})| \leq \frac{1}{\rho} \cdot 4v_d \cdot l^{d(K-1)} \cdot \sqrt{d} \cdot K^2 \cdot (2r_{\text{max}} + 1)^d \cdot e^{q \cdot e^{P_{\text{max}}}}
\]

Recalling that we assume \( r_{\text{max}} \in O(\ell) \), as mentioned at the beginning of Section 5, we obtain

\[
|Z(V, Q) - Z(G^{(\rho)}, Q^{(\rho)})| \leq \frac{1}{\rho} \cdot e^{\Theta(Kd \ln l + \ln(r_{\text{max}} + 1) + q \cdot e^{P_{\text{max}}})}.
\]

Before we get to our main result for this section, it is useful to have a closer look at \( b_d \). As we increase the resolution \( \rho \) for our discretization, we scale the radii of the continuous model accordingly to \( r_i^{(\rho)} = \rho r_i \). This causes the bound \( b_d(\rho r_i) \) to converge to the volume of the sphere \( r_i \). The following lemma gives a simple but sufficient bound for the speed of this convergence, which we use to include this effect into our approximation result for the continuous partition function.

**Lemma 18.** Let \( \delta \in (0, 1) \), \( r \in \mathbb{R}_{>0} \), and let \( b_d(\rho r) \) denote the number of integer points in a sphere of radius \( \rho r \).

Then, for all \( \rho \geq (2\sqrt{d})^d / (\delta r) \), it holds that \( b_d(\rho r) \leq (1 + \delta) \cdot v_d \cdot (\rho r)^d \).

**Proof.** We start by considering a sphere of radius \( \rho r + \sqrt{d} \) at the origin. Note that this enlarged sphere contains for each grid point \((x_1, \ldots, x_d)\) in the original sphere the cubic region \([x_1, x_1 + 1] \times \cdots \times [x_d, x_d + 1]\) of volume 1. Thus, the volume of the enlarged sphere is a trivial upper bound on the number of grid points in the original sphere.

Formally, we get

\[
b_d(\rho r) \leq v_d \cdot \left( \rho r + \sqrt{d} \right)^d,
\]

which we rewrite as

\[
v_d \cdot \left( \rho r + \sqrt{d} \right)^d = v_d \cdot (\rho r)^d + v_d \cdot \sum_{i \in [d]} \binom{d}{i} (\rho r)^{d-i} \cdot \sqrt{d}^i.
\]

Further, note that for our choice of \( \rho \) it holds that \( \rho r \geq 1 \). Thus, we get

\[
v_d \cdot (\rho r)^d + v_d \cdot \sum_{i \in [d]} \binom{d}{i} (\rho r)^{d-i} \cdot \sqrt{d}^i \leq v_d \cdot (\rho r)^d + v_d \cdot (\rho r)^{d-1} \cdot \sqrt{d}^d = v_d \cdot (\rho r)^d \cdot \left( 1 + \frac{1}{\rho r} \cdot (2\sqrt{d})^d \right).
\]

We conclude the proof by noting that \((2\sqrt{d})^d / \rho r \leq \delta\).

We now prove our main statement for approximation of the partition function of the continuous hard-sphere model. A crucial point of this proof is that the size of the polymer clique cover of the discrete model, for any fixed number of dimensions \( d \), only depends on the fraction of \( n \)
and \( r_{\text{min}} \). Both are scaled equally for any resolution \( \rho \), which means that the number of polymer cliques in the cover is independent of \( \rho \). Thus, although the number of polymers grows in \( \rho^d \), the number of polymer cliques and the mixing time of our Markov chain remains fixed, and we only have to argue that the integers that need to be drawn for running the Markov chain do not become too large.

\[ \Box \]

**Theorem 19.** Let \((V, Q)\) be a continuous hard-sphere model with \( V = [0, \ell]^d \) and \( q \) particle types \( Q = \{(r_i, p_i)\}_{i \in [q]} \), let \( r_{\text{min}} = \min_{i \in [q]} \{r_i\} \), and let \( \delta \in (0, 1/r_{\text{min}}] \). Assume that, for all \( i \in [q] \), there is an \( h_i \in \mathbb{R}_{>0} \) with

\[
\exp\left(-\frac{\ell}{r_{\text{min}}} \right)^d \leq h_i \leq \exp\left(\frac{\ell}{r_{\text{min}}} \right)^d
\]

such that, for all \( j \in [q] \), it holds that

\[
(1 + \delta)\nu_d \sum_{i \in [q]} (r_i + r_j)^d e^{p_i} \frac{h_i}{h_j} \leq 1. \tag{16}
\]

Then, for each \( \epsilon \in (0, 1] \), there is a randomized \( \epsilon \)-approximation of \( Z(V, Q) \) computable in time

\[
\text{poly}\left( \frac{\ell \sqrt{d}}{2r_{\text{min}}} \right)^d dq + d \ln(d\ell) + d \ln(1/\delta). \tag*{\Box}
\]

**Proof.** We aim to obtain an \( \epsilon' \)-approximation for the discretization \( Z(G^{(\rho)}, Q^{(\rho)}) \) by Lemma 15 for some \( \rho \). To this end, by Lemma 17, choosing

\[
\rho \geq \frac{1}{\delta r_{\text{min}}} \left( 2 \sqrt{d} \right)^d \cdot \frac{\exp\left( \Theta\left( \left( \frac{\sqrt{\ell}}{r_{\text{min}}} \right)^d \ln(I) + q \text{e}^{p_{\max}} \right) \right)}{\epsilon'}, \tag{\*}
\]

and noting that \( \rho \geq 2 \sqrt{d} \) due to \( \delta \leq 1/r_{\text{min}} \) and \( \ell \geq 1 \), we know that \( Z(G^{(\rho)}, Q^{(\rho)}) \) is an \( \epsilon' \)-approximation of \( Z(V, Q) \).

We now show that the discretization \((G^{(\rho)}, Q^{(\rho)})\) satisfies the conditions of Lemma 15. Let \( r_{\text{min}}^{(\rho)} = \min_{i \in [q]} \{r_i^{(\rho)}\} = \rho r_{\text{min}} \), and let \( n = \rho \ell \) be the number of grid points along each dimension of \( G^{(\rho)} \). It is important to note that

\[
\frac{n}{r_{\text{min}}^{(\rho)}} = \frac{\rho \ell}{r_{\text{min}}^{(\rho)}} = \frac{\ell}{r_{\text{min}}^{(\rho)}}.
\]

Consequently, for all \( i \in [q] \), it holds that

\[
\exp\left(-\frac{n}{r_{\text{min}}^{(\rho)}} \right)^d \leq h_i \leq \exp\left(\frac{n}{r_{\text{min}}^{(\rho)}} \right)^d \leftrightarrow \exp\left(-\frac{\ell}{r_{\text{min}}^{(\rho)}} \right)^d \leq h_i \leq \exp\left(\frac{\ell}{r_{\text{min}}^{(\rho)}} \right)^d.
\]

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Further, our choice of $\rho$ implies for all $i, j \in [q]$ that
\[
\rho \geq \frac{1}{\delta \cdot (r_i + r_j)} (2\sqrt{d})^d.
\]

By Lemma 18 and equation (16), we obtain
\[
\sum_{i \in [q]} b_d(r_i^{(\rho)} + r_j^{(\rho)}) e^{\rho h_i} \frac{h_i}{h_j} \leq \sum_{i \in [q]} b_d(\rho \cdot (r_i + r_j)) e^{\rho h_i} \frac{h_i}{h_j} \leq (1 + \delta) v_d \sum_{i \in [q]} (r_i + r_j)^d e^{\rho h_i} \frac{h_i}{h_j} \leq 1.
\]

Consequently, the conditions of Lemma 15 are satisfied, and it yields a runtime of
\[
\text{poly}\left(\frac{n\sqrt{d}}{2r_{\min}^{(\rho)}}\right)^d \frac{q + d \ln(n)}{\epsilon'} = \text{poly}\left(\frac{\ell\sqrt{d}}{2r_{\min}^{(\rho)}}\right)^d \frac{q + d \ln(\rho) + d \ln(\ell)}{\epsilon'}
\]
for an $\epsilon'$-approximation of $Z(G^{(\rho)}, Q^{(\rho)})$. By choosing $\rho \in \Theta(\xi)$, we bound
\[
\ln(\rho) \in O\left(\ln\left(\frac{1}{\delta}\right) + \ln\left(\frac{1}{r_{\min}^{(\rho)}}\right) + d \ln(d) + d \ln(\ell)\left(\frac{\ell\sqrt{d}}{2r_{\min}^{(\rho)}}\right)^d + q e^{\rho_{\max}}\right).
\]

Further, note that, for all $j \in [q]$, it holds that $v_d \cdot (2r_j)^d e^{\rho_j} \leq 1$ and thus $e^{\rho_{\max}} \in O\left(\left(\sqrt{d}/(2r_{\min})\right)^d\right)$, which leads to a runtime of
\[
\text{poly}\left(\frac{\ell\sqrt{d}}{2r_{\min}^{(\rho)}}\right)^d \frac{dq + d \ln(d\ell) + d \ln(1/\delta)}{\epsilon'}
\]

Last, by choosing $\epsilon' \leq \epsilon/3$, we note that the $\epsilon'$-approximation of $Z(G^{(\rho)}, Q^{(\rho)})$, which is an $\epsilon'$-approximation of $Z(V, Q)$, is an $\epsilon$-approximation of $Z(V, Q)$, as $(1 + \epsilon')^2 \leq (1 + \epsilon)$ and $(1 - \epsilon')^2 \geq (1 - \epsilon)$. This concludes the proof.

5.3 Example: $p_i = \ln\left(\frac{\lambda}{v_d \cdot (r_i)^d}\right)$

We demonstrate the application of Theorem 19 to a specific form of chemical potential. Namely, for each particle type $i \in [q]$, we choose the chemical potential $p_i = \ln(\lambda/(v_d \cdot (r_i)^d))$, where the parameter $\lambda \in \mathbb{R}_{>0}$ represents some external condition. This is a straightforward generalization of the form of chemical potential that is commonly assumed in the single-component model and, for example, discussed by Guo and Jerrum [22] and Helmuth et al. [26]. The result-
Proposition 20. Let $(V, Q)$ be a continuous hard-sphere model with $V = [0, \ell]^d$ and $q$ particle types $Q = \{(r_i, p_i)\}_{i \in [q]}$, where $p_i = \ln(\lambda/(\nu_d \cdot (r_i)^d))$ for some parameter $\lambda \in \mathbb{R}_{>0}$. Further, let $r_{\min} = \min_{i \in [q]} \{r_i\}$ and $r_{\max} = \max_{i \in [q]} \{r_i\}$, and let $\bar{\lambda} = r_{\max}/r_{\min}$. If, for some $\delta \in (0, 1)$, it holds that $\lambda \leq \frac{1}{1 + \delta} \cdot \left(2^d + (q - 1) \cdot \left(\frac{\bar{\lambda} + 1}{\sqrt{\bar{\lambda}}}\right)^d\right)^{-1}$, then, for every $\epsilon \in (0, 1)$, there is a randomized $\epsilon$-approximation of $Z(V, Q)$ computable in time $\text{poly}\left(\frac{(\ell \sqrt{d})^d dq + d \ln(d\ell) + d \ln(1/\delta)}{\epsilon}\right)$.

Proof. We aim to apply Theorem 19. To this end, for all $i \in [q]$, let $h_i = (\sqrt{\ell})^d$. Thus, for all $j \in [q]$, it holds that

\[(1 + \delta)\nu_d \sum_{i \in [q]} (r_i + r_j)^d e^{p_i} \frac{h_i}{h_j} \leq \left(2^d + (q - 1) \cdot \left(\frac{\bar{\lambda} + 1}{\sqrt{\bar{\lambda}}}\right)^d\right)^{-1} \cdot \sum_{i \in [q]} \frac{(r_i + r_j)^d}{r_i^d} \left(\frac{r_i}{r_j}\right)^{d/2}.
\]

Note that, for all $j \in [q]$, we have

\[\sum_{i \in [q]} \frac{(r_i + r_j)^d}{r_i^d} \left(\frac{r_i}{r_j}\right)^{d/2} = \sum_{i \in [q]} \left(1 + \frac{r_j}{r_i}\right)^d \left(\frac{r_i}{r_j}\right)^{d/2} = 2^d + \sum_{i \neq j} \left(\sqrt{\frac{r_i}{r_j}} + \sqrt{\frac{r_j}{r_i}}\right)^d.
\]

and that, for all $i, j \in [q]$, it holds that

\[\left(\sqrt{\frac{r_i}{r_j}} + \sqrt{\frac{r_j}{r_i}}\right)^d \leq \left(\sqrt{\frac{r_i}{r_j}} + \frac{1}{\sqrt{\frac{r_i}{r_j}}}\right)^d = \left(\frac{\bar{\lambda} + 1}{\sqrt{\bar{\lambda}}}\right)^d.
\]

Thus, we have

\[\left(2^d + (q - 1) \cdot \left(\frac{\bar{\lambda} + 1}{\sqrt{\bar{\lambda}}}\right)^d\right)^{-1} \cdot \sum_{i \in [q]} \frac{(r_i + r_j)^d}{r_i^d} \left(\frac{r_i}{r_j}\right)^{d/2} \leq 1.
\]

Applying Theorem 19 concludes the proof.


6 Truncation of polymer cliques

In Section 4, we discuss under which assumptions the partition function of a polymer model \( P \) with polymer clique cover \( \Lambda \) of size \( m \) can be approximated in time polynomial in \( m \) (Theorem 12). One of the assumptions requires to be able to sample, for all \( i \in [m] \), from \( \mu_{|\Lambda_i} \) in time poly\((m)\). Unfortunately, for many algorithmic problems, the number of polymer families of each polymer clique is large, and efficient sampling from \( \mu_{|\Lambda_i} \) is non-trivial. However, as we only require to approximately sample from \( \mu_{|\Lambda_i} \), it is sufficient to ignore polymer families with low probabilities, that is, with low weight.

We formalize this concept rigorously by defining a size function for polymers. We aim to remove polymers of large size (low weight), which still yields a sufficient approximation of \( \mu_{|\Lambda_i} \) (Lemma 23). As a consequence, we can still approximate \( Z(P) \) in time polynomial in \( m \) (Theorem 27). In Section 6.1, we showcase how this new theorem applies to bipartite \( \alpha \)-expanders with bounded degree.

\[ \text{Definition 21 (size function).} \] Given a polymer model \((C, w, +)\), a size function is a function \(|·| : C \rightarrow \mathbb{R}_{>0}\). For a fixed size function \(|·|\) and some polymer \( \gamma \in C \) we call \(|\gamma|\) the size of \( \gamma \).

A given size function, we truncate the polymer model to polymers of small size.

\[ \text{Definition 22 (truncation).} \] Given a polymer model \((C, w, +)\) equipped with a fixed size function \(|·|\) and some set of polymers \( B \subseteq C \). For all \( k \in \mathbb{R} \), we call \( B^{\leq k} = \{ \gamma \in B \mid |\gamma| \leq k \} \) the truncation of \( B \) to size \( k \). Further, we write \( B^{>k} = B \setminus B^{\leq k} \).

Note that \( B \subseteq C \) and that \( B^{\leq k}, B^{>k} \) is a partitioning of \( B \), which implies \( B^{\leq k}, B^{>k} \subseteq C \). Thus, we can apply our notions of restricted polymer families, partition function, and Gibbs distribution as stated in Section 2.1 to \( B^{\leq k} \) and \( B^{>k} \) as well. The case \( B = C \) (i.e., we truncate the entire polymer model) plays a special role, which is why we use the shorter notation \( \mathcal{F}_{\leq k} = \mathcal{F}^{\leq k}, Z_{\leq k} = Z^{\leq k} \), and \( \mu_{\leq k} = \mu^{\leq k} \). Analogously, we define \( \mathcal{F}_{>k}, Z_{>k}, \) and \( \mu_{>k} \).

\[ \text{Lemma 23 (truncation of polymer cliques).} \] Let \( P = (C, w, +) \) be a polymer model, let \( \Lambda \) be a polymer clique cover of \( P \) with size \( m \), and let \(|·|\) be a size function for \( P \). Assume that there is a \( k \in \mathbb{R} \) and an \( \epsilon \in (0, 1) \) such that, for all \( i \in [m] \), it holds that

\[
\sum_{\gamma \in \Lambda_i^{\leq k}} w_\gamma \leq \frac{\epsilon}{m}. \tag{17}
\]

Then \( e^{-\epsilon} \leq Z_{\leq k}/Z \leq 1 \) and \( d_{\text{TV}}(\mu, \mu_{\leq k}) \leq \epsilon \).

\[ \text{Proof.} \] We start by proving \( e^{-\epsilon} \leq Z_{\leq k}/Z \leq 1 \). Since \( Z_{\leq k} \leq Z \), as removing polymers does not increase the partition function, it remains to show that \( Z \leq e^\epsilon Z_{\leq k} \).

We observe that \( Z \leq Z_{\leq k} Z_{>k} \) with equality if and only if, for all \( \Gamma \in \mathcal{F}_{\leq k} \) and all \( \Gamma' \in \mathcal{F}_{>k} \), it holds that \( \Gamma \cup \Gamma' \in \mathcal{F} \). We proceed by showing that \( Z_{>k} \leq e^\epsilon \).
Note that $C^{>k} = \bigcup_{i \in [m]} A_i^{>k}$ and that each polymer family in $\mathcal{F}^{>k}$ contains at most one polymer from each $A_i^{>k}$. Thus, we obtain

$$Z_{>k} \leq \prod_{i \in [m]} Z_{|A_i^{>k}} = \prod_{i \in [m]} \left(1 + \sum_{\gamma \in A_i^{>k}} w_\gamma \right).$$

Due to equation (17), we get $Z_{>k} \leq (1 + \epsilon/m)^m \leq e^\epsilon$, which proves the first claim.

Regarding the second claim, it suffices to see that $d_{TV}(\mu, \mu_{\leq k}) = Z - Z_{\leq k} \leq kZ \leq 1 - e^{-\epsilon} \leq \epsilon$. ■

If the clique truncation condition is satisfied, by choosing a reasonable value $k$ for truncating a polymer model, only little overall weight is removed. That is, the truncated model represents a good approximation of the original.

Lemma 25. Let $\mathcal{P} = (C, w, \cdot)$ be a polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$, and let $|\cdot|$ be a size function for $\mathcal{P}$. For all $i \in [m]$, we say that $\Lambda_i$ satisfies the clique truncation condition for a monotonically increasing, invertible function $g: \mathbb{R} \to \mathbb{R}_{>0}$ and a bound $B \in \mathbb{R}_{>0}$ if and only if

$$\sum_{\gamma \in \Lambda_i} g(|\gamma|)w_\gamma \leq B.$$  

Proof. Let $\epsilon' \in (0, 1)$ and $k \geq g^{-1}(B/\epsilon')$. Due the clique truncation condition and the monotonicity of $g$, we observe that

$$g(k) \sum_{\gamma \in A_i^{>k}} w_\gamma \leq \sum_{\gamma \in A_i^{>k}} g(|\gamma|)w_\gamma \leq \sum_{\gamma \in A_i} g(|\gamma|)w_\gamma \leq B.$$  

As $g$ is positive, dividing by $g(k)$ yields $\sum_{\gamma \in A_i^{>k}} w_\gamma \leq B/g(k)$. Substituting our bound for $k$ and noting that $g$ is invertible, we conclude that

$$\sum_{\gamma \in A_i^{>k}} w_\gamma \leq \frac{B}{g(g^{-1}(B/\epsilon'))} = \epsilon'.$$  

Similar to how we required the clique dynamics condition for Theorem 12, we formalize the following condition for a polymer model with a size function.

Condition 24 (clique truncation). Let $\mathcal{P} = (C, w, \cdot)$ be a polymer model, let $\Lambda$ be a polymer clique cover of $\mathcal{P}$ with size $m$, and let $|\cdot|$ be a size function for $\mathcal{P}$. For all $i \in [m]$, we say that $\Lambda_i$ satisfies the clique truncation condition for a monotonically increasing, invertible function $g: \mathbb{R} \to \mathbb{R}_{>0}$ and a bound $B \in \mathbb{R}_{>0}$ if and only if

$$\sum_{\gamma \in \Lambda_i} g(|\gamma|)w_\gamma \leq B.$$  

Proof. Let $\epsilon' \in (0, 1)$ and $k \geq g^{-1}(B/\epsilon')$. Due the clique truncation condition and the monotonicity of $g$, we observe that

$$g(k) \sum_{\gamma \in A_i^{>k}} w_\gamma \leq \sum_{\gamma \in A_i^{>k}} g(|\gamma|)w_\gamma \leq \sum_{\gamma \in A_i} g(|\gamma|)w_\gamma \leq B.$$  

As $g$ is positive, dividing by $g(k)$ yields $\sum_{\gamma \in A_i^{>k}} w_\gamma \leq B/g(k)$. Substituting our bound for $k$ and noting that $g$ is invertible, we conclude that

$$\sum_{\gamma \in A_i^{>k}} w_\gamma \leq \frac{B}{g(g^{-1}(B/\epsilon'))} = \epsilon'.$$  

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As a direct consequence of Lemma 25, we get that the partition function of the truncated model is a useful approximation of the original partition function.

**Corollary 26.** Let \( P = (C, w, \ast) \) be a polymer model, let \( \Lambda \) be a polymer clique cover of \( P \) with size \( m \), and let \(|\cdot|\) be a size function for \( P \). Assume that there is a \( g: \mathbb{R} \to \mathbb{R}_{>0} \) and a \( B \in \mathbb{R}_{>0} \) such that, for \( i \in [m] \), the polymer clique \( A_i \) satisfies the clique truncation condition for \( g \) and \( B \).

Then, for all \( \varepsilon \in (0, 1) \) and all \( k \geq g^{-1}(Bm/\varepsilon) \), it holds that \( e^{-\varepsilon} \leq Z_{\leq k}/Z \leq 1 \) and \( d_{TV}(\mu, \mu_{\leq k}) \leq \varepsilon \).

**Proof.** The statement follows directly from Lemmas 23 and 25 by choosing \( \varepsilon' = \varepsilon / m \).

Using the truncated polymer model, we achieve an \( \varepsilon \)-approximation result of the partition function for the original model that is computable in time \( poly(m/\varepsilon) \), similar to Theorem 12.

**Theorem 27.** Let \( P = (C, w, \ast) \) be a computationally feasible polymer model, let \( \Lambda \) be a polymer clique cover of \( P \) with size \( m \), and let \(|\cdot|\) be a size function for \( P \). Further, let \( Z_{\max} = \max_{i \in [m]} \{Z_{A_i}\} \), and let \( t(k) \) denote an upper bound, for all \( i \in [m] \), on the time to enumerate \( A_i^{\leq k} \). Last, assume that

\( a) \ Z_{\max} \in poly(m), \)

\( b) \ P \) satisfies the clique dynamics condition for a function \( f \) such that, for all \( y \in C \), it holds that \( e^{-poly(m)} \leq f(y) \leq e^{poly(m)} \), and that

\( c) \ there \ are \ g: \mathbb{R} \to \mathbb{R}_{>0} \ and \ B \in \mathbb{R}_{>0} \ with \ B \in poly(m) \ and \ t(g^{-1}(x)) \in poly(x) \) (for all \( x \in \mathbb{R}_{>0} \)) such that, for all \( i \in [m] \), it holds that \( A_i \) satisfies the clique truncation condition.

Then, for all \( \varepsilon \in (0, 1] \), we can \( \varepsilon \)-approximately sample from \( \mu \) in time \( poly(m/\varepsilon) \), and there is a randomized \( \varepsilon \)-approximation of \( Z \) computable in \( poly(m/\varepsilon) \).

Note that Observation 10 applies to Theorem 27 as well. That is, by using more restrictive assumptions, assumptions (a) and (b) are satisfied. We proceed with proving the theorem.

**Proof of Theorem 27.** As in the proof of Theorem 9, we consider the polymer Markov chain \( M(P) \). Further, let \( k = g^{-1}(2Bm/\varepsilon) \), let \( M_k \) denote the polymer Markov chain on \( (C_{\leq k}, w, \ast) \), and let \( P_k \) denote its transitions. We aim to run \( M_k \) for at least \( t^* = \tau_M(\varepsilon/2) \) iterations, starting from \( \emptyset \in T_{\leq k} \).

We prove that \( d_{TV}(\mu, P_k^{t^*}(\emptyset, \cdot)) \leq \varepsilon \). By the triangle inequality, we obtain

\[
d_{TV}(\mu, P_k^{t^*}(\emptyset, \cdot)) \leq d_{TV}(\mu, \mu_{\leq k}) \leq d_{TV}(\mu_{\leq k}, P_k^{t^*}(\emptyset, \cdot)).
\]

By our choice of \( k \) and by Corollary 26 together with assumption (c), we get that \( d_{TV}(\mu, \mu_{\leq k}) \leq \varepsilon/2 \). Further, note that truncation preserves the clique dynamics condition for the same function \( f \) and does not increase any quantity that is used for bounding the mixing time. Thus, \( \tau_{M_k}(\varepsilon/2) \leq \tau_{M(P)}(\varepsilon/2) \), and we obtain \( d_{TV}(\mu_{\leq k}, P_k^{t^*}(\emptyset, \cdot)) \leq \varepsilon/2 \) for our choice of \( t^* \).
It remains to show that the runtime is bounded by \( \text{poly}(m/\varepsilon) \). Analogously to the proof of Theorem 9, due to assumptions (a) and (b), we know that \( t_{\mathcal{M}(\mathcal{P})}(\varepsilon/2) \in \text{poly}(m/\varepsilon) \), which implies \( t_{\mathcal{M}(\mathcal{P})}(\varepsilon/2) \in \text{poly}(m/\varepsilon) \). Also analogously, it holds that each step can be done in \( \text{poly}(m) \), except for sampling, for all \( i \in [m] \), from \( \mu_{|A_i} \). However, note that, for all \( i \in [m] \), we only need to sample from \( \mu_{|A_i^{\leq k}} \). We do so by enumerating \( A_i^{\leq k} \) in time \( t(k) \). By our choice of \( k \) and by assumption (c), this takes time at most

\[
t(k) = t\left( g^{-1}\left( \frac{2Bm}{\varepsilon} \right) \right) \in \text{poly}\left( \frac{m}{\varepsilon} \right),
\]

which proves that we can \( \varepsilon \)-approximately sample from \( \mu \) in the desired runtime.

Showing that we can \( \varepsilon \)-approximate \( Z \) in time \( \text{poly}(m/\varepsilon) \) is done analogously. By Corollary 26 and assumption (c), we know that for \( k = g^{-1}(2Bm/\varepsilon) \) it holds that \( e^{-\varepsilon/2} \leq Z_{\leq k}/Z \leq 1 \), which implies \( e^{-\varepsilon/2}Z \leq Z_{\leq k} \leq Z \). As argued above, the truncation of the polymer model \( \mathcal{P} \) to this size \( k \) satisfies the conditions of Theorem 9, where the sampling from each clique is done by ignoring polymers larger than \( k \). Thus, by Theorem 12, we obtain an \( \varepsilon/2 \)-approximation for \( Z_{\leq k} \) in time \( \text{poly}(2m/\varepsilon) = \text{poly}(m/\varepsilon) \). Noting that, for \( \varepsilon \leq 1 \), it holds that

\[
1 - \varepsilon \leq \left( 1 - \frac{\varepsilon}{2} \right)e^{-\varepsilon/2} \text{ and } \left( 1 + \frac{\varepsilon}{2} \right) \leq 1 + \varepsilon,
\]

which concludes the proof.

6.1 Application: hard-core model on bipartite expanders

In order to demonstrate how Theorem 27 improves known bounds for the algorithmic use of polymer models, we investigate the hard-core model for high fugacity \( \lambda \in \mathbb{R}_{>0} \) on bipartite \( \alpha \)-expanders with bounded maximum degree \( \Lambda \). For a graph \( (V, E) \) and an \( S \subseteq V \), let \( N_G(S) \) denote the set of all vertices that are adjacent to a vertex in \( S \).

**Definition 28 (bipartite \( \alpha \)-expander).** Let \( G = (V, E) \) be a bipartite graph with partition \( V = V_L \cup V_R \). For all \( i \in \{L, R\} \), we call \( S \subseteq V_i \) small if and only if \( |S| \leq |V_i|/2 \). For all \( \alpha \in (0, 1) \), graph \( G \) is a bipartite \( \alpha \)-expander if and only if, for all small sets of vertices \( S \), it holds that \( |N_G(S)| \geq (1 + \alpha)|S| \).

For any graph \( G \), the hard-core partition function is a graph polynomial of some parameter \( \lambda \in \mathbb{R}_{>0} \), called fugacity. Let \( I_G \) be the set of all independent sets in \( G \). The hard-core partition function for fugacity \( \lambda \) is now formally defined as

\[
Z(G, \lambda) = \sum_{I \in I_G} |I|^\lambda.
\]

We approximate \( Z(G, \lambda) \) in terms of the partition function of two polymer models, constructed as proposed by Jenssen et al. [30]. For a bipartite \( \alpha \)-expander \( G \) with bounded degree \( \Lambda \), we consider the graph \( G^2 \), which is the graph with vertices \( V \) and an edge between \( v, u \in V \) if \( v, u \) have at most distance 2 in \( G \). For all \( i \in \{L, R\} \), we define a polymer model \( \mathcal{P}^{(i)} = (C^{(i)}, \mathcal{W}^{(i)}, \ast) \) as follows:
• each polymer $\gamma \in \mathcal{C}(i)$ is defined by a non-empty set of vertices $\overline{\gamma} \subseteq V_i$ such that $\overline{\gamma}$ is small and induces a connected subgraph in $G^2$.

• for $\gamma \in \mathcal{C}(i)$, let $w^{(i)}(\gamma) = \lambda^{\overline{\gamma}}/((1 + \lambda)^{|\text{Net}(\overline{\gamma})|})$, and

• two polymers $\gamma, \gamma' \in \mathcal{C}(i)$ are incompatible if and only if there are vertices $v \in \overline{\gamma}, w \in \overline{\gamma}'$ with graph distance at most 1 in $G^2$.

To ease notation, for all $i \in \{L, R\}$, we write $\mu^{(i)}$ and $Z^{(i)}$ instead of $\mu^{(\mathcal{P}^{(i)})}$ and $Z(\mathcal{P}^{(i)})$, respectively.

We use $\mathcal{P}^{(L)}$ and $\mathcal{P}^{(R)}$ for approximating the hard-core partition function of bipartite $\alpha$-expanders in the following sense.

▶ **Lemma 29** ([30, Lemma 19]). Given a bipartite $\alpha$-expander $G = (V_L \cup V_R, E)$ with $|V_L \cup V_R| = n$, let $Z(G, \lambda)$ denote its hard-core partition function with fugacity $\lambda \in \mathbb{R}_{>0}$, and let the polymer models $\mathcal{P}^{(L)}, \mathcal{P}^{(R)}$ be defined as above. For all $\lambda \geq e^{11/\alpha}$, it holds that

$$ (1 - e^{-n})Z(G, \lambda) \leq (1 + \lambda)^{|V_L|}Z^{(L)} + (1 + \lambda)^{|V_R|}Z^{(R)} \leq (1 + e^{-n})Z(G, \lambda). $$

To apply Theorem 27, we have to fix a polymer clique cover $\Lambda$ for each polymer model $\mathcal{P}^{(i)}$ with $i \in \{L, R\}$. Based on the incompatibility relation, a natural choice is to define, for each $v \in V_i$, a clique $\Lambda_v$ such that $\gamma \in \Lambda_v$ if and only if $v \in \overline{\gamma}$. As we need to verify the clique dynamics condition, it is useful to have a bound on the number of incompatible polymers, which the following lemma provides.

▶ **Lemma 30** ([3, Lemma 2.1]). For an undirected graph $G = (V, E)$ with maximum degree $\Delta$ and for all $v \in V$, the number of vertex-induced subgraphs that contain $v$ and have at most $k \in \mathbb{N}_{>0}$ vertices is bounded from above by $e^k \Delta^{k-1}/(k^{3/2} \sqrt{2\pi})$.

Commonly, the bound $(e\Delta)^{k-1}/2$ is applied, as it is more convenient to work with. However, this bound actually only holds for $k \geq 2$. Further, note that the original paper used a weaker bound, namely $(e\Delta)^k$. Although this bound holds for all $k \in \mathbb{N}_{>0}$, it yields a much worse dependency on $\Delta$. For a fair comparison, we added the result of refined calculations for the approach by Jenssen et al. [30] to Table 1.

Note that the choice of the function $f$ used in the clique dynamics condition is very sensitive to the bound on the number of subgraphs. For the bound stated in Lemma 30, it turns out that using $f(\gamma) = |\overline{\gamma}|$ yields the best bounds on $\lambda$ (see the proof of Proposition 32 for details). With this choice of $f$, the condition that we identified in Observation 10 is similar to the mixing condition of Chen et al. [7, Definition 1], except that we do not require a strict inequality. Further, note that such a choice of $f$ is not possible for the Kotecký–Preiss condition [36]. If purely exponential bounds on the number of subgraphs are used, the best results are usually obtained by setting $f$ to take an exponential form. A detailed understanding of how to choose $f$ might be of interest for applications to specific graph classes and other combinatorial structures.

In order to apply truncation, we further need a notion of size for polymers. An obvious choice is to set $|\gamma| = |\overline{\gamma}|$. The following lemma then bounds the time for enumerating polymers in a clique up to some size $k \in \mathbb{N}_{>0}$.
Lemma 31 ([42, Lemma 3.7]). Let \( G = (V, E) \) be an undirected graph with maximum degree \( \Delta \), and let \( v \in V \). There is an algorithm that enumerates all connected, vertex-induced subgraphs of \( G \) that contain \( v \) and have at most \( k \in \mathbb{N}_{>0} \) vertices in time \( O(k \log(\Delta)) \).

We now prove our bound on \( \lambda \) for an efficient approximation of the hard-core partition function on bipartite \( \alpha \)-expanders. Most of the calculations are similar to those of Jenssen et al. [30], except that we use our newly obtained conditions.

Proposition 32. Let \( G(V_L \cup V_R, E) \) be a bipartite \( \alpha \)-expander with \( |V_L \cup V_R| = n \) and with maximum degree \( \Delta \in \mathbb{N}_{>0} \). For \( \lambda \geq \max\{0.81^{1/\alpha}, e^{1/\alpha}\} \) and for all \( \varepsilon \in (0, 1] \), there is an FPRAS for \( Z(G, \lambda) \) with runtime \( (n/e)^{O(\log(\Delta))} \).

Proof. If \( \varepsilon \in O(e^{-n}) \), we compute \( Z(G, \lambda) \) by enumerating all independent sets. Since there are at most \( 2^n \) independent sets, which is polynomial in \( 1/e^{-n} \), the statement then follows. It remains to analyze the case \( \varepsilon \in \Omega(e^{-n}) \). To this end, assume that \( \varepsilon \geq 4e^{-n} \).

By Lemma 29, \( Z(G, \lambda) \) can be \( e^{-n} \)-approximated using \( Z^{(L)} \) and \( Z^{(R)} \). We aim for an \( \varepsilon/4 \)-approximation of \( Z^{(L)} \) and \( Z^{(R)} \), each with failure probability at most \( 1 - \sqrt{3}/2 \). Note that

\[
1 - \varepsilon \leq (1 - e^{-\varepsilon})(1 - \frac{\varepsilon}{4}) \quad \text{and} \quad (1 + e^{-\varepsilon})(1 + \frac{\varepsilon}{4}) \leq 1 + \varepsilon.
\]

Thus, with probability at least \((\sqrt{3}/2)^2 = 3/4\) the result is an \( \varepsilon \)-approximation of \( Z(G, \lambda) \). We can obtain the desired error probability of at most \( 1 - \sqrt{3}/2 \) for the approximations of \( Z^{(L)} \) and \( Z^{(R)} \) by taking the median of \( O(\ln(2/(2 - \sqrt{3})) = O(1) \) independent approximations with failure probability at most \( 1/4 \).

Let \( i \in \{L, R\} \). In order to approximate \( Z^{(i)} \), we aim to apply Theorem 27. To this end, for all \( v \in V_i \), we define a polymer clique \( \Lambda_v \) containing all polymers \( y \in C^{(i)} \) with \( v \in \overline{y} \). This results in a polymer clique cover of size \( n \).

We proceed by proving that the polymer model satisfies the clique dynamics condition for \( f(y) = |\overline{y}| \). We use Observation 10 to simplify this step. This also implies that assumption (a) of Theorem 27 is satisfied. For any \( y \in C^{(i)} \) we start by bounding the set of polymers \( y' \ast y \) by

\[
\sum_{y' \in C^{(i)}: y' \ast y} f(y') w^{(i)}_{y'} \leq \sum_{v \in N_{G^{(i)}}(\overline{y})} \sum_{y' \in \Lambda_v} f(y') w^{(i)}_{y'} = \sum_{v \in N_{G^{(i)}}(\overline{y})} \sum_{k \in \mathbb{N}_{>0}} \sum_{|\overline{y}| = k} f(y') w^{(i)}_{y'}.
\]

Because \( G \) is a bipartite \( \alpha \)-expander, for all \( y' \in C^{(i)} \), we have \( w^{(i)}_{y'} \leq 1/\lambda^{|\overline{y}|} \). Further, note that the degree of \( G^2 \) is bounded by \( \Delta^2 \). By Lemma 30 and our definition of \( f \), we obtain

\[
\sum_{v \in N_{G^{(i)}}(\overline{y})} \sum_{k \in \mathbb{N}_{>0}} \sum_{|\overline{y}| = k} f(y') w^{(i)}_{y'} \leq \Delta^2 |\overline{y}| \sum_{k \in \mathbb{N}_{>0}} \frac{e^k (\Delta^2)^{k-1}}{k^{3/2} \sqrt{2\pi}} \cdot k \cdot \frac{1}{\lambda^{|\overline{y}|}} = \frac{|\overline{y}|}{\sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} \left( \frac{e\Delta^2}{\lambda^{|\overline{y}|}} \right)^k \frac{1}{\sqrt{k}}.
\]
For $\lambda \geq (e\Delta^2/0.8)^{1/\alpha}$, we get

$$\frac{|\gamma|}{\sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} \left(\frac{e\Delta^2}{\lambda^a}\right)^k \frac{1}{\sqrt{k}} \leq \frac{|\gamma|}{\sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} (0.8)^k \frac{1}{\sqrt{k}} \leq \frac{|\gamma|}{\sqrt{2\pi}} e^{2|\gamma|} = f(\gamma).$$

It remains to show, for all $v \in V_i$, that $\Lambda_v$ satisfies the clique truncation condition for a $g: \mathbb{R} \rightarrow \mathbb{R}_{>0}$ and a $B \in \mathbb{R}_{>0}$. To this end, for all $y \in C^{(i)}$, let $|y| = |\gamma|$, let $g(|y|) = e^{0.2|y|}$, and let $B = 1$. Analogously to our verification of the clique dynamics condition, we see, for all $v \in V_i$, that

$$\sum_{y \in \Lambda_v} g(|y|) w_y^{(i)} \leq \frac{1}{\Delta^2 \sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} \left(\frac{e\Delta^2}{\lambda^a}\right)^k \frac{1}{\sqrt{k}} e^{0.2k} = \frac{1}{\Delta^2 \sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} \left(\frac{e^{1.2\Delta^2}}{\lambda^a}\right)^k \frac{1}{\sqrt{k}} = \frac{1}{\Delta^2 \sqrt{2\pi}} e^{2|\gamma|}. $$

For $\lambda \geq (e\Delta^2/0.8)^{1/\alpha}$, we get

$$\frac{1}{\Delta^2 \sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} \left(\frac{e^{1.2\Delta^2}}{\lambda^a}\right)^k \frac{1}{\sqrt{k}} \leq \frac{1}{\Delta^2 \sqrt{2\pi}} \sum_{k \in \mathbb{N}_{>0}} (0.8e^{0.2})^k \frac{1}{\sqrt{k}} \leq \frac{1}{\Delta^2 \sqrt{2\pi}} e^{2|\gamma|} \leq B. $$

Last, we bound the runtime of the FPRAS. By Lemma 31, we can enumerate each polymer clique up to size $k$ in time $t(k) \in e^{O(k \log |\Lambda|)}$. As $g^{-1}: x \mapsto 5 \ln(x)$, we have $\Delta \mapsto x \mapsto x^{O(\ln(\Delta))}$, which is polynomial for $\Delta \in \Theta(1)$. For the runtime bound, note that we truncate to size $k = g^{-1}(n/\epsilon)$. Thus, the time for computing each step of the polymer Markov chain is bounded by $t(k) \leq (n/\epsilon)^{O(\ln(\Lambda))}$, which dominates the runtime.

The results for the remaining applications in Table 1 are derived via similar calculations. For the Potts model on expander graphs and the hard-core model on unbalanced bipartite graphs, we use Lemmas 30 and 31 together with the same function $f$ for the clique dynamics condition as in the proof of Proposition 32. For the perfect matching polynomial, we use the bounds for the number of polymers and for polymer enumeration that are stated by Casel et al. [6], and we choose $f(\gamma) = e^{a|\gamma|}$ for $a \approx 0.2$.

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Appendix

We discuss Theorem 2 in detail. First, we explain why the assumptions of the original theorem by Greenberg et al. [20, Theorem 3.3] are insufficient. With Example 33, we provide a counterexample. Last, we prove our version of the theorem.

Besides some minor generalizations, the most important difference between Theorem 2 and Theorem 3.3 by Greenberg et al. [20] is that we assume the coupling to be defined for all pairs of states. We also require the expected change of $\delta$ as well as the probability bound to hold for all pairs of states. In contrast, Greenberg et al. [20] claim that it is sufficient if these properties hold for neighboring states with respect to some adjacency structure. In what follows, we argue that this does not always suffice.

It is well known that couplings on adjacent states can be extended to all pairs of states such that the expected decrease of $\delta$ for adjacent states implies an expected decrease for all pairs of states [12]. However, a similar argument does not necessarily hold for bounds on the probability that $\delta$ changes by at least a certain amount. More precisely, it is possible to construct a Markov chain and a coupling such that

$$\Pr[|\delta(X_{t+1}, Y_{t+1}) - \delta(x, y)| \geq \eta \delta(x, y) \mid X_t = x, Y_t = y] \geq \kappa$$

holds for all pairs of adjacent states $x, y \in \Omega$ but not for all pairs of non-adjacent states.

Thus, Theorem 3.3 by Greenberg et al. [20] can be used to deduce upper bounds for mixing times that contradict known lower bounds. We demonstrate this by giving a simple counterexample (Example 33). Using Theorem 3.3 by Greenberg et al. [20], we bound the mixing time of a symmetric random walk on a cycle of size $n$ by $O(\ln(n)^2 \ln(1/\epsilon))$. This contradicts the lower bound of $\Omega(n \ln(1/\epsilon))$ that results from the diameter of the state space [37, Chapter 7.1.2].

Example 33. We consider a symmetric random walk on a cycle of length $n \in \mathbb{N}_{>2}$ (i.e., $\Omega = \{0\} \cup \{n - 1\}$). In what follows, let all $+1$ and $-1$ operations on the state space be defined modulo $n$. In order to have the desired self-loop probability, we define the transitions $P$, for all $x \in \Omega$, by $P(x, x) = 1/2$ and $P(x, x + 1) = P(x, x - 1) = 1/4$.

We say two states $x, y \in \Omega$ with $x \neq y$ are adjacent if and only if $x = y + 1$ or $x = y - 1$. Further, we define $\delta$ to be the shortest-path distance in the cycle. Note that, for all $x, y \in \Omega$ with $x \neq y$, it holds that $\delta(x, y) \in [1, \lceil n/2 \rceil]$.

Let $(X_t)_{t \in \mathbb{N}}$ and $(Y_t)_{t \in \mathbb{N}}$ be two copies of the chain $(\Omega, P)$, and let $x, y \in \Omega$ be adjacent. Without loss of generality, assume $x = y + 1$. For $X_t = x, Y_t = y$ we construct the following coupling:

- With probability $1/4$, choose $X_{t+1} = x$ and $Y_{t+1} = x$, resulting in $\delta(X_{t+1}, Y_{t+1}) = 0$.
- With probability $1/4$, choose $X_{t+1} = y$ and $Y_{t+1} = y$, resulting in $\delta(X_{t+1}, Y_{t+1}) = 0$.
- With probability $1/4$, choose $X_{t+1} = x$ and $Y_{t+1} = y$, resulting in $\delta(X_{t+1}, Y_{t+1}) = 1$.
- With the remaining probability of $1/4$, choose $X_{t+1} = x + 1$ and $Y_{t+1} = y - 1$, resulting in $\delta(X_{t+1}, Y_{t+1}) = 3$.
Note that $E[\delta(X_{t+1}, Y_{t+1}) \mid X_t = x, Y_t = y] = \delta(x, y)$.

For $\eta = 0.999$ and $\kappa = 3/4$, it holds that

$$\Pr[|\delta(X_{t+1}, Y_{t+1}) - \delta(x, y)| \geq \eta \delta(x, y) \mid X_t = x, Y_t = y] \geq \kappa.$$ 

Theorem 3.3 by Greenberg et al. [20] then yields a mixing time bound of $O(\ln(n)^2 \ln(1/\epsilon))$, which contradicts the linear lower bound stated by Levin and Peres [37, Chapter 7.1.2].

Note that Example 33 is not a counterexample for Theorem 2, as there are, for all $\eta \in \omega(1/n)$, non-adjacent states $x, y \in \Omega$ with $\Pr[|\delta(X_{t+1}, Y_{t+1}) - \delta(x, y)| \geq \eta \delta(x, y) \mid X_t = x, Y_t = y] = 0$.

**Proof of our version**

We closely follow the proof of Greenberg et al. [20]. Central to this is the following theorem, which we present in a slightly different fashion than Greenberg et al. [21, Lemma 3.5].

**Theorem 34.** Let $d, D \in \mathbb{R}$ with $d \leq D$, let $q \in [d, D]$, and let $(S_t)_{t \in \mathbb{N}}$ be a stochastic process adapted to a filtration $(\mathcal{F}_t)_{t \in \mathbb{N}}$. Further, let $T = \inf\{t \in \mathbb{N} \mid S_t \leq q\}$. Assume that, for all $t \in \mathbb{N}$, it holds that $S_t \cdot 1\{t \leq T\} \in [d, D]$, that

$$E[S_{t+1} \cdot 1\{t < T\} \mid \mathcal{F}_t] \leq S_t \cdot 1\{t < T\},$$  \hspace{1cm} (18)

and that there is a $Q \in \mathbb{R}_{>0}$ such that

$$E[(S_{t+1} - S_t)^2 \cdot 1\{t < T\} \mid S_t] \geq Q \cdot 1\{t < T\}.$$  \hspace{1cm} (19)

Then

$$E[T] \leq \frac{E[(D - S_T)^2] - E[(D - S_0)^2]}{Q}. \hspace{1cm} \blacksquare$$

Different to the original theorem by Greenberg et al. [21, Lemma 3.5], we include a filtration, indicator functions, and define the predicate of the stopping time via an inequality. Our reasons are as follows. The proof of Theorem 34 aims to apply the optional-stopping theorem for submartingales. A submartingale is, by definition, a stochastic process $(Z_t)_{t \in \mathbb{N}}$ adapted to a filtration $(\mathcal{F}_t)_{t \in \mathbb{N}}$ such that, for all $t \in \mathbb{N}$, the expectation of $Z_t$ is finite and $E[Z_{t+1} \mid \mathcal{F}_t] \geq Z_t$.

It is important to note that the expectation $E[Z_{t+1} \mid \mathcal{F}_t]$ is itself a random variable and that the inequality $E[Z_{t+1} \mid \mathcal{F}_t] \geq Z_t$ is stronger than $E[Z_{t+1}] \geq E[Z_t]$ (which follows by the law of total expectation). Hence, we require a filtration.

Second, the indicator functions make sure that equations (18) and (19) (and the boundedness of $S$) only have to hold as long as $S$ did not stop. Afterward, they are trivially satisfied. This is important, as $S$ is bounded from below by $d$ and its expectation does not increase. Assume that we did not use indicator functions. If there is a $t \in \mathbb{N}$ such that $S_t = d$, then $S_{t+1} = d$ holds as well, as otherwise the inequality $E[S_{t+1}] \leq E[S_t]$ (which follows by the law of total expectation from equation (18)) does not hold. However, this implies that $E[(S_{t+1} - S_t)^2 \mid \mathcal{F}_t] = 0$ (since the process is now almost surely deterministic), which violates equation (19) if not for the indicator functions.
Last, the inequality with respect to \( q \) in the definition of \( T \) is important, as \( S \) does not need to take on exactly \( q \). If this never happens, equation (19) may eventually not hold, due to the same argument as in the previous paragraph. Using the inequality in the definition of \( T \) guarantees that \( E[T] \) is finite.

Note that our additional assumptions in Theorem 34 only fixes issues in the proof of Greenberg et al. [21, Lemma 3.5]. The proof itself remains mostly unchanged.

While we state Theorem 34 in an elaborate fashion, we use it in a slightly different way in the following proof of Theorem 2. First, in order to ease notation, we ignore the indicator functions and check equations (18) and (19) for values of \( t \in \mathbb{N} \) such that \( t < T \) is true. Second, instead of using a filtration and calculating expectations that are random variables, such as \( E[S_{t+1} \mid \mathcal{F}_t] \) (ignoring the indicator function), we use normal expectations but do so for every possible outcome of \( S_t \). That is, we make sure that equations (18) and (19) are satisfied pointwise. Since we only consider countable state spaces, this approach is valid.

**Proof of Theorem 2.** We aim to bound the expected time until \( \delta \) hits 0 for the coupled copies \( (X_t)_{t \in \mathbb{N}} \) and \( (Y_t)_{t \in \mathbb{N}} \) of \( M \) and for all pairs of starting states \( x, y \in \Omega \). This results in a bound on the expected coupling time, and, because \( M \) is ergodic, also bounds \( \tau_M \) (see, for example, Chapter 11 by Mitzenmacher and Upfal [40] for a detailed discussion).

We start by defining a scaled potential \( \delta' \) such that, for all \( x, y \in \Omega \), it holds that \( \delta'(x, y) = \delta(x, y)/d \). Note that \( \delta' \) takes values in \( \{0\} \cup [1, D/d] \), and, for all \( t \in \mathbb{N} \), it holds that

\[
X_t = Y_t \iff \delta(X_t, Y_t) = 0 \iff \delta'(X_t, Y_t) = 0.
\]

Further, for all \( x, y \in \Omega \), by the linearity of expectation and by equation (3), it holds that

\[
E[\delta'(X_{t+1}, Y_{t+1}) \mid X_t = x, Y_t = y] = \frac{1}{d} E[\delta(X_{t+1}, Y_{t+1}) \mid X_t = x, Y_t = y] \leq \frac{1}{d} \delta(x, y) = \delta'(x, y)
\]

and, by equation (4), that

\[
\Pr[|\delta'(X_{t+1}, Y_{t+1}) - \delta'(x, y)| \geq \eta \delta'(x, y) \mid X_t = x, Y_t = y] = \Pr[|\delta(X_{t+1}, Y_{t+1}) - \delta(x, y)| \geq \eta \delta(x, y) \mid X_t = x, Y_t = y] \geq \kappa.
\]

We define the stochastic processes whose expected hitting times we bound, as follows. For all \( x, y \in \Omega \), let \( (\phi_t^{xy})_{t \in \mathbb{N}} \), where \( \phi_t^{xy} = \delta'(X_t, Y_t) \), given \( X_0 = x, Y_0 = y \). Further, for all \( x \in [0, D/d] \), let

\[
\ln(x) = \begin{cases} 2 \ln(2) x - 2 \ln(2) & \text{if } x \in [0, 1), \\ \ln(x) & \text{if } x \in [1, D/d], \end{cases}
\]

and, for all \( x, y \in \Omega \) and all \( t \in \mathbb{N} \), let \( \psi_t^{xy} = \ln(\phi_t^{xy}) \). Note that

\[
\psi_t^{xy} = -2 \ln(2) \iff \phi_t^{xy} = 0 \iff X_t = Y_t, \text{ given } X_0 = x, Y_0 = y.
\]

Thus, for all \( x, y \in \Omega \), we bound the expectation of \( T_{x,y} = \inf_{t \in \mathbb{N}} \{ \psi_t^{xy} \leq -2 \ln(2) \} \) from above.
We aim to apply Theorem 34, which requires showing, for all \( t \in \mathbb{N} \) with \( t < T_{x,y} \), and all \( s \in \text{rng}(S_t) \), that \( E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s \right] < s \) (equation (18)) and obtaining a lower bound on \( E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s \right] \) (equation (19)) (as we discuss after Theorem 34).

Let \( t \in \mathbb{N} \), and assume that \( t < T_{x,y} \). Further, let \( s \in [0, \ln(D/d)] \) such that \( \psi_t^{x,y} = s \). Note that \( \ln \) is a concave function and that \( \varphi_t^{x,y} \geq 1 \). By Jensen’s inequality, we obtain

\[
E[\psi_{t+1}^{x,y} \mid \psi_t^{x,y} = s] \leq \ln(E[\psi_{t+1}^{x,y} \mid \ln(\varphi_t^{x,y}) = s]) = \ln(E[\psi_{t+1}^{x,y} \mid \varphi_t^{x,y} = e^s]) \leq \ln(e^s) = s,
\]

which shows equation (18).

Again, let \( t \in \mathbb{N} \), and assume that \( t < T_{x,y} \). Further, let \( s \in [0, \ln(D/d)] \) such that \( \psi_t^{x,y} = s \). We proceed by bounding \( E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s \right] \) from below. Let \( A \) be the event that \( \psi_t^{x,y} \) jumps from \( \psi_t^{x,y} = s \geq 0 \) directly to \( \psi_{t+1}^{x,y} = -2\ln(2) \) (i.e., \( \varphi_t^{x,y} \geq 1 \) and \( \varphi_{t+1}^{x,y} = 0 \)). The positive self-loop probability of \( M \) implies that \( \Pr[A] < 1 \) and \( \Pr[\overline{A}] > 0 \). By the law of total expectation, we obtain

\[
E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s \right] = E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s, A \right] \Pr[A] + E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s, \overline{A} \right] (1 - \Pr[A]).
\]

We lower-bound each term in the sum separately. Because of \( \psi_t^{x,y} \geq 0 \), we have

\[
E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s, A \right] \Pr[A] = (-2\ln(2) - s)^2 \cdot \Pr[A] \geq 4\ln(2)^2 \cdot \Pr[A]. \tag{20}
\]

Furthermore, because \( \eta > 0 \), by Markov’s inequality, we get

\[
E\left[ (\psi_{t+1}^{x,y} - s)^2 \mid \psi_t^{x,y} = s, \overline{A} \right] \geq \ln(1 + \eta)^2 \Pr\left[ (\psi_{t+1}^{x,y} - s)^2 \geq \ln(1 + \eta)^2 \mid \psi_t^{x,y} = s, \overline{A} \right] = \ln(1 + \eta)^2 \Pr\left[ |\psi_{t+1}^{x,y} - s| \geq \ln(1 + \eta) \mid \psi_t^{x,y} = s, \overline{A} \right].
\]

We decomposed the probability on the right-hand side as

\[
\Pr\left[ |\psi_{t+1}^{x,y} - s| \geq \ln(1 + \eta) \mid \psi_t^{x,y} = s, \overline{A} \right] = \Pr\left[ \psi_{t+1}^{x,y} - s \geq \ln(1 + \eta) \mid \psi_t^{x,y} = s, \overline{A} \right] + \Pr\left[ \psi_{t+1}^{x,y} - s \leq -\ln(1 + \eta) \mid \psi_t^{x,y} = s, \overline{A} \right].
\]

We rewrite the first of these probabilities as

\[
\Pr\left[ \psi_{t+1}^{x,y} - s \geq \ln(1 + \eta) \mid \psi_t^{x,y} = s, \overline{A} \right] = \Pr\left[ \ln\left( \frac{\psi_{t+1}^{x,y}}{e^s} \right) \geq \ln(1 + \eta) \mid \varphi_t^{x,y} = e^s, \overline{A} \right]
\]

\[
= \Pr\left[ \frac{\psi_{t+1}^{x,y}}{e^s} \geq 1 + \eta \mid \varphi_t^{x,y} = e^s, \overline{A} \right] = \Pr\left[ \psi_{t+1}^{x,y} - e^s \geq \eta e^s \mid \varphi_t^{x,y} = e^s, \overline{A} \right]. \tag{21}
\]
Since, for all $x \in (0, 1)$, it holds that $-\ln(1 + x) \geq \ln(1 - x)$, we bound the second probability by

\[
\Pr \left[ \psi_t^{xy} - s' \geq -\ln(1 + \eta) \left| \psi_t^{xy} = s, \overline{A} \right. \right] \geq \Pr \left[ \psi_t^{xy} - s' \geq -\ln(1 - \eta) \left| \psi_t^{xy} = s, \overline{A} \right. \right] \\
= \Pr \left[ \ln \left( \frac{\phi_t^{xy}}{\varepsilon^s} \right) \leq -\ln(1 - \eta) \left| \phi_t^{xy} = e^s, \overline{A} \right. \right] \\
= \Pr \left[ \frac{\phi_t^{xy}}{e^s} \leq 1 - \eta \left| \phi_t^{xy} = e^s, \overline{A} \right. \right] \\
= \Pr \left[ \phi_{t+1}^{xy} - e^s \leq -\eta e^s \left| \phi_t^{xy} = e^s, \overline{A} \right. \right].
\]

(22)

Combining equations (21) and (22), we obtain

\[
\Pr \left[ \left| \psi_{t+1}^{xy} - s' \right| \geq \ln(1 + \eta) \left| \psi_t^{xy} = s, \overline{A} \right. \right] \geq \Pr \left[ \left| \phi_{t+1}^{xy} - e^s \right| \geq \eta e^s \left| \phi_t^{xy} = e^s, \overline{A} \right. \right].
\]

(23)

For bounding the right-hand side of equation (23), assume that $\phi_t^{xy} = s' \geq 1$. Consider the probability that $\phi^{xy}$ takes steps of at least size $\eta s'$. By the law of total probability,

\[
\Pr \left[ \phi_{t+1}^{xy} - s' \geq \eta s' \{ \phi_t^{xy} = s' \} \right] = \Pr \left[ \phi_{t+1}^{xy} - s' \geq \eta s' \{ \phi_t^{xy} = s', A \} \Pr[A] \right. \\
+ \Pr \left[ \phi_{t+1}^{xy} - s' \geq \eta s' \{ \phi_t^{xy} = s', \overline{A} \} \right](1 - \Pr[A]).
\]

Since $A$ is the event to go from $\phi_t^{xy} \geq 1$ to $\phi_{t+1}^{xy} = 0$, for all $\eta \in (0, 1)$, it holds that

\[
\Pr \left[ \left| \phi_{t+1}^{xy} - s' \right| \geq \eta s' \left| \phi_t^{xy} = s', A \right. \right] = 1.
\]

Thus and by equation (4), we obtain

\[
\Pr \left[ \left| \phi_{t+1}^{xy} - s' \right| \geq \eta s' \left| \phi_t^{xy} = s', \overline{A} \right. \right] = \frac{\Pr \left[ \left| \phi_{t+1}^{xy} - s' \right| \geq \eta s' \left| \phi_t^{xy} = s' \right. \right] - \Pr[A]}{1 - \Pr[A]} \\
\geq \frac{\kappa - \Pr[A]}{1 - \Pr[A]}.
\]

(24)

By combining equations (23) and (24) with $s' = e^s$, we get

\[
\mathbb{E} \left[ (\psi_{t+1}^{xy} - s)^2 \left| \psi_t^{xy} = s, \overline{A} \right. \right] \geq \ln(1 + \eta)^2 \Pr \left[ \left| \psi_{t+1}^{xy} - s \right| \geq \ln(1 + \eta) \left| \psi_t^{xy} = s, \overline{A} \right. \right] \\
\geq \ln(1 + \eta)^2 \frac{\kappa - \Pr[A]}{1 - \Pr[A]}.
\]

(25)

Last, we use equations (20) and (25) and that $\eta < 1$ implies $\ln(1 + \eta) \leq \ln(2)$ to obtain

\[
\mathbb{E} \left[ (\psi_{t+1}^{xy} - s)^2 \left| \psi_t^{xy} = s \right. \right] \geq 4 \ln(2)^2 \Pr[A] + (1 - \Pr[A]) \ln(1 + \eta)^2 \frac{\kappa - \Pr[A]}{1 - \Pr[A]} \\
= 4 \ln(2)^2 \Pr[A] + \ln(1 + \eta)^2 \kappa - \ln(1 + \eta)^2 \Pr[A]
\]

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\[ \geq 3 \ln(2)^2 \Pr[A] + \ln(1 + \eta)^2 \kappa \geq \ln(1 + \eta)^2 \kappa, \]

which shows equation (19).

By Theorem 34, for all \( x, y \in \Omega \), we get

\[
E[T_{x,y}] \leq \frac{\left( \ln(D/d) + 2 \ln(2) \right)^2 - E\left[ \left( \ln(D/d) - \psi_0 \right)^2 \right]}{\ln(1 + \eta)^2 \kappa}
\leq \frac{\left( \ln(D/d) + 2 \ln(2) \right)^2}{\ln(1 + \eta)^2 \kappa}.
\]

This results in the desired mixing time bound of

\[
\tau_M(\epsilon) \leq \frac{\left( \ln(D/d) + 2 \ln(2) \right)^2}{\ln(1 + \eta)^2 \kappa} \ln\left( \frac{1}{\epsilon} \right).
\]

\[ \square \]