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A spectral independence view on hard spheres via block dynamics

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Abstract

The hard-sphere model is one of the most extensively studied models in statistical physics. It describes the continuous distribution of spherical particles, governed by hard-core interactions. An important quantity of this model is the normalizing factor of this distribution, called the *partition function*. We propose a Markov chain Monte Carlo algorithm for approximating the grand-canonical partition function of the hard-sphere model in d dimensions. Up to a fugacity of $\lambda < e/2^d$, the runtime of our algorithm is polynomial in the volume of the system. This covers the entire known real-valued regime for the uniqueness of the Gibbs measure.

Key to our approach is to define a discretization that closely approximates the partition function of the continuous model. This results in a discrete hard-core instance that is exponential in the size of the initial hard-sphere model. Our approximation bound follows directly from the correlation decay threshold of an infinite regular tree with degree equal to the maximum degree of our discretization. To cope with the exponential blow-up of the discrete instance we use clique dynamics, a Markov chain that was recently introduced in the setting of abstract polymer models. We prove rapid mixing of clique dynamics up to the tree threshold of the univariate hard-core model. This is achieved by relating clique dynamics to block dynamics and adapting the spectral expansion method, which was recently used to bound the mixing time of Glauber dynamics within the same parameter regime.

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1 Introduction

Statistical physics models particle systems as probability distributions. One of the most fundamental and mathematically challenging models in this area is the hard-sphere model, which plays a central role in understanding the thermodynamic properties of monoatomic gases and liquids [7, 29]. It is a continuous model that studies the distribution and macroscopic behavior of indistinguishable spherical particles, assuming only hard-core interactions, i.e., no two particles can occupy the same space.

We focus on computational properties of the *grand-canonical ensemble* of the hard-sphere model in a finite d -dimensional cubic region $V = [0, \ell]^d$ in the Euclidean space. In the



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44 grand-canonical ensemble, the system can exchange particles with its surrounding based on
 45 a fugacity parameter λ , which is inverse to the temperature of the system. For the rest of
 46 the paper, we make the common assumption that the system is normalized such that the
 47 particles have unit volume. That means we fix their radii to $r = (1/v_d)^{1/d}$, where v_d is the
 48 volume of a unit sphere in d dimensions.

49 A simple probabilistic interpretation of the distribution of particles in the grand-canonical
 50 ensemble is that centers of points that are drawn from a Poisson point process on \mathbb{V} with
 51 intensity λ , conditioned on the event that no two particles overlap (i.e., every pair of centers
 52 has distance at least $2r$). The resulting distribution over particle configurations in \mathbb{V} is
 53 called the *Gibbs distribution* of the model. An important quantity in such models is the
 54 so called partition function $Z(\mathbb{V}, \lambda)$, which can be seen as the normalizing constant of the
 55 Gibbs distribution. Formally, it is defined as

$$56 \quad Z(\mathbb{V}, \lambda) = 1 + \sum_{k \in \mathbb{N}_{>0}} \frac{\lambda^k}{k!} \int_{\mathbb{V}^k} D(x^{(1)}, \dots, x^{(k)}) \, d\nu^{d \times k},$$

57 where

$$58 \quad D(x^{(1)}, \dots, x^{(k)}) = \begin{cases} 1 & \text{if } d(x^{(i)}, x^{(j)}) \geq 2r \text{ for all } i, j \in [k] \text{ with } i \neq j \\ 0 & \text{otherwise} \end{cases}$$

59 and $\nu^{d \times k}$ is the Lebesgue measure on $\mathbb{R}^{d \times k}$. Commonly, two computational task are
 60 associated with the grand-canonical hard-sphere model: (1) approximating its partition
 61 function $Z(\mathbb{V}, \lambda)$, and (2) approximately sampling from the Gibbs distribution.

62 Studying computational aspects of the hard-sphere model carries a historical weight, as in
 63 the seminal work of Metropolis [41], the Monte Carlo method was introduced to investigate
 64 a two-dimensional hard-sphere model. Approximate-sampling Markov chain approaches have
 65 been mainly focused on the canonical ensemble of the model, that is, the system does not
 66 exchange particles with its surrounding and thus, the distribution is defined over a fixed
 67 number of spheres [31, 36, 34]. Considering the grand canonical ensemble, exact sampling
 68 algorithms have appeared in the literature for the two-dimensional model without asymptotic
 69 runtime guarantees [37, 38, 43]. A result that is more aligned with theoretical computer
 70 science was given in [28], where the authors introduced an exact sampling algorithm for the
 71 grand-canonical hard-sphere model in d -dimensions. Their algorithm is based on partial
 72 rejection sampling with a runtime linear in the volume of the system $|\mathbb{V}|$ when assuming a
 73 continuous computational model and access to a sampler from a continuous Poisson point
 74 process. Their approach is guaranteed to apply for $\lambda < 2^{-(d+1/2)}$.

75 Besides such sampling results, there is an ongoing effort to improve the known fugacity
 76 regime where the Gibbs measure is unique and correlations decay exponentially fast [22, 14,
 77 32, 42]. Note that for many discrete spin systems, such as the hard-core model, correlation
 78 decay is closely related to the applicability of different methods for efficient approximation of
 79 the partition function [50, 24, 54]. Recently, the correlation decay bounds for the hard-sphere
 80 model were improved in [32] to $\lambda < 2/2^d$, using probabilistic arguments, and in [42] to
 81 $\lambda < e/2^d$, based on an analytic approach. A common feature of [32] and [42] is that they
 82 translated tools originally developed in theoretical computer science for investigating the
 83 discrete hard-core model to the continuous domain.

84 Our work is in line with the computational view on the hard-sphere model but more
 85 algorithmic in nature. We investigate the range of the fugacity λ for which an approximation
 86 of $Z(\mathbb{V}, \lambda)$ can be obtained efficiently in terms of the volume of the system $|\mathbb{V}|$, assuming a

87 discrete computational model. Our main result is that for all $\lambda < e/2^d$ there is a randomized
 88 algorithm for ε -approximating the partition function in time polynomial in $|\mathbb{V}|$ and $1/\varepsilon$.

89 ► **Theorem 1.** *Let (\mathbb{V}, λ) be an instance of the continuous hard-sphere model with $\mathbb{V} = [0, \ell]^d$.
 90 If there is a $\delta \in (0, 1]$ such that*

$$91 \quad \lambda \leq (1 - \delta) \frac{e}{2^d},$$

92 *then for each $\varepsilon \in (0, 1]$ there is a randomized ε -approximation of $Z(\mathbb{V}, \lambda)$ computable in time
 93 polynomial in $|\mathbb{V}|^{1/\delta^2}$ and $\frac{1}{\varepsilon}$.*

94 Note that this bound on λ precisely coincides with the best known bound for the uniqueness
 95 of the Gibbs measure in the thermodynamic limit, recently established in [42]. For many
 96 discrete spin systems, such as the hard-core model or general anti-ferromagnetic 2-state spin
 97 systems, the region of efficient approximation of the partition function is closely related to
 98 uniqueness of the Gibbs measure. More precisely, it can be shown that the partition function
 99 of every graph of maximum degree Δ can be approximated efficiently if the corresponding
 100 Gibbs distribution on an infinite Δ regular tree is unique [39, 53]. A detailed discussion for
 101 the discrete hard-core model can be found in the next subsection. In a sense, Theorem 1
 102 can be seen as the algorithmic counterpart of the recent uniqueness result for the continuous
 103 hard-sphere model. This answers an open question, asked in [42].

104 The way we prove our result is quite contrary to [32] and [42]. Instead of translating
 105 discrete tools from computer science into the continuous domain, we rather discretize the
 106 hard-sphere model. By this, existing algorithmic and probabilistic techniques for discrete
 107 models become available, and we avoid continuous analysis.

108 Our applied discretization scheme is fairly intuitive and results in an instance of the
 109 discrete hard-core model. This model has been extensively studied in the computer science
 110 community. However, as this hard-core instance is exponential in the size of the continuous
 111 system $|\mathbb{V}|$, existing approaches for approximating its partition function, such a Markov
 112 chain Monte Carlo methods based on Glauber dynamics, are not feasible. We overcome
 113 this problem by applying a Markov chain Monte Carlo approach based on clique dynamics,
 114 which were introduced in [23] in the setting of abstract polymer models. Previously known
 115 conditions for the rapid mixing of clique dynamics were developed for the multivariate version
 116 of the hard-core model. Due to this generality, those conditions do not result in the desired
 117 bound in our univariate setting. Instead we relate those clique dynamics to another Markov
 118 chain, called *block dynamics*. We then prove the desired mixing time for the block dynamics
 119 by adapting a recently introduced technique for bounding the mixing time of Markov chains,
 120 based on local spectral expansion [2]. Together with a known self-reducibility scheme for
 121 clique dynamics, this results in the desired approximation algorithm.

122 Note that we aim for a rigorous algorithmic result for approximating the partition
 123 function of the continuous hard-sphere model. To be in line with commonly used discrete
 124 computational models, our Markov chain Monte Carlo algorithm does not assume access to
 125 a continuous sampler but instead samples approximately from a discretized version of the
 126 Gibbs distribution. Note that sampling from the continuous hard-sphere partition function
 127 cannot be done using a discrete computation model as this would involve infinite float pointer
 128 precision. For practical matters, our discretization of the Gibbs distribution can be seen as
 129 an approximation of the original continuous Gibbs measure. However, a rigorous comparison
 130 between both distributions based on total variation distance is not applicable, due to the
 131 fact that one is discrete whereas the other is continuous in nature.

132 Assuming access to a continuous sampler, we believe that our approach can be used to
 133 obtain an approximation of the Gibbs distribution of the continuous model within the same
 134 fugacity regime, by adding small perturbations to the drawn sphere centers. This would be
 135 in line with the relation between the mixing time of continuous heat-bath dynamics and
 136 strong spatial mixing, pointed out in [32], combined with the uniqueness bound from [42].

137 In Sections 1.1–1.3 we discuss our contributions in more detail and explain how they
 138 relate to the existing literature. Finally in Section 1.4 we discuss possible extensions and
 139 future work. All technical details, statements and proofs are presented the full version of the
 140 paper.

141 1.1 Discretization and hard-core model

142 Our discretization scheme expresses the hard-sphere partition function as the partition
 143 function of an instance of the (univariate) hard-core model. An instance of the hard-core
 144 model is a tuple (G, λ) where $G = (V, E)$ is an undirected graph and $\lambda \in \mathbb{R}_{>0}$. Its partition
 145 function is defined as

$$146 \quad Z(G, \lambda) := \sum_{I \in \mathcal{I}(G)} \lambda^{|I|},$$

147 where $\mathcal{I}(G)$ denotes the independent sets of G . A common way to obtain an approximation
 148 for the partition function is by applying a Markov chain Monte Carlo algorithm. This involves
 149 sampling from the Gibbs distribution $\mu^{(G, \lambda)}$ of (G, λ) , which is a probability distribution on
 150 $\mathcal{I}(G)$ that assigns each independent set $I \in \mathcal{I}(G)$ the probability

$$151 \quad \mu^{(G, \lambda)}(I) = \frac{\lambda^{|I|}}{Z(G, \lambda)}.$$

152 Conditions for efficient approximation of the hard-core partition function have been
 153 studied extensively in the theoretical computer science community. Due to hardness results
 154 in [50] and [24], it is known that for general graphs of maximum degree $\Delta \in \{3\} \cup \mathbb{N}_{>5}$
 155 there is a critical parameter value $\lambda_c(\Delta) = (\Delta - 1)^{\Delta-1} / (\Delta - 2)^\Delta$, such that there is no
 156 FPRAS for the partition function of (G, λ) for $\lambda > \lambda_c(\Delta)$, unless $\text{RP} = \text{NP}$. On the other
 157 hand, in [54] it was proven that there is a deterministic algorithm for approximating the
 158 partition function of (G, λ) for $\lambda < \lambda_c(\Delta)$ that runs in time $|V|^{O(\Delta)}$. The critical value
 159 $\lambda_c(\Delta)$ is especially interesting, as it precisely coincides with the upper bound on λ for
 160 which the hard-core model on an infinite Δ -regular tree exhibits strong spatial mixing and a
 161 unique Gibbs distribution [54]. For this reason, it is also referred to as the *tree threshold*.
 162 This relation between computational hardness and phase transition in statistical physics is
 163 one of the most celebrated results in the area. Both, the hardness results [25, 3] and the
 164 approximation algorithms [46, 30] were later generalized for complex λ .

165 Note that the computational hardness above the tree threshold $\lambda_c(\Delta)$ for general graphs
 166 of maximum degree Δ applies to both, randomized and deterministic algorithms. However,
 167 in the randomized setting, Markov chain Monte Carlo methods are known to improve
 168 the runtime of the algorithm introduced in [54]. Those approaches use the vertex-wise
 169 self-reducibility of the hard-core model to construct a randomized approximation of the
 170 partition function based on an approximate sampler for the Gibbs distribution. Commonly,
 171 a Markov chain on the state space $\mathcal{I}(G)$, called *Glauber dynamics*, is used to construct
 172 the sampling scheme. At each step, a vertex $v \in V$ is chosen uniformly at random. With
 173 probability $\lambda / (1 + \lambda)$ the chain tries to add v to the current independent set and otherwise
 174 it tries to remove it. The resulting Markov chain is ergodic and reversible with respect

175 to the Gibbs distribution, meaning that it eventually converges to $\mu^{(G,\lambda)}$. A sequence of
 176 results has shown that for all $\Delta \geq 3$ there is a family of graphs with maximum degree Δ ,
 177 such that the Glauber dynamics are torpidly mixing for $\lambda > \lambda_c(\Delta)$, even without additional
 178 complexity-theoretical assumptions [17, 27, 45]. Whether the Glauber dynamics are rapidly
 179 mixing for the entire regime $\lambda < \lambda_c(\Delta)$ remained a long-standing open problem, until recently
 180 the picture was completed [2]. By relating spectral expansion properties of certain random
 181 walks on simplicial complexes to the Glauber dynamics, it was shown that the mixing time is
 182 polynomial in $|V|$ below the tree threshold. The mixing time was recently further improved
 183 in [12] for a broader class of spin systems by combining simplicial complexes with entropy
 184 factorization and using the modified log-Sobolev inequality.

185 By mapping the hard-sphere model to an instance of the hard-core model we can make use
 186 of the existing results about approximation and sampling below the tree threshold. Roughly,
 187 our discretization scheme restricts the positions of sphere centers to an integer grid, while
 188 scaling the radii of spheres and the fugacity appropriately. For a hard-sphere instance (\mathbb{V}, λ)
 189 with $\mathbb{V} = [0, \ell)^d$ the hard-core representation for resolution $\rho \in \mathbb{R}_{\geq 1}$ is a hard-core instance
 190 (G_ρ, λ_ρ) with $G_\rho = (V_\rho, E_\rho)$. Each vertex $v \in V_\rho$ represents a grid point in the finite integer
 191 lattice of side length $\rho\ell$. Two distinct vertices in V_ρ are connected by an edge in E_ρ if the
 192 Euclidean distance of the corresponding grid points is less than $2\rho r$. Furthermore, we set
 193 $\lambda_\rho = \lambda/\rho^d$. We provide the following result on the rate of convergence of $Z(G_\rho, \lambda_\rho)$ to the
 194 hard-sphere partition function $Z(\mathbb{V}, \lambda)$ in terms of ρ .

195 **► Lemma 2.** *Let (\mathbb{V}, λ) be an instance of the continuous hard-sphere model in d dimensions.*
 196 *For each resolution $\rho \geq 2\sqrt{d}$ it holds that*

$$197 \quad 1 - \rho^{-1}e^{\Theta(|V|\ln|V|)} \leq \frac{Z(\mathbb{V}, \lambda)}{Z(G_\rho, \lambda_\rho)} \leq 1 + \rho^{-1}e^{\Theta(|V|\ln|V|)}.$$

198 Although proving this rate of convergence involves some detailed geometric arguments,
 199 there is an intuitive reason why the partition functions converge eventually as $\rho \rightarrow \infty$.
 200 Increasing the resolution ρ also linearly increases the side length of the grid and the minimum
 201 distance that sphere centers can have. This is equivalent to putting a grid into \mathbb{V} with
 202 increasing granularity but fixing the radii of spheres instead. However, only scaling the
 203 granularity of this grid increases the number of possible configurations by roughly ρ^d , which
 204 would cause the partition function of the hard-core model to diverge as $\rho \rightarrow \infty$. To
 205 compensate for this, we scale the weight of each vertex in the hard-core model by the inverse
 206 of this factor.

207 Using this discretization approach, the fugacity bound from Theorem 1 results from
 208 simply considering Δ_ρ , the maximum degree of G_ρ and comparing λ_ρ with the corresponding
 209 tree threshold $\lambda_c(\Delta_\rho)$. Recall that we assume $r = (1/v_d)^{1/d}$. A simple geometric argument
 210 shows that Δ_ρ is roughly upper bounded by $2^d \rho^d$ for sufficiently large ρ . Now, observe that

$$211 \quad \lambda_\rho = \frac{\lambda}{\rho^d} < \lambda_c(2^d \rho^d),$$

212 for $\lambda < \rho^d \lambda_c(2^d \rho^d)$. This follows from the fact that $\rho^d \lambda_c(2^d \rho^d)$ converges to $e/2^d$ from above
 213 for $\rho \rightarrow \infty$. Thus, the approximation bound from Theorem 1 and the uniqueness bound in
 214 [42] coincide with the regime of λ , for which λ_ρ is below the tree threshold $\lambda_c(\Delta_\rho)$ in the
 215 limit $\rho \rightarrow \infty$.

216 The arguments above show that for a sufficiently high resolution ρ the partition function
 217 of the hard-sphere model $Z(\mathbb{V}, \lambda)$ is well approximated by the partition function of our
 218 discretization (G_ρ, λ_ρ) and that (G_ρ, λ_ρ) is below the tree threshold for $\lambda < e/2^d$. However,

219 this does not immediately imply an approximation algorithm within the desired runtime
 220 bounds. Based on Lemma 2, we still need to choose ρ exponentially large in the volume $|\mathbb{V}|$.
 221 Note that the number of vertices in G_ρ is roughly $|V_\rho| \in \Theta(\rho^d |\mathbb{V}|)$. Even without explicitly
 222 constructing the graph, this causes problems, as the best bound for the mixing time of the
 223 Glauber dynamics is polynomial in $|V_\rho|$ and thus exponential in $|\mathbb{V}|$. Intuitively, the reason
 224 for this mixing time is that the Glauber dynamics only change one vertex at each step.
 225 Assuming that each vertex should be updated at least once to remove correlations with the
 226 initial state, any mixing time that is sublinear in the number of vertices is unlikely. We
 227 circumvent this problem by applying dynamics that update multiple vertices at each step
 228 but still allow each step to be computed efficiently without constructing the graph explicitly.

229 1.2 Block and clique dynamics

230 Most of the results that we discuss from now on apply to the multivariate version of the
 231 hard-core model, that is, each vertex $v \in V$ has its own weight λ_v . For a given graph
 232 $G = (V, E)$ we denote the set of such vertex weights by $\boldsymbol{\lambda} = \{\lambda_v\}_{v \in V}$ and write $(G, \boldsymbol{\lambda})$ for
 233 the resulting multivariate hard-core instance. In the multivariate setting, the contribution of
 234 an independent set $I \in \mathcal{I}(G)$ to the partition function is defined as the product of its vertex
 235 weights (i.e., $\prod_{v \in I} \lambda_v$), where the contribution of the empty set is fixed to 1. Similar to the
 236 univariate hard-core model, the Gibbs distribution assigns a probability to each independent
 237 set proportionally to its contribution to the partition function.

238 As we discussed before, the main problem with approximating the partition function of
 239 our discretization (G_ρ, λ_ρ) is that the required graph G_ρ is exponential in the volume of
 240 the original continuous system $|\mathbb{V}|$. As the Glauber dynamics Markov chain only updates
 241 a single vertex at each step, the resulting mixing time is usually polynomial in the size of
 242 the graph, which is not feasible in our case. Various extensions to Glauber dynamics for
 243 updating multiple vertices in each step have been proposed in the literature, two of which
 244 we discuss in the following.

245 Clique dynamics

246 Recently, in [23] a Markov chain, called *clique dynamics*, was introduced in order to efficiently
 247 sample from the Gibbs distribution of abstract polymer models. Note that this is similar
 248 to our algorithmic problem, as abstract polymer models resemble multivariate hard-core
 249 instances. For a given graph $G = (V, E)$, we call a set $\Lambda = \{\Lambda_i\}_{i \in [m]} \subseteq 2^V$ a clique cover
 250 of size m if and only if its union covers all vertices V and each $\Lambda_i \in \Lambda$ induces a clique in
 251 G . For an instance of the multivariate hard-core model $(G, \boldsymbol{\lambda})$ and a given clique cover Λ of
 252 G with size m the clique dynamics Markov chain $\mathcal{C}(G, \boldsymbol{\lambda}, \Lambda)$ is defined as follows. First, a
 253 clique $\Lambda_i \in \Lambda$ for $i \in [m]$ is chosen uniformly at random. Let us write $G[\Lambda_i]$ for the subgraph,
 254 induced by Λ_i , and $\boldsymbol{\lambda}[\Lambda_i] = \{\lambda_v\}_{v \in \Lambda_i}$ for the corresponding set of vertex weights. Next, an
 255 independent set from $\mathcal{I}(G[\Lambda_i])$ is chosen according to the Gibbs distribution $\mu^{(G[\Lambda_i], \boldsymbol{\lambda}[\Lambda_i])}$.
 256 Note that, as the vertices Λ_i form a clique, such an independent set is either the empty set
 257 or contains a single vertex from $v \in \Lambda_i$. If the empty set is drawn, all vertices from Λ_i are
 258 removed from the current independent set. Otherwise, if a single vertex $v \in \Lambda_i$ is drawn, the
 259 chain tries to add v to the current independent set.

260 Using a coupling argument, it was proven in [23] that the so-called *clique dynamics*
 261 *condition* implies that for any clique cover of size m the clique dynamics are mixing in time
 262 polynomial in m and Z_{\max} , where $Z_{\max} = \max_{i \in [m]} \{Z(G[\Lambda_i], \boldsymbol{\lambda}[\Lambda_i])\}$ denotes the maximum
 263 partition function of a clique in Λ . This is important for the application to polymer models, as

264 they are usually used to model partition functions of other spin systems, which often results
 265 in a multivariate hard-core model of exponential size [33, 9, 35, 10, 6, 8, 26]. As discussed in
 266 [23], those instances tend to have polynomial size clique covers that arise naturally from the
 267 original spin system. In such cases, the mixing time of clique dynamics is still polynomial in
 268 the size of original spin system, as long as the clique dynamics condition is satisfied.

269 This is very similar to our discretization (G_ρ, λ_ρ) . To see this, set $a = \frac{2\rho}{\sqrt{d}}r$ and divide the
 270 d -dimensional integer lattice of side length $\rho\ell$ into cubic regions of side length a . Every pair of
 271 integer points within such a cubic region has Euclidean distance less than $2\rho r$, meaning that
 272 the corresponding vertices in G_ρ are adjacent. Thus, each such cubic region forms a clique,
 273 resulting in a clique cover of size $(\rho\ell/a)^d \in O(|V|)$. This means, there is always a clique
 274 cover with size linear in $|V|$ and independent of the resolution ρ . By showing that, for the
 275 univariate hard-core model, the mixing time of clique dynamics is polynomial in the size of
 276 the clique cover for all $\lambda_\rho < \lambda_c(\Delta_\rho)$, we obtain a Markov chain with mixing time polynomial
 277 in $|V|$ independent of the resolution ρ . Unfortunately, the clique dynamics condition does
 278 not hold for the entire regime up to the tree threshold in the univariate hard-core model.
 279 We overcome this problem by proving a new condition for rapid mixing of clique dynamics
 280 based on a comparison with block dynamics.

281 Block dynamics

282 Block dynamics are a very natural generalization of Glauber dynamics to arbitrary sets of
 283 vertices. For a given graph $G = (V, E)$, we call a set $\Lambda = \{\Lambda_i\}_{i \in [m]} \subseteq 2^V$ a block cover of size
 284 m if and only if its union covers all vertices V . We refer to the elements of Λ as blocks. Note
 285 that the clique cover discussed before is a special case of a block cover, where all blocks are
 286 restricted to be cliques. At each step, the block dynamics Markov chain $\mathcal{B}(G, \lambda, \Lambda)$ chooses
 287 a block $\Lambda_i \in \Lambda$ uniformly at random. Then, the current independent set is updated on Λ_i
 288 based on the projection of the Gibbs distribution onto Λ_i and conditioned on the current
 289 independent set outside Λ_i .

290 In fact, block dynamics are defined for a much more general class of spin systems than
 291 the hard-core model. However, due to the fact that each step of the Markov chain involves
 292 sampling from a conditional Gibbs distribution, block dynamics are rarely used as an
 293 algorithmic tool on its own. Instead, they are usually used to deduce rapid mixing of other
 294 dynamics.

295 For spin systems on lattice graphs, close connections between the mixing time of block
 296 dynamics and Glauber dynamics are known [40]. Such connections were for example applied
 297 to improve the mixing time of Glauber dynamics of the Monomer Dimer model on torus
 298 graphs [51]. Moreover, block dynamics were used to improve conditions for rapid mixing
 299 of Glauber dynamics on specific graph classes, such as proper colorings [16, 18, 19, 44] or
 300 the hard-core model [18, 44] in sparse random graphs. A very general result for the mixing
 301 time of block dynamics was achieved in [4], who proved that for all spin systems on a finite
 302 subgraph of the d -dimensional integer lattice the mixing time of block dynamics is polynomial
 303 in the number of blocks if the spin system exhibits strong spatial mixing. This result was
 304 later generalized in [5] for the Ising model on arbitrary graphs. Very recently, block dynamics
 305 based random equally-sized blocks were used in [12] to prove entropy factorization and
 306 improve the mixing time of Glauber dynamics for a variety of discrete spin systems up to
 307 the tree threshold.

308 Although our discretization works by restricting sphere positions to the integer lattice,
 309 the resulting graph is rather different from the lattice. Thus, results like those in [4] do not
 310 apply to our setting. However, on the other hand, we do not need to prove rapid mixing for

311 arbitrary block covers. Instead, in order to obtain rapid mixing for clique dynamics, it is
 312 sufficient to establish this result for cases where all blocks are cliques.

313 Applying block dynamics directly would involve sampling from a conditional Gibbs
 314 distribution within each clique. Due to the exponential size of the cliques in our discretization,
 315 this would impose additional algorithmic challenges. Instead, similar to the previous literature,
 316 we rather use block dynamics as a tool for proving rapid mixing of another Markov chain,
 317 namely clique dynamics.

318 Improved mixing condition for clique dynamics via block dynamics

319 We analyze the mixing time of clique dynamics for a given clique cover by relating it to the
 320 mixing time of block dynamics, using the cliques as blocks. This is done by investigating
 321 a notion of pairwise influence between vertices that has also been used to establish rapid
 322 mixing of Glauber dynamics up to the tree threshold [2]. Let $\mathbb{P}_G[w]$ denote the probability
 323 of the event that a vertex $w \in V$ is in an independent set drawn from $\mu^{(G, \lambda)}$. Further, let
 324 $\mathbb{P}_G[\bar{w}]$ denote the probability that w is not in an independent set. We extend this abuse
 325 of notation to conditional probabilities, so $\mathbb{P}_G[\cdot | \bar{w}]$ for example denotes the probability of
 326 some event conditioned on w not being in an independent set. For a pair of vertices $v, w \in V$
 327 the influence $\Psi_G(v, w)$ of v on w is defined as

$$328 \quad \Psi_G(v, w) = \begin{cases} 0 & \text{if } v = w, \\ \mathbb{P}_G[w | v] - \mathbb{P}_G[w | \bar{v}] & \text{otherwise.} \end{cases}$$

329 The following condition in terms of pairwise influence is central to our analysis.

330 ► **Condition 3.** *Let (G, λ) be an instance of the multivariate hard-core model. There is a*
 331 *constant $C \in \mathbb{R}_{>0}$ and a function $q: V \rightarrow \mathbb{R}_{>0}$ such that for all $S \subseteq V$ and $r \in S$ it holds*
 332 *that*

$$333 \quad \sum_{v \in S} |\Psi_G(r, v)| q(v) \leq Cq(r).$$

334 Note that this condition appeared before in [13], where it was used for bounding the mixing
 335 time of Glauber dynamics for anti-ferromagnetic spin systems. Given Condition 3, we obtain
 336 the following result for the mixing time of block dynamics based on a clique cover.

337 ► **Theorem 4.** *Let (G, λ) be an instance of the multivariate hard-core model that satisfies Con-*
 338 *dition 3. Let Λ be a clique cover for G of size m , and let $Z_{\max} = \max_{i \in [m]} \{Z(G[\Lambda_i], \lambda[\Lambda_i])\}$.*
 339 *The mixing time of the block dynamics $\mathcal{B}(G, \lambda, \Lambda)$, starting from $\emptyset \in \mathcal{I}(G)$, is bounded by*

$$340 \quad \tau_{\mathcal{B}}^{(\emptyset)}(\varepsilon) \leq m^{\mathcal{O}((2+C)C)} Z_{\max}^{\mathcal{O}((2+C)C)} \ln\left(\frac{1}{\varepsilon}\right).$$

341 Using a bound for the sum of absolute pairwise influences that was recently established
 342 in [13], it follows that the univariate hard-core model satisfies Condition 3 up to the tree
 343 threshold. As a result, we know that the mixing time of block dynamics is polynomial in m
 344 and Z_{\max} for any clique cover of size m . To the best of our knowledge, this is the first result
 345 for the mixing time of block dynamics for the univariate hard-core model on general graphs
 346 that holds in this parameter range.

347 As we aim to apply clique dynamics to avoid sampling from the conditional Gibbs
 348 distribution in each step, we still need to prove that Theorem 4 also holds in terms of clique
 349 dynamics. To this end, we apply a Markov chain comparison argument from [15] to prove

350 that using clique dynamics instead of block dynamics for the same clique cover Λ increases
 351 the mixing time by at most a factor $2Z_{\max}$. The following corollary, which is central for
 352 proving Theorem 1, follows immediately.

353 ► **Corollary 5.** *Let (G, λ) be an instance of the univariate hard-core model such that
 354 the degree of G is bounded by Δ . Let Λ be a given clique cover of size m with $Z_{\max} =$
 355 $\max_{i \in [m]} \{Z(G[\Lambda_i], \lambda)\}$. Denote by $\mathcal{C} = \mathcal{C}(G, \lambda, \Lambda)$ the corresponding clique dynamics. If
 356 there is some $\delta \in \mathbb{R}_{>0}$ such that $\lambda \leq (1 - \delta)\lambda_c(\Delta)$ then the mixing time of the clique dynamics
 357 \mathcal{C} , starting from $\emptyset \in \mathcal{I}(G)$, is bounded by*

$$358 \quad \tau_{\mathcal{C}}^{(\emptyset)}(\varepsilon) \leq m^{O(1/\delta^2)} Z_{\max}^{O(1/\delta^2)} \ln\left(\frac{1}{\varepsilon}\right).$$

359 A side journey: comparison to multivariate conditions

360 In fact, Corollary 5 is sufficient for our application to the hard-sphere model. However, we
 361 also aim to set Condition 3 in the context of other conditions for rapid mixing of clique
 362 dynamics for the multivariate hard-core model. Note that such a rapid mixing result for
 363 clique dynamics carries over to Glauber dynamics by taking each vertex as a separate clique
 364 of size 1.

365 To this end, we compare Condition 3 to a strict version of the clique dynamics condition,
 366 originally introduced in [23] in the setting of clique dynamics for abstract polymer models. It
 367 turns out that this strict version of the clique dynamics condition directly implies Condition 3.
 368 This is especially interesting, as the clique dynamics condition was initially introduced as a
 369 local condition (only considering the neighborhood of each vertex) and is based on a coupling
 370 argument. However, we show that it can as well be understood as a sufficient condition for
 371 the global decay of pairwise influence with increasing distance between vertices.

372 Formally, we say that the strict clique dynamics condition is satisfied for an instance of
 373 the multivariate hard-core model (G, λ) if there is a function $f: V \rightarrow \mathbb{R}_{>0}$ and a constant
 374 $\alpha \in (0, 1)$ such that for all $v \in V$ it holds that

$$375 \quad \sum_{w \in N(v)} \frac{\lambda_w}{1 + \lambda_w} f(w) \leq (1 - \alpha)f(v),$$

376 where $N(v)$ is the neighborhood of v in G . This is a strict version of the clique dynamics
 377 condition in that the original clique dynamics condition would correspond to the case $\alpha = 0$
 378 (i.e., the strict clique dynamics condition requires some strictly positive slack α).

379 The result of our comparison is summarized in the following statement.

380 ► **Lemma 6.** *Let (G, λ) be an instance of the multivariate hard-core model. If (G, λ) satisfies
 381 the strict clique dynamics condition for a function f and a constant α , then it also satisfies
 382 Condition 3 for $q = f$ and $C = \frac{1}{\alpha}$.*

383 Lemma 6 is proven by translating the calculation of pairwise influences to the self-avoiding
 384 walk tree of the graph, based on a result in [13], and applying a recursive argument on this
 385 tree.

386 Despite being an interesting relationship between local coupling arguments and global
 387 pairwise influence, Lemma 6 also implies that, from an algorithmic perspective, Theorem 4
 388 can be used to produce similar results as those obtained in [23] for abstract polymer models.
 389 Further, note that for the univariate model, using pairwise influence yields strictly better
 390 results than any coupling approach in the literature. This raises the question if a refined

391 argument based on pairwise influences can be used in the multivariate setting to improve on
 392 the clique dynamics condition, leading to better approximation results on abstract polymer
 393 models.

394 1.3 Analyzing spectral expansion

395 As core technique for obtaining Theorem 4, we adapt an approach for bounding the mixing
 396 time that was recently used to prove rapid mixing of Glauber dynamics for the entire regime
 397 below the tree threshold for several applications, such as the hard-core model [2], general
 398 two-state spin systems [13], and proper colorings [11, 21]. The idea is to map the desired
 399 distribution to a weighted simplicial complex.

400 A simplicial complex X over a groundset U is a set family $X \subseteq 2^U$ such that for each
 401 $\tau \in X$ every subset of τ is also in X . We call the elements $\tau \in X$ the faces of X and refer to
 402 its cardinality $|\tau|$ as dimensionality.

403 For a univariate hard-core instance (G, λ) , the authors of [2] construct a simplicial complex
 404 over a ground set U that contains two elements $x_v, x_{\bar{v}} \in U$ for each vertex $v \in V$. For every
 405 independent set $I \in \mathcal{I}(G)$, a face $\tau_I \in X$ is introduced such that $x_v \in \tau_I$ if $v \in I$ and $x_{\bar{v}} \in \tau_I$
 406 otherwise. The simplicial complex is completed by taking the downward closure of these faces.
 407 Note that by construction all maximum faces of the resulting complex are $|V|$ -dimensional
 408 and there is a one-to-one correspondence between the maximum faces and the independent
 409 sets in $\mathcal{I}(G)$. By assigning each maximum face $\tau_I \in X$ an appropriate weight, the Glauber
 410 dynamics can be represented as a random walk on those maximum faces, which is sometimes
 411 referred to as the two-step walk or down-up walk. Using a local-to-global theorem [1], the
 412 mixing time of this two-step walk can then be bounded based on certain local expansion
 413 properties of the simplicial complex X . It is then proved that such local expansion properties
 414 are well captured by the largest eigenvalue of the pairwise influence matrix Ψ_G , which is
 415 a $|V| \times |V|$ matrix that contains the pairwise influence $\Psi_G(v, w)$ for all $v, w \in V$. Finally,
 416 by bounding those influences a bound on this largest eigenvalue of Ψ_G is obtained. This
 417 analysis was later refined and generalized in [13] to general two-state spin systems.

418 This method was independently extended in [11] and [21] to the non-Boolean domain
 419 by applying it to the Glauber dynamics for proper colorings. The main differences to the
 420 Boolean domain are that elements of the simplicial complex now represent combinations of a
 421 vertex and a color. Furthermore, the bound on the local spectral expansion was obtained by
 422 using a different influence matrix, which captures the effect of selecting a certain color for
 423 one vertex on the distribution of colors for another vertex.

424 Although we are dealing with the hard-core model, which is Boolean in nature, the way
 425 that we model block dynamics is mainly inspired by the existing work on proper colorings
 426 [11]. Assume we have an instance of the multivariate hard-core model (G, λ) and let Λ be a
 427 clique cover for G of size m such that every pair of distinct cliques is vertex-disjoint (i.e., Λ
 428 is a partition of G into cliques). We construct a simplicial complex X based on a ground
 429 set U that contains one element $x_v \in U$ for each vertex $v \in V$ and one additional element
 430 \emptyset_i for each clique $\Lambda_i \in \Lambda$. We introduce a face $\tau_I \in X$ for each independent set $I \in \mathcal{I}(G)$
 431 such that for every $\Lambda_i \in \Lambda$ we have $\emptyset_i \in \tau_I$ if $\Lambda_i \cap I = \emptyset$ and $x_v \in \tau_I$ if $\Lambda_i \cap I = \{v\}$ for
 432 some $v \in \Lambda_i$. The simplicial complex is completed by taking the downward closure of these
 433 faces. All maximum faces of the resulting complex are m -dimensional and there is a bijection
 434 between the maximum faces and the independent sets of G . Furthermore, there is a natural
 435 partitioning $\{U_i\}_{i \in [m]}$ of the ground set U , each partition U_i corresponding to a clique Λ_i ,
 436 such that every maximum face in X contains exactly one element from each partition U_i .

437 By weighting each maximum face of X by the contribution of the corresponding inde-

438 pendent set to the partition function, the block dynamics based on Λ are equivalent to the
 439 two-step walk on X . Thus, in order to bound the mixing time of the block dynamics, it is
 440 sufficient to study the local expansion properties of X . To this end, we adapt the influence
 441 matrix used for proper colorings in [11]. For $x \in U$, let $\mathbb{P}_G[x]$ denote the probability that
 442 $x \in \tau_I$ for an independent set $I \in \mathcal{I}(G)$ drawn from $\mu^{(G, \lambda)}$ and corresponding maximum face
 443 $\tau_I \in X$. Similarly as for defining pairwise influences, we extend this notation to conditional
 444 probabilities. The clique influence matrix $\Phi_{G, \Lambda}$ contains an entry $\Phi_{G, \Lambda}(x, y)$ for each $x, y \in U$
 445 with

$$446 \quad \Phi_{G, \Lambda}(x, y) = \begin{cases} 0 & \text{if } x, y \in U_i \text{ for some } i \in [m], \\ \mathbb{P}_G[y \mid x] - \mathbb{P}_G[y] & \text{otherwise.} \end{cases}$$

447 By using similar linear-algebraic arguments as in [11] we prove that the maximum eigenvalue
 448 of $\Phi_{G, \Lambda}$ can be used to upper bound the local spectral expansion of X . To obtain Theorem 4
 449 it is then sufficient to relate Condition 3 to the maximum eigenvalue of $\Phi_{G, \Lambda}$. The following
 450 lemma establishes this connection.

451 **► Lemma 7.** *Let (G, λ) be an instance of the multivariate hard-core model that satisfies*
 452 *Condition 3 for a function q and a constant C . For every $S \subseteq V$ and every disjoint clique*
 453 *cover Λ of $G[S]$ it holds that the largest eigenvalue of $\Phi_{G[S], \Lambda}$ is at most $(2 + C)C$.*

454 Note that our simplicial-complex representation is only given under the assumption that
 455 the cliques in the clique cover Λ are pairwise disjoint. Indeed, this is a necessary requirement
 456 to map the block dynamics to the two-step walk such that the local-global-theorem from [1]
 457 can be applied. Thus, Lemma 7 only helps to prove Theorem 4 for disjoint clique covers.
 458 However, we relax this requirement by proving that for every clique cover Λ a disjoint clique
 459 cover K can be constructed such that the block dynamics $\mathcal{B}(G, \lambda, \Lambda)$ and $\mathcal{B}(G, \lambda, K)$ have
 460 asymptotically the same mixing time. By this comparison argument, we extend Theorem 4
 461 to arbitrary clique covers.

462 We are aware that, in the case of Glauber dynamics, more recent techniques for combining
 463 simplicial complex representations with entropy factorization as proposed in [12] yield superior
 464 mixing time results. However, in case of the hard-core model, this approach comes with
 465 an additional multiplicative factor of $\Delta^{O(\Delta^2)}$ in the mixing time (see section 8 of [12]).
 466 Although negligible for bounded degree graphs, this would be too much for our application,
 467 as the degree of our discretization gets exponentially large in the continuous volume $|V|$ of
 468 the system. Thus, directly relating local spectral expansion with the spectral gap of block
 469 dynamics is more suitable in our case. We leave as an open question, whether a modification
 470 of the approach in [12] can be applied to further improve our mixing time result.

471 1.4 Outlook

472 We obtain the fugacity bound from Theorem 1 based on the tree threshold $\lambda_c(\Delta)$ of the
 473 hard-core model. An obvious question is whether there are any structural properties of our
 474 discretization that can be used to improve this bound. Similar results are known for specific
 475 graph classes, such as the 2-dimensional square lattice [48, 52, 54]. In [42] the authors discuss
 476 that a generalization of the connective constant to the continuous Euclidean space might
 477 be applicable to improve their uniqueness result for the hard-sphere model. A comparable
 478 algorithmic result was already established for the discrete hard-core model in [49]. However,
 479 any such improvement for our discretization would require the connective constant of G_ρ to
 480 be at least by a constant factor small than its maximum degree Δ_ρ . Unfortunately, due to a

481 result in [47], this is not the case. Although this does not necessarily imply that a similar
 482 concept does not work in continuous space, it gives a strong evidence that a more specialized
 483 tool instead of the connective constant might be required.

484 A different direction for future work is to see which other quantities and properties of the
 485 model are preserved under discretization. This would especially include the thermodynamic
 486 pressure and its analyticity. As a matter of fact, non-analytic points of the pressure along the
 487 positive real axis of fugacity in the thermodynamic limit are known to mark phase transitions
 488 in infinite volume systems (see for example [42]). One way to approach this could be to prove
 489 a relation between zero-freeness of the continuous and the discretized partition function in a
 490 complex neighborhood of the real axis by extending our convergence result to the complex
 491 domain. Along this line, insights could be gained in how far properties like correlation decay
 492 and phase transitions (or their absence) are preserved under sufficiently fine discretization.

493 From a purely technical point of view, it is interesting to see if our result on the mixing
 494 time of block dynamics in Theorem 4 also holds without the requirement of using cliques as
 495 blocks. Especially: is the mixing time for block dynamics for the univariate hard-core model
 496 polynomial in the number of blocks for any block cover? Most of our techniques that we use
 497 for clique covers, such as modeling the distribution as a simplicial complex and relating its
 498 local spectral expansion to the clique influence matrix, can be generalized in a straightforward
 499 way for different choices of blocks. However, the main difficulty is to relate generalized
 500 versions of the clique influence matrix to pairwise influences, as we do in Lemma 7. One way
 501 to circumvent this might be to not rely on pairwise influences at all but to rather investigate
 502 the influence matrix directly, for example, via different computational-tree methods.

503 Finally, it would be interesting to see if approaches like ours can be extended to other
 504 continuous models from statistical physics (see for example coarse-graining [20]). We believe
 505 that the variety of tools that are already established for discrete spin systems are useful in
 506 this setting to establish rigorous computational results for different continuous models. We
 507 emphasize that clique and block dynamics are a useful computational tool to handle the
 508 exponential blow-ups caused by discretization.

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