

# Sequential Cavity Method for Computing Free Energy and Surface Pressure

David Gamarnik · Dmitriy Katz

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**Abstract** We propose a new method for the problems of computing free energy and surface pressure for various statistical mechanics models on a lattice  $\mathbb{Z}^d$ . Our method is based on representing the free energy and surface pressure in terms of certain marginal probabilities in a suitably modified sublattice of  $\mathbb{Z}^d$ . Then recent deterministic algorithms for computing marginal probabilities are used to obtain numerical estimates of the quantities of interest. The method works under the assumption of Strong Spatial Mixing (SSP), which is a form of a correlation decay.

We illustrate our method on the hard-core and monomer-dimer models, on which we improve several earlier estimates. For example we show that the exponential of the monomer-dimer coverings of  $\mathbb{Z}^3$  belongs to the interval  $[0.78595, 0.78599]$ , improving best previously known estimate of  $[0.7850, 0.7862]$  obtained in (Friedland and Peled in Adv. Appl. Math. 34:486–522, 2005; Friedland et al. in J. Stat. Phys., 2009). Moreover, we show that given a target additive error  $\epsilon > 0$ , the computational effort of our method for these two models is  $(1/\epsilon)^{O(1)}$  both for the free energy and surface pressure values. In contrast, prior methods, such as the transfer matrix method, require  $\exp((1/\epsilon)^{O(1)})$  computation effort.

**Keywords** Partition function · Spatial mixing · Independent sets · Matchings · Algorithm

## 1 Introduction

It is a classical fact in statistical physics that the logarithm of the partition function of a general statistical mechanics model on  $[-n, n]^d \subset \mathbb{Z}^d$ , appropriately normalized, has a well-defined limit as  $n \rightarrow \infty$  [15, 31]. This limit is called free energy or pressure (the difference

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D. Gamarnik (✉)  
Operations Research Center, MIT, Cambridge, MA 02139, USA  
e-mail: [gamarnik@mit.edu](mailto:gamarnik@mit.edu)

D. Katz  
Department of Mathematical Sciences, IBM T.J. Watson Research Center, Yorktown Heights,  
NY 10598, USA  
e-mail: [dimdim@mit.edu](mailto:dimdim@mit.edu)

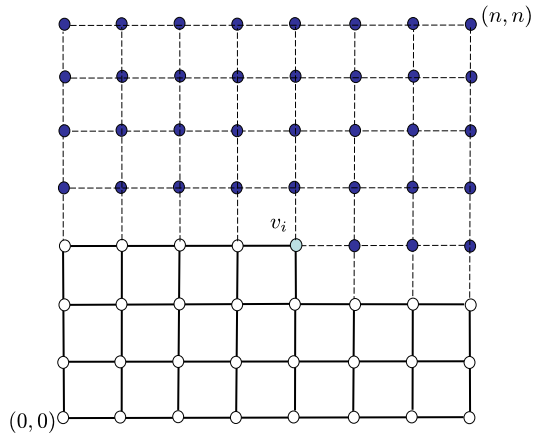
between the two is in the normalization constant). Similarly, the limit of its first order correction, *surface pressure*, exists, though such limit depends on the shape of the underlying finite box and the existing proofs assume soft core interactions,  $H < \infty$  (see Sect. 2) [31]. It is a different matter to compute these limits, and this question interested researchers both in the statistical physics and combinatorics communities. In very special cases, free energy can be computed analytically. The most widely known such an example is Fisher-Kasteleyn-Temperley's formula for the dimer model on  $\mathbb{Z}^2$  [11, 23, 33]. This formula was used in [30] for obtaining complete parametrization of different Gibbs measures for the pure dimer model on  $\mathbb{Z}^2$ . The formula, unfortunately, extends neither to a dimer model in other dimensions nor to the closely related monomer-dimer model. Another example of an exactly solvable model is hard-core model on a hexagonal lattice [3]. We refer the reader to [4], as a standard reference on such models.

Short of these special cases, the existing methods for computing free energy mostly rely on numerical approximations. These include randomized methods such as Monte-Carlo [22, 26] and deterministic methods such as transfer matrices. The Monte-Carlo method can be used to estimate free energy in finite graphs, say  $[-n, n]^d$ , with some probabilistic approximation guarantee, provided that some underlying Markov chain is rapidly mixing. One then has to relate a finite graph to infinite lattices to approximate free energy for an infinite lattice. The drawback of this method is its dependence on the sampling error. The transfer matrix method, on the other hand is a deterministic method and provides rigorous deterministic bounds on the free energy. In Sect. 3.3 we show that in order to get a target additive error  $\epsilon$ , the transfer matrix method requires computation time  $\exp(O((1/\epsilon)^{d-1}))$ . While, for low dimensions  $d$ , this is a substantial saving over a brute force method, which requires time  $\exp(O((1/\epsilon)^d))$ , the method stops being effective for larger  $d$ . Some additional computational savings can be achieved using underlying automorphisms group structure, see Friedland and Peled [14], but we are not aware of any formal analysis of the computational savings produced by this method. The complexity of computing surface pressure using the transfer matrix method further increases to  $\exp(O((1/\epsilon)^{2d-2}))$ , see Sect. 3.3.

The transfer matrix method was used to obtain some of the best known bounds on the free energy in several models. For the hard-core model (see Sect. 4) with activity  $\lambda = 1$ , which corresponds to counting independent sets in  $\mathbb{Z}^d$ , the exponential of the free energy is known to be in the range  $[1.503047782, 1.5035148]$ , as obtained by Calkin and Wilf [8]. A far more accurate but non-rigorous estimate was obtained by Baxter [5]. This was recently confirmed rigorously by Friedland et al. [13] with estimate 1.50304808247533. Similarly, the transfer matrix method was used to compute the free energy of the monomer-dimer (matchings) model (see Sect. 5). The problem has a long history. Earlier studies include Hammersley [17, 18], Hammersley and Menon [21], Baxter [2], where some non-rigorous estimates and crude bounds were obtained. Recently Friedland and Peled [14] obtained rigorously a range  $0.6627989727 \pm 0.0000000001$  for  $d = 2$ , and  $[0.7653, 0.7863]$  for  $d = 3$  using the transfer matrix method and Friedland-Tveberg inequality. A tighter lower bound 0.7849602275 was recently obtained using techniques related to the asymptotic matching conjectures [12]. A bit earlier a similar non-rigorous estimate  $[0.7833, 0.7861]$  was obtained in [20], via reduction from the permanent problem. Exact values for monomer-dimer entropy on two dimensional infinite strip were obtained by Kong [25].

In this paper we propose a new approach for the problem of computing numerically free energy and surface pressure. Our approach takes advantage of the fact that some of these models, including the two models above, are in the so-called uniqueness regime. Namely, the Gibbs measure on the infinite lattice is unique. This is an implication of the Strong Spatial Mixing (SSM) property [7], see Sect. 2.4 for the definition. SSM is a stronger notion

**Fig. 1**  $\mathbb{G}_i$  is obtained by removing all dark nodes



of a classical notion of spatial mixing known as Dobrushin-Shlosman condition [9, 15, 31]. The SSM property asserts that the marginal probability that a node  $v$  attains a particular spin value  $\sigma_v$  is asymptotically independent from the spin configurations for nodes  $u$  which are far away from  $v$ . Our main theoretical result is Theorem 1, which provides a simple representation of the free energy and the surface pressure in terms of such a marginal probability, provided that the SSM holds. This representation is particularly easy to explain for the special case of hard-core model in two dimensions, and now we provide a key idea of our method. Consider the subset  $\mathbb{Z}_{<0}^2$  of  $\mathbb{Z}^2$  consisting of points  $\mathbf{v} = (r, m)$  with either  $r < 0$  or  $r = 0, m \leq 0$ . Our representation theorem states that the free energy equals  $\log(1/p^*)$  where  $p^*$  is the probability that a random independent set in  $\mathbb{Z}_{<0}^2$  does not contain the origin  $(0, 0)$ . As the model satisfies SSM (see Sect. 4) this probability is well-defined. The idea of the proof is simple. Let  $v_1 < v_2 < \dots < v_{(2n+1)^2}$  be the lexicographic ordering of nodes in  $[-n, n]^2$ . That is  $(v_1, v_2) > (u_1, u_2)$  iff  $v_2 > u_2$  or  $v_2 = u_2$  and  $v_1 > u_1$ . Observe the following telescoping identity  $Z^{-1} = \prod_{i=0}^{(2n+1)^2-1} Z(i)/Z(i+1)$ , where  $Z(i)$  is the number of independents sets in the subgraph  $\mathbb{G}_i$  of  $[-n, n]^2$  when all nodes  $v_j, j > i$  and incident edges are removed, see Fig. 1. The convention  $Z(0) = 1$  is used. Observe that  $Z(i)/Z(i+1)$  is the probability that a randomly chosen independent set in  $\mathbb{G}_{i+1}$  does not contain  $v_{i+1}$ . This probability is then approximately  $p^*$  for “most” of the nodes in  $[-n, n]^2$ . The required representation is then obtained by taking logarithms of both sides. Such representation is called cavity method in statistical physics and has been used heavily for analyzing statistical models on sparse random graphs, [1, 27–29]. Here due to a particular sequencing of removed vertices, we call our approach the *sequential cavity method*. A similar approach based on successively removing nodes is known for the representation of the relative entropy, see Proposition 15.16 in [15], though no interpretation of the relative entropy in terms of marginal probabilities is provided. We are not aware of a similar expression in the context of the surface pressure. We note that our results provide an independent proof of the existence of the free energy and surface pressure, not relying on the sub-additivity arguments, albeit in the special case of SSM.

Theorem 1 reduces the problem of computing the free energy and surface pressure to the one of computing marginal probabilities, and the latter problem is solved using recent deterministic algorithms for computing such marginals in certain models satisfying SSM property [6, 16, 34]. These results are based on establishing even stronger property, namely the correlation decay on a computation tree property, and lead to efficient algorithms for

computing such marginals. We have implemented these algorithm for the hard-core [34] and monomer-dimer [6] models in the special case of  $\mathbb{Z}^d$ . Using our approach we improve existing bounds and obtain some new bounds for these models. For example we show that the exponential of the free-energy of the hard-core model in two dimensions  $d = 2, 3$  and  $4$  are in the ranges  $[1.503034, 1.503058]$ ,  $[1.434493, 1.449698]$  and  $[1.417583, 1.444713]$ , respectively. While our bounds for the case  $d = 2$  are weaker than the existing bounds, we are not aware of any bounds for the cases  $d = 3, 4$  and suspect that the bounds obtainable from the transfer matrix method will be substantially weaker than the ones obtained by our method.

For the case of monomer-dimer model when  $d = 3$  we obtained a range  $[0.78595, 0.78599]$ , substantially improving earlier bounds [10, 12, 14] (see above). Further we show that our method provides an exponential improvement over the transfer matrix method in terms of the computation effort. Specifically, we show that the numerical complexity of obtaining  $\epsilon$ -additive approximation using our approach is  $(1/\epsilon)^{O(1)}$  for both free energy and surface pressure. The constant in  $O(1)$  may depend on model parameters and dimensions. For example, for the case of monomer-dimer model, this constant is  $Cd^{\frac{1}{2}} \log d$ , where  $C$  is some universal constant (Proposition 4). This is a exponential improvement over the computation efforts  $\exp(O((1/\epsilon)^{d-1}))$  and  $\exp(O((1/\epsilon)^{2d-2}))$  needed for the transfer matrix method for computing free energy and surface pressure, respectively. On the other hand our method is applicable only to the models satisfying SSM property, whereas the transfer matrix method does not require this restriction. Extending our approach to models undergoing phase transition and thus falling outside of the SSM regime is an interesting open problem.

The rest of the paper is organized as follows. In the following section we provide a necessary background on Gibbs measures on general graphs and lattices, free energy, surface pressure, and define the Strong Spatial Mixing property. Our main theoretical result is Theorem 1 which represents free energy and surface pressure in terms of marginal probabilities. This result and its several variations are stated and proven in Sect. 3. Sections 4 and 5 are devoted to application of Theorem 1 and its variations to the problem of numerically estimating free energy for hard-core and monomer-dimer models specifically. Additionally, in these sections we compare the algorithmic complexity of our method with the complexity of the transfer matrix method. Concluding thoughts and open questions are in Sect. 6.

## 2 Model, Assumptions and Notations

### 2.1 Finite and Locally Finite Graphs

Consider a finite or infinite locally finite simple undirected graph  $\mathbb{G}$  with node set  $V$  and edge set  $E \subset V \times V$ . The locally-finite property means every node is connected to only finitely many neighbors. The graph is undirected and simple (no loops, no multiple edges). For every  $v, u \in V$  let  $d(u, v)$  be the length (number of edges) in the shortest path connecting  $u$  and  $v$ . For every node  $v$ , we let  $N(v)$  stand for the set of neighbors of  $v$ :  $N(v) = \{u : (u, v) \in E\}$ . We will write  $N_{\mathbb{G}}(v)$  when we need to emphasize the underlying graph  $\mathbb{G}$ . The quantity  $\Delta = \Delta_{\mathbb{G}} \triangleq \max_v |N(v)|$  is called the degree of the graph. For every  $r \in \mathbb{Z}_+$  let  $B_r(v) = \{u : d(v, u) \leq r\}$ . For every set  $A \subset V$ , let  $B_r(A) = \bigcup_{v \in A} B_r(v)$ . Thus locally finite property means  $|B_r(v)| < \infty$  for all  $v, r$ . Given  $A \subset V$ , let  $\partial A = \{v \in A^c : N(v) \cap A \neq \emptyset\}$  and let  $\partial_r A = \partial B_r(A)$ . For every subset  $A \subset V$ , we have an induced subgraph obtained by taking nodes in  $A$  and all edges  $(v, u) \in E \cap A^2$ . The corresponding edge set of the induced graph is denoted by  $E(A)$ .

Let  $\mathbb{R}_+(\mathbb{Z}_+)$  denote the set of all non-negative real (integer) values. Let  $\mathbb{R}_{>0}(\mathbb{Z}_{>0})$  be the set of all positive real (integer) values. Our main example of an infinite locally-finite graph is the  $d$ -dimensional lattice  $\mathbb{Z}^d$  with  $V = \{(v_1, \dots, v_d) : v_i \in \mathbb{Z} \text{ and } E = \{(v, u) \in V^2 : \|v - u\| = 1\}$ , where  $\|w\| = \sum_{1 \leq j \leq d} |w_j|$ . We denote the origin  $(0, 0, \dots, 0)$  by  $0$  for short. Given a vector  $a = (a_1, \dots, a_d) \in \mathbb{R}_+^d$ , and  $v = (v_1, \dots, v_d) \in \mathbb{Z}^d$ , let  $B_{an}(v) = \{u \in \mathbb{Z}^d : |u_j - v_j| \leq a_j n, j = 1, 2, \dots, d\}$ . In the special case  $\mathbb{G} = \mathbb{Z}^d, v = 0$ , we write  $B_r$  instead of  $B_r(0)$  and  $B_{an}$  instead of  $B_{an}(0)$ . For each  $j \leq d, k \in \mathbb{Z}_+$ , let  $\mathbb{Z}_{j,k,+}^d = \{v \in \mathbb{Z}^d : v_j \leq k\}$ ,  $\mathbb{Z}_{j,k,-}^d = \{v \in \mathbb{Z}^d : v_j \geq -k\}$ . Each of these is a  $d$ -dimensional half-plane in  $\mathbb{Z}^d$ . Let  $<$  denote a lexicographic full order on  $\mathbb{Z}^d$ . Namely,  $v < u$  iff either  $u_d > v_d$  or  $\exists k \in \{1, 2, \dots, d - 1\}$  such that  $u_k > v_k$  and  $v_j = u_j, j = k + 1, \dots, d$ . For every  $v \in \mathbb{Z}^d$  and  $k = 1, 2, \dots, d$ , let  $\mathbb{Z}_{<v}^d = \{u \in \mathbb{Z}^d : u < v\} \cup \{v\}$ . Similarly we define  $\mathbb{Z}_{j,k,+,<v}^d$  and  $\mathbb{Z}_{j,k,-,<v}^d$  with  $\mathbb{Z}_{j,k,+}^d$  and  $\mathbb{Z}_{j,k,-}^d$  replacing  $\mathbb{Z}^d$ .

Throughout the paper we write  $f(n) = O(g(n))$  and  $f(n) = o(g(n)), n \in \mathbb{Z}_+$  if  $|f(n)| \leq C|g(n)|$ , respectively  $f(n)/g(n) \rightarrow 0$ , for all  $n$ , for some constant  $C$ . This constant may in general depend on model parameters such as  $H, h$  (see the next section) or dimension  $d$ . However, in some places the constant is universal, namely independent from any model parameters. We will explicitly say so if this is the case.

### 2.2 Gibbs Measures

Consider a finite set of spin values  $\chi = \{s_1, \dots, s_q\}$ , a Hamiltonian function  $H : \chi^2 \rightarrow \mathbb{R} \cup \{\infty\}$ , and an external field  $h : \chi \rightarrow \mathbb{R} \cup \{\infty\}$ . Given a graph  $\mathbb{G} = (V, E)$  we consider the associated spin configuration space  $\Omega = \chi^V$  equipped with product  $\sigma$ -field  $\mathcal{F}$ . If the graph  $\mathbb{G}$  is finite, a probability measure  $\mathbb{P}$  on  $(\Omega, \mathcal{F})$  is defined to be Gibbs measure if for every spin assignment  $(s_v) \in \chi^V$

$$\mathbb{P}(\sigma_v = s_v, \forall v \in V) = Z^{-1} \exp\left(- \sum_{(v,u) \in E} H(s_v, s_u) - \sum_{v \in V} h(s_v)\right), \tag{1}$$

where  $Z$  is the normalizing partition function:

$$Z = \sum_{(s_v) \in \chi^V} \exp\left(- \sum_{(v,u) \in E} H(s_v, s_u) - \sum_{v \in V} h(s_v)\right).$$

We will often write  $\mathbb{P}_{\mathbb{G}}$  and  $Z_{\mathbb{G}}$  in order to emphasize the underlying graph. The case  $H(a, a') = \infty$  corresponds to a hard-core constraint prohibiting assigning  $a \in \chi$  and  $a' \in \chi$  to neighbors. The possibility of such hard-core constraints is important for us when we discuss the problems of counting independent sets and matchings.

When  $\mathbb{G}$  is infinite, a probability measure  $\mathbb{P}(\cdot)$  is defined to be Gibbs measure, if it satisfies the following spatial Markovian property. For every finite  $A \subset V$  and every spin assignment  $(s_v) \in \chi^{|\partial A|}$  on the boundary  $\partial A$  of  $A$ , the conditional probability measure  $\mathbb{P}(\cdot | (s_v))$  on the finite graph  $(V(A), E(A))$  induced by  $A$  is a Gibbs measure with the same  $H$  as the original graph and external field  $h'$  given as  $h'_v(a) = h(a) + \sum_{u \in N(v) \setminus A} H(s_u, a)$  for every  $a \in \chi$ . Here the external field becomes node dependent, but the Hamiltonian remains the same for all nodes. Since every node  $u \in N(v) \setminus A$  belongs to  $\partial A$  and thus its spin value  $s_u$  is well defined. This is called spatial Markovian property of Gibbs measure. One can construct Gibbs measures as a weak limit of Gibbs measures on cylinder sets in  $\mathcal{F}$  obtained from finite induced subgraphs of  $\mathbb{G}$ , see [15, 31] for details. Generally there are multiple Gibbs

measures and the space of Gibbs measures of  $\mathbb{G}$  is denoted by  $\mathcal{M}$  or  $\mathcal{M}_{\mathbb{G}}$ . We say that the model  $(\mathbb{G}, H, h)$  is in the uniqueness regime if  $\mathcal{M}$  consists of a unique measure  $\mathcal{M} = \{\mathbb{P}\}$ . Most of the results in this paper correspond to the uniqueness case, and more specifically to the case of Strong Spatial Mixing (SSM) defined below. Given a model  $(\mathbb{G}, H, h)$  and a subset  $A \subset V$ , we have a naturally defined induced submodel on the induced subgraph  $\mathbb{G}(A) = (V(A), E(A))$ , given by the same  $\chi, H$  and  $h$  (but different partition function). In order to emphasize the underlying subgraph  $\mathbb{G}$  we write, with abuse of notation,  $\mathbb{Z}_A$  and  $\mathbb{P}_A$  for the partition function and the Gibbs measure on the subsystem  $(\mathbb{G}(A), H, h)$ , when it is unique. By default we drop the subscript when the underlying graph is the entire lattice  $\mathbb{Z}^d$ .

The definitions above are “node” centered: the spins are associated with nodes of a graph. In order to study the monomer-dimer model we need to consider a similar “edge” model where spins are associated with edges. Thus given a finite graph  $\mathbb{G} = (V, E)$ , and a finite set of spin values  $\chi$ , we consider a probability space  $\Omega = \chi^{|E|}$ . Then (1) is restated as follows. Write  $e \sim e'$  if edges  $e, e'$  are distinct and incident (share a node). For every spin assignment  $(s_e) \in \chi^{|E|}$  we assign probability measure

$$\mathbb{P}(\sigma_e = s_e, \forall e \in E) = Z^{-1} \exp\left(- \sum_{e \sim e' \in E} H(s_e, s_{e'}) - \sum_{e \in E} h(s_e)\right). \tag{2}$$

It is clear that “edge” model can be reduced to “node” model by considering a line graph of  $\mathbb{G}$ : the nodes of this graph are edges of  $\mathbb{G}$  and two nodes  $e, e'$  form an edge in the line graph if and only if  $e \sim e'$ . For simplicity, however, we prefer not to switch to the line graph model.

### 2.3 Free Energy, Pressure and Surface Pressure

Given  $\mathbb{G} = \mathbb{Z}^d$ , Hamiltonian  $H$  and an external field  $h$ , consider an arbitrary infinite sequence of finite subsets  $\emptyset \in \Lambda_1 \subset \Lambda_2 \subset \dots \subset \mathbb{Z}^d$ , such that the sequence  $r_n \triangleq \max\{r : B_r \subset \Lambda_n\}$  diverges to infinity as  $n \rightarrow \infty$ . Consider the corresponding sequence of Gibbs measures  $\mathbb{P}_{\Lambda_n}$  and partition functions  $Z_{\Lambda_n}$  on the graphs induced by  $\Lambda_n$ . It follows from the sub-additivity property of partition functions that the limit

$$\mathcal{P}(d, H, h) \triangleq \lim_{n \rightarrow \infty} \frac{\log Z_{\Lambda_n}}{|\Lambda_n|} \tag{3}$$

exists and is independent from the choice of the sequence of subsets [15, 31]. This quantity is called *pressure*. Given a positive  $\beta > 0$  one usually also considers limits  $\lim_{n \rightarrow \infty} \log Z_{\Lambda_n} / (\beta |\Lambda_n|)$  where  $H$  and  $h$  are replaced by  $\beta H$  and  $\beta h$ , respectively. The corresponding limit is called *free energy*. For our purposes, this difference is insubstantial, as it is just a matter of redefining  $H, h$  and changing the normalization.

The first order correction to the limit (3) is known as *surface pressure* and is defined as follows. Unlike pressure, this quantity is “shape” dependent. In this paper we only consider the case of the rectangular shape, although our results can be extended to more complicated shapes as well. Given a vector  $a = (a_i) \in \mathbb{R}_{>0}^d$ , let  $A_j(a) \triangleq \prod_{k \neq j} (2a_k)$ ,  $j = 1, 2, \dots, d$ , and let  $A(a) = \sum_{j \leq d} A_j(a)$ . Observe that surface area of  $B_{an}$  (the number of boundary nodes in  $B_{an}$ ) is  $A(a)n^{d-1} + o(n^{d-1})$ . The surface pressure is defined as

$$s\mathcal{P}(d, H, h, a) \triangleq \lim_{n \rightarrow \infty} A^{-1}(a)n^{-d+1} \left( \log Z_{B_{an}(0)} - n^d \mathcal{P}(d, H, h) \prod_{1 \leq i \leq d} (2a_i) \right). \tag{4}$$

The surface pressure is interpreted as the first order correction of the free energy, scaled by the surface area. The existence of this limit is a classical fact [31] for the case  $\max_{s,s' \in \chi} H(s, s') < \infty$ . The hard-core case  $H = \infty$  is trickier and we are not aware of results on the existence of the limit for this case. Our proofs however imply the existence of the limit under the assumption of SSM, see below.

### 2.4 Strong Spatial Mixing

The following technical assumption is needed for our analysis. The assumption essentially says that there is always a choice of a spin value  $s^* \in \chi$  which allows any other choice of spin values for its neighbors without rendering the Hamiltonian infinite.

**Assumption 1** There exist  $s^* \in \chi$  such that  $\max_{s \in \chi} |H(s, s^*)| < \infty$ .

The assumption implies that under any Gibbs measure, for every node  $v$

$$c^* \triangleq \min_{(s_u)} \mathbb{P}(\sigma_v = s^* | \sigma_u = s_u, \forall u \in N(v)) > 0 \tag{5}$$

where the minimum is over all possible spin assignments  $(s_u) \in \chi^{|N(v)|}$  of the neighbors of  $v$ . We now introduce the Strong Spatial Mixing assumption, which, in particular, implies the uniqueness of the Gibbs measure on an infinite graph. We first informally discuss this notion. Loosely speaking, a model  $(\mathbb{G}, H, h)$  exhibits just *spatial mixing* if for every finite set  $A \subset \mathbb{G}$  the joint probability law for spins in  $A$  is asymptotically independent from the values of spins which are far away from  $A$ . A form of this condition is known to be equivalent to the uniqueness of the Gibbs measure. Instead, a strong spatial mixing means the same except that values for any other subset  $B \subset \mathbb{Z}^d$  are allowed to be fixed. In other words, strong spatial mixing is spatial mixing, but for the *reduced* model on  $V \setminus B$  when values of spins in  $B$  are fixed and values of the external field  $h$  on the remaining graph are appropriately modified. Strong spatial mixing is strictly stronger than spatial mixing (hence the separate definition), see [7] for counterexamples and discussion.

We now introduce the definition formally.

**Definition 1**  $(\mathbb{G}, H, h)$  satisfies the Strong Spatial Mixing property if for every finite set  $X \subset V(\mathbb{G})$ , possibly infinite set  $Y \in V(\mathbb{G})$  there exists a function  $R(r)$  satisfying  $\lim_{r \rightarrow \infty} R(r) = 0$ , such that for every positive integer  $r$

$$\begin{aligned} & \max \left\| \mathbb{P}(\sigma_v, v \in X | \sigma_v = s_v^1, v \in Y; \sigma_v = s_v^2, v \in \partial_r X) \right. \\ & \left. - \mathbb{P}(\sigma_v, v \in X | \sigma_v = s_v^1, v \in Y; \sigma_v = s_v^3, v \in \partial_r X) \right\|_{\text{VAR}} \leq R(r), \end{aligned}$$

where the maximum is over all possible spin assignments  $(s_v^1) \in \chi^{|Y|}$ ,  $(s_v^2), (s_v^3) \in \chi^{|\partial_r X|}$ , and  $\| \cdot \|_{\text{VAR}}$  denotes the variational distance of the Gibbs measure restricted to the subset  $X$ .  $(\mathbb{G}, H, h)$  satisfies exponential strong spatial mixing if there exist  $\kappa, \gamma > 0$  such that  $R(r) \leq \kappa \exp(-\gamma r)$  for all  $r \geq 0$ .

It is known that if  $(\mathbb{G}, H, h)$  exhibits SSM, then the Gibbs measure is unique:  $\mathcal{M} = \{\mathbb{P}\}$ , [7]. We note that in this paper we will exclusively consider the case  $|X| = 1$ .

### 3 Sequential Cavity Method

In this section we present a theoretical result which serves as a basis for our subsequent computational work. Specifically, we provide the representation of the free energy and surface pressure on  $\mathbb{Z}^d$  in terms of some conditional marginal probabilities  $\mathbb{P}(\sigma_0 = s|\cdot)$  defined on suitably modified subsets of  $\mathbb{Z}^d, \mathbb{Z}_{j,k,+}^d, \mathbb{Z}_{j,k,-}^d$ . The idea is to sequentially remove nodes from a rectangle  $B_{an}$  one by one and observe that the log-partition function can be written in terms of the log-marginal probabilities (cavity) of the removed nodes.

#### 3.1 Representation Theorem

Given a graph  $\mathbb{G} = (V, E)$  with some full order  $\succ$ , a node  $v$  and  $s \in \chi$ , let  $\mathcal{E}_{v,s}$  denote the event “ $\sigma_u = s$  for all  $u \succ v, u \in V$ ”. By convention we assume that  $\mathcal{E}_{v,s}$  is the full event  $\Omega$ , if the set  $u \succ v, u \in V$  is empty. In the special case when  $\mathbb{G} = \mathbb{Z}^d, v = 0$  and  $\succ$  is the lexicographic order, this event is denoted by  $\mathcal{E}_s$ , see Fig. 2 for the case  $d = 2$ . We remind the reader, that we drop the subscripts in  $\mathbb{P}_{\mathbb{G}}, Z_{\mathbb{G}}$  when the underlying graph is  $\mathbb{Z}^d$ .

**Theorem 1** *Suppose  $(\mathbb{Z}^d, H, h)$  satisfies the SSM property and the Assumption 1 holds. Then*

$$\mathcal{P}(d, H, h) = -\log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) - dH(s^*, s^*) - h(s^*). \tag{6}$$

If, in addition, the SSM is exponential, then for every  $a = (a_j) \in \mathbb{R}_{>0}^d$

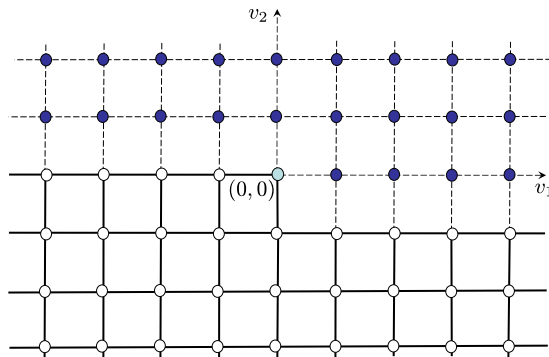
$$\begin{aligned} s\mathcal{P}(d, H, h, a) &= -H(s^*, s^*) + \sum_{1 \leq j \leq d} \frac{A_j(a)}{A(a)} \sum_{k=0}^{\infty} (2 \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) - \log \mathbb{P}_{\mathbb{Z}_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*}) \\ &\quad - \log \mathbb{P}_{\mathbb{Z}_{j,-k,-}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*})). \end{aligned} \tag{7}$$

In particular, the infinite sum is convergent.

*Remark*

- We stress that our proof does not rely on the existence of a limit in (3) and thus provides an independent proof for it, albeit in the restricted case of SSM. Preempting the formal

**Fig. 2** Event  $\mathcal{E}_{s^*}$  on  $\mathbb{Z}^2$ . Every dark node is assigned spin  $s^*$





discussion, the convergence of the infinite sum in (7) is an almost immediate consequence of the exponential SSM, which gives

$$|\mathbb{P}_{Z_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*}) - \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})| \leq \kappa \exp(-\gamma k).$$

A similar conclusion for difference of the logarithms is obtained then using the Assumption 1. This observation implies that  $\epsilon$ -additive approximation of this infinite sum is obtained by considering the partial sum with first  $O(\log(1/\epsilon))$  terms. As we shall discuss in the following subsection, the main import from this observation is that the overhead of computing surface pressure vs free energy is very small.

- A representation similar to the one of (6) is known for the relative entropy, see Proposition 15.16 in [15]. Here it is important for us that the representation connects free energy and marginal probabilities, since, as is discussed in the latter part of the paper, we have tools for numerical computation of the marginal probabilities approximately. We are not aware of an expression similar to (7) existing in the prior literature.

*Proof* We first prove (6). Let  $v_1 \succ v_2 \succ \dots \succ v_{|B_n|}$  be the labeling of nodes in  $B_n$  according to the lexicographic order. Note that the number of edges in  $B_n$  is  $d|B_n| + o(|B_n|)$ . We have

$$\begin{aligned} &\mathbb{P}_{B_n}(\sigma_v = s^*, \forall v \in B_n) \\ &= Z_{B_n}^{-1} \exp(-d|B_n|H(s^*, s^*) - o(|B_n|)H(s^*, s^*) - |B_n|h(s^*)), \end{aligned}$$

from which we infer that

$$\begin{aligned} Z_{B_n}^{-1} &= \exp(d|B_n|H(s^*, s^*) + o(|B_n|)H(s^*, s^*) + |B_n|h(s^*)) \\ &\times \mathbb{P}_{B_n}(\sigma_v = s^*, \forall v \in B_n). \end{aligned} \tag{8}$$

On the other hand, by the telescoping property

$$\begin{aligned} \mathbb{P}_{B_n}(\sigma_v = s^*, \forall v \in B_n) &= \prod_{v \in B_n} \mathbb{P}_{B_n}(\sigma_v = s^* | \sigma_u = s^*, \forall u \succ v, u \in B_n) \\ &= \prod_{v \in B_n} \mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*}). \end{aligned} \tag{9}$$

Fix  $\epsilon > 0$  and find  $r = r(\epsilon)$  such that according to Definition 1,  $R(r) < \epsilon$  for  $X = \{0\}$ ,  $Y = \{u > 0\}$ . Let  $B^o = \{v \in B_n : B_r(v) \subset B_n\}$ . Observe that  $|B^o|/|B_n| \rightarrow 1$  as  $n \rightarrow \infty$ . By the choice of  $r$  we have for every  $v \in B^o$

$$|\mathbb{P}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*})| \leq \epsilon. \tag{10}$$

By translation invariance we have

$$\mathbb{P}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) = \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}).$$

For every  $v \in B_n \setminus B^o$  we have the generic lower bound (5)

$$\mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \geq c^* \tag{11}$$

which is strictly positive by Assumption 1. A similar inequality with the same constant holds for  $\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})$ . Combining this with (8) and (9) we obtain

$$\begin{aligned} Z_{B_n}^{-1} &= \exp(d|B_n|H(s^*, s^*) + o(|B_n|)H(s^*, s^*) + |B_n|h(s^*)) \\ &\quad \times \prod_{v \in B^o} \mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \prod_{v \in B_n \setminus B^o} \mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \\ &\geq \exp(d|B_n|H(s^*, s^*) + o(|B_n|)H(s^*, s^*) + |B_n|h(s^*)) \\ &\quad \times (\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) - \epsilon)^{|B^o|} (c^*)^{|B_n \setminus B^o|}. \end{aligned}$$

Since  $|B^o|/|B_n| \rightarrow 1$  as  $n \rightarrow \infty$  and  $c^* > 0$ , then we obtain

$$\liminf_{n \rightarrow \infty} \frac{\log Z_{B_n}^{-1}}{|B_n|} \geq dH(s^*, s^*) + h(s^*) + \log(\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) - \epsilon)$$

Recalling  $\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) \geq c^* > 0$ , since  $\epsilon$  was arbitrary, we conclude

$$\liminf_{n \rightarrow \infty} \frac{\log Z_{B_n}^{-1}}{|B_n|} \geq H(s^*, s^*)d + h(s^*) + \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}).$$

Similarly we show

$$\limsup_{n \rightarrow \infty} \frac{\log Z_{B_n}^{-1}}{|B_n|} \leq H(s^*, s^*)d + h(s^*) + \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}),$$

where for the case  $v \in B_n \setminus B_n^o$  we use a trivial inequality  $\mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \leq 1$  in place of (11). We obtain

$$\lim_{n \rightarrow \infty} \frac{\log Z_{B_n}^{-1}}{|B_n|} = H(s^*, s^*)d + h(s^*) + \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}). \tag{12}$$

This concludes the proof of (6).

Now we establish (7). Thus consider a rectangle  $B_{an}$ . The proof is based on a more refined estimates for the elements of the telescoping product (9) with  $B_{an}$  replacing  $B_n$ . We begin by refinement of (8). The number of edges in  $B_{an}$  is  $d|B_{an}| - A(a)n^{d-1} + o(n^{d-1})$ . Repeating the derivation of (8) and (9), we obtain

$$\begin{aligned} Z_{B_{an}}^{-1} &= \exp(d|B_{an}|H(s^*, s^*) - A(a)n^{d-1}H(s^*, s^*) + h(s^*)|B_{an}| + o(n^{d-1})) \\ &\quad \times \prod_{v \in B_{an}} \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}). \end{aligned} \tag{13}$$

Let

$$B_{an}^o = \{v \in B_{an} : |a_i n - v_i|, |a_i n + v_i| \geq C \log n, 1 \leq i \leq d\},$$

and for each  $j = 1, \dots, d$  and  $0 \leq k < C \log n$  let

$$\begin{aligned} B_{an,j,k,+} &= \{v \in B_{an} : v_j = \lfloor a_j n \rfloor - k; |a_i n - v_i|, |a_i n + v_i| \geq C \log n, i \neq j\}, \\ B_{an,j,k,-} &= \{v \in B_{an} : v_j = -\lfloor a_j n \rfloor + k; |a_i n - v_i|, |a_i n + v_i| \geq C \log n, i \neq j\}. \end{aligned}$$

Here  $C > 0$  is a large yet unspecified constant. In other words,  $B_{an,j,k,+} \cup B_{an,j,k,-}$  consists of nodes which have distance  $k$  from the boundary of  $B_{an}$  in the  $j$  coordinate, but have distance at least  $C \log n$  in all the other coordinates  $i \neq j$ . Observe that the sets  $B_{an,j,k,+}$ ,  $B_{an,j,k,-}$  are non-intersecting, for sufficiently large  $n$ . Observe also that

$$\begin{aligned} & \left| B_{an} \setminus \left( B_{an}^o \cup \bigcup_{1 \leq j \leq d, 0 \leq k \leq C \log n} (B_{an,j,k,+} \cup B_{an,j,k,-}) \right) \right| \\ &= O(n^{d-2} \log^2 n). \end{aligned} \tag{14}$$

For every  $v \in B_{an}^o$  we have by exponential SSM

$$|\mathbb{P}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*})| \leq \kappa \exp(-\gamma C \log n) = O(n^{-\gamma C}).$$

By translation invariance we have

$$\mathbb{P}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) = \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}).$$

Recalling  $\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) \geq c^*$ , we obtain using the Taylor expansion,

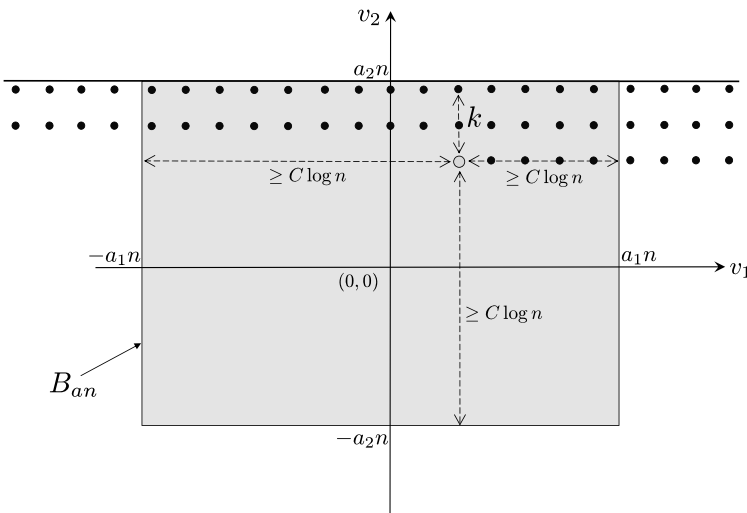
$$|\log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})| = O(n^{-\gamma C}). \tag{15}$$

Fix  $v \in B_{an,j,k,+}$ . Since  $v_j = \lfloor a_j n \rfloor - k$  and for every  $i \neq j$ ,  $v_i$  is at least  $C \log n$  away from the boundary of  $B_{an}$ , then by the exponential SSM property we have

$$|\mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \mathbb{P}_{\mathbb{Z}_{j,\lfloor a_j n \rfloor,+}^d}(\sigma_v = s^* | \mathcal{E}_{v,s^*})| \leq \kappa \exp(-\gamma C \log n) = O(n^{-\gamma C}),$$

(see Fig. 3 for the two-dimensional illustration with  $j = 2$ ). Recalling  $v_j = \lfloor a_j n \rfloor - k$  and using translation invariance we have

$$\mathbb{P}_{\mathbb{Z}_{j,\lfloor a_j n \rfloor,+}^d}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) = \mathbb{P}_{\mathbb{Z}_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*})$$



**Fig. 3** Event  $\mathcal{E}_{s^*}$  on  $\mathbb{Z}_{2,\lfloor a_2 n \rfloor,+}^2$ . Every dark node is assigned spin  $s^*$

Using again the Taylor expansion, we obtain

$$|\log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}_{\mathbb{Z}_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*})| = O(n^{-\gamma C}). \tag{16}$$

Similarly, if  $v \in B_{an,j,k,-}$ , then

$$|\mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \mathbb{P}_{\mathbb{Z}_{j,-[aj]n,-}^d}(\sigma_v = s^* | \mathcal{E}_{v,s^*})| \leq \exp(-\gamma C \log n) = O(n^{-\gamma C}).$$

By translation invariance and since  $v_j = -[aj]n + k$ , then

$$\mathbb{P}_{\mathbb{Z}_{j,-[aj]n,-}^d}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) = \mathbb{P}_{\mathbb{Z}_{j,-k,-}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*}),$$

and again applying Taylor expansion

$$|\log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}_{\mathbb{Z}_{j,-k,-}^d}(\sigma_0 = s^* | \mathcal{E}_{s^*})| = O(n^{-\gamma C}). \tag{17}$$

We now take log of both sides of (13) and divide by  $n^{d-1}$  to obtain

$$\begin{aligned} & \frac{-\log Z_{B_{an}} + |B_{an}| \mathcal{P}(d, H, h)}{n^{d-1}} \\ &= \frac{|B_{an}|}{n^{d-1}} \mathcal{P}(d, H, h) + \frac{|B_{an}|}{n^{d-1}} dH(s^*, s^*) - A(a)H(s^*, s^*) + \frac{|B_{an}|}{n^{d-1}} h(s^*) + o(1) \\ &+ n^{-d+1} \sum_{v \in B_{an}^o} \log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \\ &+ n^{-d+1} \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} \sum_{v \in B_{an,j,k,+}} \log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \\ &+ n^{-d+1} \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} \sum_{v \in B_{an,j,k,-}} \log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \end{aligned}$$

Here we use (14) and the fact  $\mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \geq c^* > 0$  for all  $v$ . Applying (15)

$$\begin{aligned} & \sum_{v \in B_{an}^o} \log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) \\ &= |B_{an}^o| \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) + |B_{an}^o| O(n^{-\gamma C}) \\ &= |B_{an}| \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*}) \\ &\quad \times \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} (|B_{an,j,k,+}| + |B_{an,j,k,-}|) + o(n^{d-1}), \end{aligned}$$

where we used (14) in the last inequality and assume that  $C > 1/\gamma$ . Using the established identity (6) we conclude

$$\begin{aligned} & \frac{-\log Z_{B_{an}} + |B_{an}| \mathcal{P}(d, H, h)}{n^{d-1}} \\ &= -A(a)H(s^*, s^*) \\ &\quad + n^{-d+1} \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} \sum_{v \in B_{an,j,k,+}} (\log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})) \end{aligned}$$

$$\begin{aligned}
 &+ n^{-d+1} \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} \sum_{v \in B_{an,j,k,-}} (\log \mathbb{P}_{B_{an}}(\sigma_v = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})) \\
 &+ o(1)
 \end{aligned}$$

Further applying (16) and (17) and using  $C > 1/\gamma$ , we obtain the following expression

$$\begin{aligned}
 &-A(a)H(s^*, s^*) \\
 &+ n^{-d+1} \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} |B_{an,j,k,+}| (\log \mathbb{P}_{\mathbb{Z}_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})) \\
 &+ n^{-d+1} \sum_{1 \leq j \leq d} \sum_{k \leq C \log n} |B_{an,j,k,-}| (\log \mathbb{P}_{\mathbb{Z}_{j,-k,-}^d}(\sigma_0 = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})) \\
 &+ o(1)
 \end{aligned}$$

We have

$$\begin{aligned}
 |B_{an,j,k,+}| &= A_j(a)n^{d-1} + o(n^{d-1}), \\
 |B_{an,j,k,-}| &= A_j(a)n^{d-1} + o(n^{d-1}).
 \end{aligned}$$

The resulting expression is then

$$\begin{aligned}
 &-A(a)H(s^*, s^*) \\
 &+ \sum_{1 \leq j \leq d} A_j(a) \sum_{k \leq C \log n} (\log \mathbb{P}_{\mathbb{Z}_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})) \\
 &+ \sum_{1 \leq j \leq d} A_j(a) \sum_{k \leq C \log n} (\log \mathbb{P}_{\mathbb{Z}_{j,-k,-}^d}(\sigma_0 = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})) \\
 &+ o(1)
 \end{aligned}$$

Applying the exponential SSM property and the Taylor expansion, we have for every  $k \geq C \log n$

$$\begin{aligned}
 &|\log \mathbb{P}_{\mathbb{Z}_{j,k,+}^d}(\sigma_0 = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})| \leq \kappa \exp(-\gamma k) \\
 &|\log \mathbb{P}_{\mathbb{Z}_{j,-k,-}^d}(\sigma_0 = s^* | \mathcal{E}_{v,s^*}) - \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})| \leq \kappa \exp(-\gamma k).
 \end{aligned}$$

This means that we can replace the sums  $\sum_{k \leq C \log n}$  with infinite sums  $\sum_{k \geq 0}$ , with a resulting error  $O(\exp(-\gamma C \log n) = O(n^{-\gamma C})$ . Dividing by  $A(a)$  we obtain the result.  $\square$

### 3.2 Extensions and Variations

In this subsection we establish several variations of the first part of Theorem 1, namely the representation (6) of the free energy in terms of the marginal probability. First we extend identity (6) for the case when we do not necessarily have SSM, but instead have an upper or lower bound on marginal probability  $\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})$ . In this case we obtain an analogue of (6) in the form of inequalities. These inequalities will be useful for obtaining numerical bounds on free energy for hard-core model in dimensions  $d = 3, 4$  in Sect. 4.

Given  $r > 0$  consider an arbitrary spin assignment  $(s_u) \in \chi^{|\partial B_r|}$  which is consistent with the event  $\mathcal{E}_{s^*}$ . Namely,  $s_u = s^*$  for all  $u \succ 0, u \in \partial B_r$ . Let  $p_{\max}(r)$  ( $p_{\min}(r)$ ) be the maximum (minimum) of  $\mathbb{P}_{B_r}(\sigma_0 = s^* | \mathcal{E}_{s^*})$  when we vary over all such assignments.

**Corollary 1** For every  $(\mathbb{Z}^d, H, h)$  and  $r \geq 0$

$$\begin{aligned}
 -\log p_{\max}(r) - dH(s^*, s^*) - h(s^*) &\leq \mathcal{P}(d, H, h) \\
 &\leq -\log p_{\min}(r) - dH(s^*, s^*) - h(s^*). \quad (18)
 \end{aligned}$$

While the result holds for arbitrary  $r$  the quality of the bounds presumably improves with increasing  $r$ . We will see in Sect. 4 that in some cases  $p_{\max}(r)$  and  $p_{\min}(r)$  are fairly close for large  $r$  even though the model is outside of provably exponential SSM regime.

*Proof* The proof is a minor variation of the proof of (6). Instead of estimate (10) we use  $p_{\min}(r) \leq \mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v, s^*}) \leq p_{\max}(r)$  for every  $n > r$ . □

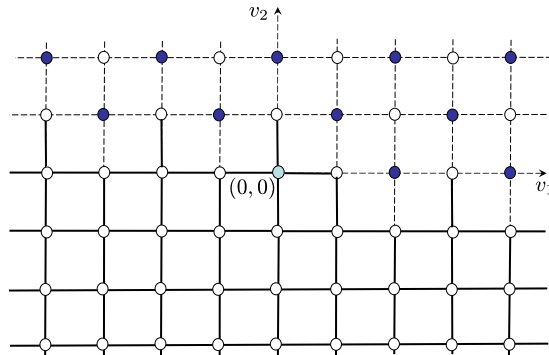
Our second variation is a “chess-pattern” version of Theorem 1 where in representation (9) we sequentially remove only vertices with even sum of coordinates. As it turns out this version provides substantial gains in computing numerical estimates of free energy both for hard-core and monomer-dimer models, though we do not have a theoretical explanation for this gain.

Let  $\mathbb{Z}_{\text{even}}^d = \{v = (v_1, \dots, v_d) \in \mathbb{Z}^d : \sum_i v_i \text{ is even}\}$ . Similarly define  $\mathbb{Z}_{\text{odd}}^d$ . Given a subgraph  $\mathbb{G} = (V, E)$  of  $\mathbb{Z}^d$ , let  $\mathcal{E}_{v, s, \text{even}}$  denote the event  $\sigma_u = s, \forall u \succ v, u \in V \cap \mathbb{Z}_{\text{even}}^d$ . The special case  $v = 0$  is denoted by  $\mathcal{E}_{s, \text{even}}$ . See Fig. 4 for this chess-pattern version of the event  $\mathcal{E}_{s^*}$ .

**Theorem 2** Suppose  $(\mathbb{Z}^d, H, h)$  satisfies the SSM property and the Assumption 1 holds. Then

$$\mathcal{P}(d, H, h) = -\frac{1}{2} \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*, \text{even}}) + \frac{1}{2} \log \left( \sum_{s \in \chi} \exp(-2dH(s, s^*) - h(s)) \right). \quad (19)$$

**Fig. 4** Event  $\mathcal{E}_{s^*, \text{even}}$  on  $\mathbb{Z}^2$ . Every dark node is assigned spin  $s^*$



*Proof* Let  $B_{n,\text{even}} = B_n \cap \mathbb{Z}_{\text{even}}^d$ . Observe that every node  $v \in B_n \setminus B_{n,\text{even}}$  has only neighbors in  $B_{n,\text{even}}$ . Let  $\Delta(v)$  denote the degree of  $v$  in  $B_n$ . As a result,

$$\mathbb{P}_{B_n}(\sigma_v = s^*, \forall v \in B_{n,\text{even}}) = Z_{B_n}^{-1} \prod_{v \in B_n \setminus B_{n,\text{even}}} \sum_{s \in \chi} \exp(-\Delta(v)H(s, s^*) - h(s)),$$

from which we obtain

$$Z_{B_n}^{-1} = \prod_{v \in B_n \setminus B_{n,\text{even}}} \left( \sum_{s \in \chi} \exp(-\Delta(v)H(s, s^*) - h(s)) \right)^{-1} \mathbb{P}_{B_n}(\sigma_v = s^*, \forall v \in B_{n,\text{even}}).$$

On the other hand, by telescoping property

$$\begin{aligned} \mathbb{P}_{B_n}(\sigma_v = s^*, \forall v \in B_{n,\text{even}}) &= \prod_{v \in B_{n,\text{even}}} \mathbb{P}_{B_n}(\sigma_v = s^* | \sigma_u = s^*, \forall u \succ v, u \in B_{n,\text{even}}) \\ &= \prod_{v \in B_{n,\text{even}}} \mathbb{P}_{B_n}(\sigma_v = s^* | \mathcal{E}_{v,s^*,\text{even}}). \end{aligned} \tag{20}$$

The remainder of the proof is very similar to the proof of Theorem 1 and details are omitted. Notice that for  $|B_n| - o(|B_n|)$  nodes in  $B_n$ , the degree  $\Delta(v) = 2d$ . Then in place of (12) we obtain

$$\begin{aligned} \lim_n \frac{\log Z_{B_n}^{-1}}{|B_n|} &= - \lim_{n \rightarrow \infty} \frac{|B_n \setminus B_{n,\text{even}}|}{|B_n|} \log \left( \sum_{s \in \chi} \exp(-2dH(s, s^*) - h(s)) \right) \\ &\quad + \lim_{n \rightarrow \infty} \frac{|B_{n,\text{even}}|}{|B_n|} \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*,\text{even}}) \\ &= -\frac{1}{2} \log \left( \sum_{s \in \chi} \exp(-2dH(s, s^*) - h(s)) \right) \\ &\quad + \frac{1}{2} \log \mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*,\text{even}}). \end{aligned} \quad \square$$

Now let us present a version of Theorem 1 for the model (2) where spins are assigned to edges rather than nodes. We need this for application to the monomer-dimer model. Let  $\mathcal{E}_{v,s,\text{edges}}$  denote the event  $\sigma_{u,w} = s, \forall u \succ v, w \in N(u)$ , and let  $\mathcal{E}_{v,s,\text{edges,even}}$  denote the event  $\sigma_{u,w} = s, \forall u \succ v, u \in \mathbb{Z}_{\text{even}}^d, w \in N(u)$ . Let  $\mathcal{E}_{s,\text{edges}}, \mathcal{E}_{s,\text{edges,even}}$  denote the same events when  $v = 0$ .

**Theorem 3** Consider a model  $(\mathbb{Z}^d, H, h)$  given by (2) with spins assigned to edges. Suppose  $(\mathbb{Z}^d, H, h)$  satisfies the SSM property and the Assumption 1 holds. Then

$$\begin{aligned} \mathcal{P}(d, H, h) &= -\log \mathbb{P}(\sigma_{(0,v)} = s^*, \forall v \in N(0) | \mathcal{E}_{s^*,\text{edges}}) \\ &\quad - d(2d - 1)H(s^*, s^*) - dh(s^*) \end{aligned} \tag{21}$$

$$\begin{aligned} &= -\frac{1}{2} \log \mathbb{P}(\sigma_{(0,v)} = s^*, \forall v \in N(0) | \mathcal{E}_{s^*,\text{edges,even}}) \\ &\quad - d(2d - 1)H(s^*, s^*) - dh(s^*). \end{aligned} \tag{22}$$

*Remark* Contrast this result with Theorem 2. There the extra term  $\log(\sum_{s \in \chi} \cdot)$  appears since every odd node surrounded by even nodes with preset spin value  $s^*$  still has  $\chi$  choices for the spin selection. For the edge version this is not the case: all edges are preselected to take spin values  $s^*$ .

*Proof* We first prove (21). Let  $E(B_n)$  denote the edge set of  $B_n$ . Note that  $E(B_n) = d|B_n| + o(|B_n|)$  and the number of edges with  $4d - 2$  incident edges is also  $d|B_n| + o(|B_n|)$ . The number of pairs of incident edges is then  $d(2d - 1)|B_n| + o(|B_n|)$ . We have

$$\begin{aligned} &\mathbb{P}_{B_n}(\sigma_e = s^*, \forall e \in E(B_n)) \\ &= Z_{B_n}^{-1} \exp(-d(2d - 1)|B_n|H(s^*, s^*) - o(|B_n|)H(s^*, s^*) - d|B_n|h(s^*)). \end{aligned}$$

On the other hand, by telescoping property

$$\begin{aligned} &\mathbb{P}_{B_n}(\sigma_e = s^*, \forall e \in E(B_n)) \\ &= \prod_{v \in B_n} \mathbb{P}_{B_n}(\sigma_{(v,u)} = s^*, \forall u \in N(v) | \sigma_{(u,w)} = s^*, \forall u \succ v, w \in N(u), u, w \in B_n) \\ &= \prod_{v \in B_n} \mathbb{P}_{B_n}(\sigma_{(v,u)} = s^*, \forall u \in N(v) | \mathcal{E}_{v,s^*,\text{edges}}). \end{aligned}$$

The remainder of the proof of (21) is similar to the one of Theorem 1 and is omitted.

Turning to (22), observe that every edge in  $\mathbb{Z}^d$  has exactly one end point in  $\mathbb{Z}_{\text{even}}^d$ . Then we have again by the telescoping property

$$\begin{aligned} &\mathbb{P}_{B_n}(\sigma_e = s^*, \forall e \in E(B_n)) \\ &= \prod_{v \in B_{n,\text{even}}} \mathbb{P}_{B_n}(\sigma_{(v,u)} = s^*, \forall u \in N(v) | \sigma_{(u,w)} = s^*, \\ &\quad \forall u \succ v, w \in N(u), u \in B_{n,\text{even}}, w \in B_n) \\ &= \prod_{v \in B_{n,\text{even}}} \mathbb{P}_{B_n}(\sigma_{(v,u)} = s^*, \forall u \in N(v) | \mathcal{E}_{v,s^*,\text{edges,even}}). \end{aligned}$$

The remainder of the proof of (21) is similar to the one of Theorem 1. The fact  $|B_{n,\text{even}}|/|B_n| \rightarrow 1/2$  as  $n \rightarrow \infty$  leads to a factor 1/2 in (22). □

### 3.3 Applications and the Numerical Complexity

Theorem 1 reduces the problem of computing  $\mathcal{P}$  and  $s\mathcal{P}$  to the problem of computing conditional marginal probabilities  $\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})$ . This is certainly not the only way to represent free energy and surface pressure in terms of marginal probabilities. For example, consider a modified system  $(\mathbb{G}, \beta H, \beta h)$  on a finite graph  $\mathbb{G}$ , and observe that

$$\frac{d \log Z_{\mathbb{G}}}{d\beta} = - \sum_{v \in V} \mathbb{E}[h(\sigma_v)] - \sum_{(v,u) \in E} \mathbb{E}[H(\sigma_v, \sigma_u)],$$



both expectations are taken wrt the Gibbs measure  $\mathbb{P}$ . Thus knowing the marginal probabilities  $\mathbb{P}(\sigma_v)$  and joint probabilities  $\mathbb{P}(\sigma_v, \sigma_u)$ ,  $(v, u) \in E$  lets us recover  $\log Z_{\mathbb{G}}$  approximately in principle. Unfortunately, this means we have to integrate the answers over  $\beta \in [0, 1]$ , which in practice has to be approximated by summation. In order then to guarantee the target level of accuracy, one would have to control the derivatives of marginal probabilities wrt  $\beta$ . Additionally, one would have to compute marginal probabilities for a whole range of  $\beta$ , over which the integration takes place. The advantage of the representation (6) and (7) is that it allows us computing free energy and surface pressure by computing *only one* marginal probability  $\mathbb{P}(\sigma_0 = s^* | \mathcal{E}_{s^*})$ . In this paper we will compute these marginal quantities approximately using recent deterministic algorithms for computing such marginal probabilities in general graphs, where appropriately defined computation tree (see following sections) satisfies exponential SSM. As we will see below, when we have such a property, our method provides an additive  $\epsilon$  approximation of free energy in time  $(1/\epsilon)^{O(1)}$ , where the constant  $O(1)$  may depend on the model parameters and  $d$ . Let us now compare this performance with the performance of the transfer matrix method. While we are not aware of any systematic numerical complexity analysis of the transfer matrix method, it can be deduced from the following considerations. The transfer matrix method is based on first computing the partition function on a strip  $[-n, n]^{d-1} \times \mathbb{Z}$ . The latter is done by constructing certain  $|\chi|^{(2n+1)^{d-1}}$  by  $|\chi|^{(2n+1)^{d-1}}$  transfer matrix. For the hard-core case with  $\lambda = 1$  (see Sect. 4) the matrix is  $0 - 1$  with 1 corresponding to allowed pair of neighboring configurations and 0 corresponding to pairs of configurations which are not allowed. The spectral radius of the transfer matrix is then used to deduce the growth rate of the partition function, namely the free energy. Constructing such matrix takes time  $\exp(O(n^{d-1}))$ . Since the partition function on  $[-n, n]^{d-1} \times \mathbb{Z}$  converges to the one of  $\mathbb{Z}^d$  at the rate  $O(1/n)$  [31], then in order to achieve an additive error  $\epsilon > 0$ , one needs  $\exp(O((1/\epsilon)^{d-1}))$  computation effort.

Suppose one then wishes to use this method to approximate the surface pressure with an additive error  $\epsilon$ . What is the required numerical effort? We are not aware of applications of the transfer matrix method for computing surface pressure. Thus the reasonable alternative approach is to (1) select a rectangle  $an$  for some large value  $n$ , (2) Compute the partition function  $Z_{an}$  in this rectangle using perhaps the brute force method and (3) Compute the approximation  $\hat{P}$  of the free energy  $\mathcal{P}$  using perhaps the transfer matrix method. The approximate surface pressure is then obtained from the fact that the convergence rate in the limit (4) is  $O(1/n)$  [31]. Let us show that this approach requires  $\exp(O((1/\epsilon)^{2d-2}))$  numerical effort in order to obtain  $\epsilon$  additive approximation, regardless of how quickly one is able to compute  $Z_{an}$ . Indeed, observe that this approach leads to an error  $n^d |\hat{P} - \mathcal{P}|/n^{d-1} = n |\hat{P} - \mathcal{P}|$ . Thus for the target  $\epsilon$  additive error, we need to set  $n \geq 1/\epsilon$ . But this further requires that  $(1/\epsilon) |\hat{P} - \mathcal{P}| = O(\epsilon)$ , namely  $|\hat{P} - \mathcal{P}| = O(\epsilon^2)$ . Thus we need to achieve  $\epsilon^2$  additive error accuracy in estimating the free energy. This requires  $\exp(O((1/\epsilon)^{2d-2}))$  per our earlier calculations, and the assertion is established. This is a stark contrast with complexity  $(1/\epsilon)^{O(1)}$  of the method proposed in this paper both for free energy and surface pressure for the cases of hard-core and monomer-dimer models. However, one should note that our method takes explicit advantage of the exponential SSM, while the transform matrix method does not rely on this assumption.

### 4 Hard-Core (Independent Set) Model

The hard-core lattice gas model, commonly known as independent set model in combinatorics, is given by  $\chi = \{0, 1\}$ ,  $H(0, 0) = H(0, 1) = H(1, 0) = 0$ ,  $H(1, 1) = \infty$ ,  $h(0) =$

$0, h(1) = \beta$  for some parameter  $\beta$ . Case of interest is  $\beta \leq 0$  as it corresponds to Gibbs measure putting larger weight on larger cardinality independent set. Choosing  $s^* = 0$  we obtain that Assumption 1 holds.

It is common to set  $\lambda = \exp(-\beta) > 0$  and let  $\lambda$  be the parameter of the hard-core model. This parameter is usually called *activity*. Note that in terms of  $\lambda$ , for every finite graph  $\mathbb{G}$

$$Z_{\mathbb{G}} = \sum \lambda^{|\{v \in V: \sigma_v=1\}|} \tag{23}$$

where the sum is over all spin configurations  $(\sigma_v) \in \{0, 1\}^V$  such that  $\sigma_v \sigma_u = 0$  for all  $(v, u) \in E$ . Equivalently, a subset of nodes  $I \subset V(\mathbb{G})$  is called an independent (also sometimes called a stable set) if for no edge  $(u, v)$  we have both  $u$  and  $v$  belong to  $I$ . Then we may rewrite (23) as

$$Z_{\mathbb{G}} = \sum_I \lambda^{|I|} \tag{24}$$

where the summation is over all independent sets of  $\mathbb{G}$ . The summation in (24) is sometimes called an independent set polynomial in the combinatorics literature. From now on we let  $I$  denote the random independent set selected according to a Gibbs measure (multiply defined if there are many Gibbs measures). In the case of finite graph  $\mathbb{G}$ , for every independent set  $I$  we have

$$\mathbb{P}_{\mathbb{G}}(I = I) = Z_{\mathbb{G}}^{-1} \lambda^{|I|}.$$

The special case  $\lambda = 1$  corresponds to a uniform distribution on the set of all independent sets in  $\mathbb{G}$ . We denote the free energy and surface pressure on  $\mathbb{Z}^d$  by  $\mathcal{P}(d, \lambda)$  and  $s\mathcal{P}(d, \lambda, a)$ , respectively. In the special case  $\lambda = 1$ , the free energy is also the entropy of the Gibbs distribution, since it is uniform. Conditioning on spins taking value  $s^* = 0$  simplifies significantly in the context of hard-core model as the following proposition shows, a simple proof of which we include for completeness.

**Proposition 1** *If a hard-core model on a graph  $\mathbb{G} = (V, E)$  satisfies SSM for some  $\lambda$ , then so does any subgraph of  $\mathbb{G}$ . The same assertion applies to exponential SSM. Moreover, for every  $W_1, W_2 \subset V(\mathbb{G})$  the following identity holds with respect to the unique Gibbs measure.*

$$\mathbb{P}_{\mathbb{G}}(v \in I | W_1 \cap I = \emptyset, W_2 \subset I) = \mathbb{P}_{\hat{\mathbb{G}}}(v \in I), \tag{25}$$

for every  $v \in V \setminus (W_1 \cup B_1(W_2))$ , where  $\hat{\mathbb{G}}$  is the subgraph induced by nodes in  $V \setminus (W_1 \cup B_1(W_2))$ .

*Proof* Fix any positive integer  $r$  and consider any spin assignment  $(s_u), u \in \partial B_r(v) \setminus (W_1 \cup B_1(W_2))$ . Extend this to a spin assignment to entire  $\partial B_r(v)$  by setting  $s_u = 1$  (that is  $u \in I$ ), for  $u \in \partial B_r(v) \cap W_2$  and  $s_u = 0$  (that is  $u \notin I$ ) for  $u \in \partial B_r(v) \cap (W_1 \cup (B_1(W_2) \setminus W_2))$ . Call this spin assignment  $\mathcal{S}$ . Applying spatial Markovian property we have

$$\begin{aligned} &\mathbb{P}_{\mathbb{G}}(\sigma_v = 0 | \sigma_u = 0, u \in W_1, \sigma_u = 1, u \in W_2, \mathcal{S}) \\ &= \frac{\mathbb{P}_{\mathbb{G}}(\sigma_v = 0, \sigma_u = 0, u \in W_1, \sigma_u = 1, u \in W_2, | \mathcal{S})}{\mathbb{P}_{\mathbb{G}}(\sigma_u = 0, u \in W_1, \sigma_u = 1, u \in W_2 | \mathcal{S})} \\ &= \frac{\sum_{I \in \mathcal{I}_1} \lambda^{|I|}}{\sum_{I \in \mathcal{I}_2} \lambda^{|I|}}, \end{aligned}$$

where  $\mathcal{I}_1$  is the set of independent sets in  $B_r(v)$  such that  $v \notin I, I \cap W_1 = \emptyset, W_2 \subset I$  and  $u \in I \cap \partial B_r(v)$  iff  $s_u = 1$  (according to  $\mathcal{S}$ ). The set  $\mathcal{I}_2$  is defined similarly, except the condition  $v \notin I$  is dropped. Then the ratio is equal to

$$\frac{\sum_{I \in \mathcal{I}_1} \lambda^{|I|-|W_2|}}{\sum_{I \in \mathcal{I}_2} \lambda^{|I|-|W_2|}} = \frac{\sum_{I \in \mathcal{I}_3} \lambda^{|I|}}{\sum_{I \in \mathcal{I}_4} \lambda^{|I|}}$$

where  $\mathcal{I}_4$  is the set of independent subsets of  $B_r(0) \setminus (W_1 \cup B_1(W_2))$  such that  $u \in I \cap \partial B_r(v)$  iff  $s_u = 1$ , and  $\mathcal{I}_3$  is defined similarly, except in addition  $v \notin I$  for every  $I \in \mathcal{I}_3$ . We recognize this ratio as  $\mathbb{P}_{\hat{\mathbb{G}}}(\sigma_v = 0 | \mathcal{S})$ . We conclude

$$\mathbb{P}_{\mathbb{G}}(\sigma_v = 0 | \sigma_u = 0, u \in W_1, \sigma_u = 1, u \in W_2, \mathcal{S}) = \mathbb{P}_{\hat{\mathbb{G}}}(\sigma_v = 0 | \mathcal{S}).$$

Now consider any induced subgraph  $\mathbb{G}_1$  of  $\mathbb{G}$  and any two sets  $W_1, W_2$  in  $\mathbb{G}_1$ . Applying a similar argument we obtain

$$\begin{aligned} &\mathbb{P}_{\mathbb{G}_1}(\sigma_v = 0 | \sigma_u = 0, u \in W_1, \sigma_u = 1, u \in W_2, \mathcal{S}) \\ &= \mathbb{P}_{\mathbb{G}}(\sigma_v = 0 | \sigma_u = 0, u \in W_1 \cup (V \setminus V_1), \sigma_u = 1, u \in W_2, \mathcal{S}) \\ &= \mathbb{P}_{\hat{\mathbb{G}}_1}(\sigma_v = 0 | \mathcal{S}) \end{aligned}$$

where  $\hat{\mathbb{G}}_1$  is induced by nodes  $V_1 \setminus (W_1 \cup B_1(W_2))$ . By SSM property, the second quantity has a limit as  $r \rightarrow \infty$  which is independent from assignment  $\mathcal{S}$  on the boundary  $\partial B_r(v)$ . Therefore the same applies to the first and third quantities. The first conclusion implies that  $\mathbb{G}_1$  satisfies SSM. The second conclusion gives (25) when applied to  $\mathbb{G}_1 = \mathbb{G}$ . □

In light of Proposition 1 we obtain the following simplification of Theorems 1 and 2 in the hard-core case. Let

$$\mathbb{Z}_{<0, \text{even}}^d = \mathbb{Z}_{<0}^d \cup \{u \in \mathbb{Z}_{\text{odd}}^d : 0 < u\},$$

see Fig. 4.

**Corollary 2** *Suppose the hard-core model on  $\mathbb{Z}^d$  satisfies SSM for a given  $\lambda$ . Then*

$$\mathcal{P}(d, \lambda) = -\log \mathbb{P}_{\mathbb{Z}_{<0}^d}(0 \notin I) \tag{26}$$

$$= -\frac{1}{2} \log \mathbb{P}_{\mathbb{Z}_{<0, \text{even}}^d}(0 \notin I) + \frac{1}{2} \log(1 + \lambda). \tag{27}$$

Thus we now focus on developing an algorithm for numerically estimating marginal probabilities appearing in (26) and (27).

#### 4.1 Recursion, Sequential Cavity Algorithm and Correlation Decay

Let us now introduce a recursion satisfied by the hard-core model. This identity in a different form using a self-avoiding tree construction was established recently by Weitz [34]. We repeat here some of the developments in [34], with some minor modifications, which are indicated as necessary.

**Theorem 4** Given a finite graph  $\mathbb{G} = (V, E)$  and  $v \in V$ , let  $N(v) = \{v_1, \dots, v_k\}$ . Then

$$\mathbb{P}_{\mathbb{G}}(v \notin I) = \frac{1}{1 + \lambda \prod_{1 \leq i \leq k} \mathbb{P}_{\mathbb{G}_{i-1}}(v_i \notin I)} \tag{28}$$

where  $\mathbb{G}_i$  is the graph induced by  $V \setminus \{v, v_1, \dots, v_i\}$ ,  $\mathbb{G}_0$  is induced by  $V \setminus \{v\}$  and  $\prod_{1 \leq i \leq k} 1 = 1$  when  $k = 0$ .

*Proof* We have

$$Z_{\mathbb{G}} = \sum_{I: v \notin I} \lambda^{|I|} + \sum_{I: v \in I} \lambda^{|I|} = \sum_{I: I \subset V \setminus \{v\}} \lambda^{|I|} + \lambda \sum_{I: I \subset V \setminus \{v, v_1, \dots, v_k\}} \lambda^{|I|} \tag{29}$$

where everywhere the sums are over independent sets  $I$ . Note that  $\sum_{I: I \subset V \setminus \{v\}} \lambda^{|I|} = Z_{\mathbb{G}_0}$  and  $\sum_{I: I \subset V \setminus \{v, v_1, \dots, v_k\}} \lambda^{|I|} = Z_{\mathbb{G}_k}$ . Dividing both sides of the identity (29) by  $Z_{\mathbb{G}_0}$  we obtain

$$\frac{Z_{\mathbb{G}}}{Z_{\mathbb{G}_0}} = 1 + \lambda \frac{Z_{\mathbb{G}_k}}{Z_{\mathbb{G}_0}}$$

It is immediate that  $Z_{\mathbb{G}_0}/Z_{\mathbb{G}} = \mathbb{P}_{\mathbb{G}}(v \notin I)$ . In order to interpret  $Z_{\mathbb{G}_k}/Z_{\mathbb{G}_0}$  similarly we rewrite it as

$$\frac{Z_{\mathbb{G}_k}}{Z_{\mathbb{G}_0}} = \prod_{i=1}^k \frac{Z_{\mathbb{G}_i}}{Z_{\mathbb{G}_{i-1}}}$$

and note that  $Z_{\mathbb{G}_i}/Z_{\mathbb{G}_{i-1}} = \mathbb{P}_{\mathbb{G}_{i-1}}(v_i \notin I)$ . Combining these observations we obtain (28).  $\square$

The identity (28) suggests a recursion for computing marginal probabilities  $\mathbb{P}_{\mathbb{G}}(v \notin I)$  approximately. The idea is to apply the identity recursively several times and then set the initial values arbitrarily. One then establishes further that a correlation decay property holds on this recursion which implies that any initialization of the values at the beginning of the recursion leads to approximately correct values at the end of the recursion. This principle was underlying the algorithm proposed in [34] for computing approximately the number of independent sets in general graphs. The original approach taken in [34] was slightly different—first a self-avoiding tree corresponding to the recursive computation tree described above is constructed. Then it is shown that  $\mathbb{P}(v \notin I)$  on this tree equals the same probability in the underlying graph. The approach proposed here is slightly simpler as it bypasses the extra argument of showing equivalence of two marginal probabilities.

We now provide details of this approach. Given a finite graph  $\mathbb{G}$ , for every subgraph  $\hat{\mathbb{G}} = (\hat{V}, \hat{E})$  of  $\mathbb{G}$ , every vertex  $v \in \hat{V}$  and every  $t \in \mathbb{Z}_+$  we introduce a quantity  $\Phi_{\hat{\mathbb{G}}}(v, t)$  defined inductively as follows.

$$\Phi_{\hat{\mathbb{G}}}(v, t) = \begin{cases} 1, & t = 0; \\ (1 + \lambda)^{-1}, & t > 0, N(v) = \emptyset, \\ (1 + \prod_{1 \leq i \leq k} \Phi_{\hat{\mathbb{G}}_{i-1}}(v_i, t - 1))^{-1}, & t > 0, N(v) = \{v_1, \dots, v_k\} \neq \emptyset. \end{cases} \tag{30}$$

Here again  $\hat{\mathbb{G}}_0$  is induced by  $\hat{V} \setminus \{v\}$  and  $\hat{\mathbb{G}}_i$  is induced by  $\hat{V} \setminus \{v, v_1, \dots, v_i\}$ . The recursion (30) is naturally related to the identity (28). Specifically if  $\Phi_{\hat{\mathbb{G}}_{i-1}}(v_i, t - 1) = \mathbb{P}_{\hat{\mathbb{G}}_{i-1}}(v_i \notin I)$  for all  $i$  then  $\Phi_{\hat{\mathbb{G}}}(v, t) = \mathbb{P}_{\hat{\mathbb{G}}}(v \notin I)$ . However, this will not occur in general, as we set

$\Phi_{\hat{\mathbb{G}}}(v, 0) = 1$ , due to the lack of knowledge of actual values of the corresponding probabilities.

Similarly to  $\Phi$ , we introduce values  $\Psi_{\hat{\mathbb{G}}}(v, t)$  with the only exception that  $\Psi_{\hat{\mathbb{G}}}(v, 0) = 0$  for all  $\hat{\mathbb{G}} = (\hat{V}, \hat{E})$  and  $v \in \hat{V}$ . The following lemma follows from Theorem 4 and the definitions of  $\Phi$  and  $\Psi$  using a simple induction argument

**Lemma 1** *For every  $v$  and  $t \in \mathbb{Z}_+$*

$$\begin{aligned} \Psi_{\mathbb{G}}(v, 2t) &\leq \mathbb{P}_{\mathbb{G}}(v \notin I) \leq \Phi_{\mathbb{G}}(v, 2t), \\ \Phi_{\mathbb{G}}(v, 2t + 1) &\leq \mathbb{P}_{\mathbb{G}}(v \notin I) \leq \Psi_{\mathbb{G}}(v, 2t + 1) \end{aligned}$$

Next we provide bounds on the computational effort required to compute  $\Phi$  and  $\Psi$ .

**Lemma 2** *For every finite graph  $\mathbb{G}$  with degree  $\leq \Delta$ ,  $v \in \mathbb{G}$  and  $t$ , the values  $\Phi_{\mathbb{G}}(v, t)$ ,  $\Psi_{\mathbb{G}}(v, t)$  can be computed in time  $\exp(O(t \log \Delta))$ , where the constant in  $O(\cdot)$  is universal.*

*Proof* The result follows immediately from the recursive definitions of  $\Phi$  and  $\Psi$ . □

The crucial correlation decay property is formulated in the following proposition.

**Theorem 5** ([34]) *For every  $\Delta \geq 3$  and for every*

$$\lambda < (\Delta - 1)^{\Delta-1} / (\Delta - 2)^{\Delta}, \tag{31}$$

*there exists  $\rho = \rho(\lambda, \Delta) < 1$  such that for every finite graph  $\mathbb{G} = (V, E)$  with degree at most  $\Delta$  and every  $v \in V, t \in \mathbb{Z}_+$ :*

$$|\log \Phi_{\mathbb{G}}(v, t) - \log \Psi_{\mathbb{G}}(v, t)| \leq \log(1 + \lambda)\rho^t. \tag{32}$$

*As a result,  $\mathbb{G}$  satisfies exponential SSM for  $\lambda$  satisfying (31).*

*Proof* The details of the proof can be found in [34]. It is shown there that the absolute value in (32) is upper bounded by the same quantity, when applied to  $\mathbb{G} = \mathbb{T}_{\Delta,t}$ —the  $\Delta$ -regular depth- $t$  tree. Then a classical results by Spitzer [32] and Kelly [24] are invoked to show the existence of  $\rho$ . The existence of  $\rho$  then implies SSM via Proposition 1 and observing that changing values of  $\sigma$  for nodes  $u$  which have distance bigger than  $t$  from a given node  $v$ , does not affect the values of  $\Phi_{\mathbb{G}}(v, t)$  and  $\Psi_{\mathbb{G}}(v, t)$ . □

#### 4.2 Free Energy and Surface Pressure on $\mathbb{Z}^d$ . Numerical Results

We are now equipped to obtain bounds on the free energy and the surface pressure for the hard-core model on  $\mathbb{Z}^d$ .

Denote by  $\Phi(t)$  and  $\Psi(t)$  the values of  $\Phi_{\mathbb{G}}(v, t)$ ,  $\Psi_{\mathbb{G}}(v, t)$  when applied to a graph  $\mathbb{G} = \mathbb{Z}_{>0}^d \cap B_n$ , for sufficiently large  $n$  and  $v = 0$ . Observe that the values  $\Phi_{\mathbb{G}}(v, t)$ ,  $\Psi_{\mathbb{G}}(v, t)$  are the same for all values of  $n$  sufficiently larger than  $t$  (for example  $n \geq t + 1$  suffices). Thus the notations are justified. The following relations are the basis for computing bounds on the free energy and surface pressure.

**Corollary 3** For every  $t \in \mathbb{Z}_+$  and  $\lambda$  satisfying (31)

$$-\log \Phi(2t) \leq \mathcal{P}(d, \lambda) \leq -\log \Psi(2t), \tag{33}$$

$$-\log \Psi(2t + 1) \leq \mathcal{P}(d, \lambda) \leq -\log \Phi(2t + 1). \tag{34}$$

*Proof* By Theorem 5 we have exponential SSM. Thus

$$\mathbb{P}_{\mathbb{Z}_{<0}^d} (0 \notin I) = \lim_{n \rightarrow \infty} \mathbb{P}_{B_n \cap \mathbb{Z}_{<0}^d} (0 \notin I).$$

$B_n \cap \mathbb{Z}_{<0}^d$  is finite graph for which bounds from Lemma 1 are applicable. □

Our algorithm for computing  $\mathcal{P}(d, \lambda)$  and  $s\mathcal{P}(\mathbb{Z}^d, \lambda)$  is based on relations (33) and (34), and will be called *Sequential Cavity Algorithm* or shortly SCA.

We have numerically computed values  $\Phi(t), \Psi(t)$  for the cases  $d = 2, 3, 4$  using the chessboard pattern method. Our results provide the following bounds on the free energy for the case  $\lambda = 1$ . Since previous bounds were stated in terms of  $\exp(\mathcal{P}(d, 1))$ , we do the same here:

$$1.503034 \leq \exp(\mathcal{P}(2, 1)) \leq 1.503058,$$

$$1.434493 \leq \exp(\mathcal{P}(3, 1)) \leq 1.449698,$$

$$1.417583 \leq \exp(\mathcal{P}(4, 1)) \leq 1.444713.$$

The computations were done at the level  $t = 27$  for the case  $d = 2, t = 16$  for the case  $d = 3$  and  $t = 12$  for the case  $d = 4$ . Our bounds for the case  $d = 2$  are weaker than a more accurate estimate 1.50304808247533 first derived by Baxter [5] and recently rigorously confirmed by Friedland et al. [13]. However, we are not aware of any estimates for the cases  $d = 3, 4$  and we believe that our bounds are the best known. We have not done computations of the surface pressure and we are not aware of any previously existing benchmarks. Note that in the case  $d = 3$  we have  $\Delta = 6$ , and  $\lambda = 1$  no longer satisfies (31). Thus we have no guarantee that SCA will provide converging estimates as  $t$  increases. The correctness of our bounds for this case is guaranteed by Corollary 1. It is encouraging to see that the bounds are close and based on this fact we conjecture that  $\lambda = 1$  corresponds to the uniqueness regime.

It is instructive to compare our numerical results, which were obtained using the chess-pattern approach (identity (27)) with results which could be obtained directly from (26). The computations based on (26) for the case  $d = 2, \lambda = 1$  at depth  $t = 12$  lead to bounds  $1.0942 \leq \exp(\mathcal{P}(2, 1)) \leq 1.8377$ . At the same time, the computations using chess pattern method at the depth only  $t = 3$  already lead to a much tighter bounds  $1.4169 \leq \exp(\mathcal{P}(2, 1)) \leq 1.5565$ .

Notice, that while Theorem 5 is not used in computing actual bounds on the free energy and surface pressure, it provides the guarantee for the quality of such bounds. Let us use it now to analyze the computation effort required to obtain a particular level of accuracy in bounds.

**Proposition 2** For every  $d, \lambda < (d - 1)^{d-1} / (d - 2)^d$  and  $\epsilon > 0$  SCA produces an  $\epsilon$ -additive estimate of  $\mathcal{P}(d, \lambda)$  and  $s\mathcal{P}(\mathbb{Z}^d, \lambda)$  in time  $(\frac{1}{\epsilon})^{O(1)}$ , where the constant in  $O(\cdot)$  depends on  $\lambda$  and  $d$ .

*Proof* Applying Theorem 5, an additive error  $\epsilon$  is achieved provided that  $\log(1 + \lambda)\rho^t < \epsilon$  or  $t \geq \log(\log(1 + \lambda)/\epsilon) \log^{-1}(1/\rho) = O(\log(1/\epsilon))$ . Hence the result for free energy follows from Lemma 2.

For surface pressure observe that applying Theorem 5

$$|\log \mathbb{P}_{\mathbb{Z}_{<0}^d}(\sigma_0 = 0) - \log \mathbb{P}_{\mathbb{Z}_{j,k,+,<0}^d}(\sigma_0 = 0)| \leq (1 + \lambda)\rho^k.$$

A similar bound holds for  $\mathbb{P}_{\mathbb{Z}_{j,-k,-,<0}^d}(\sigma_0 = 0)$ . Thus if we take  $k_0$  such that  $\log(1 + \lambda)\rho^{k_0}/(1 - \rho) < \epsilon$ , then the partial sum in (7) corresponding to terms  $k \geq k_0$  is at most  $2\epsilon$ . The required  $k_0$  is  $O(\log((1 - \rho)^{-1}\epsilon^{-1} \log(1 + \lambda))/\log(1/\rho)) = O(\log(1/\epsilon))$ . For the remaining terms  $k < k_0$  we compute  $\mathbb{P}_{\mathbb{Z}_{j,k,+,<0}^d}(\sigma_0 = 0)$  and  $\mathbb{P}_{\mathbb{Z}_{j,-k,-,<0}^d}(\sigma_0 = 0)$  using SCA with accuracy  $\hat{\epsilon} = \epsilon/k_0$ . Since  $\log(1/\hat{\epsilon}) = \log(1/\epsilon) + \log \log(1/\epsilon) = O(\log(1/\epsilon))$ , the result then follows from our estimate for computing  $\mathcal{P}(d, \lambda)$ . □

### 5 Monomer-Dimer (Matching) Model

The monomer-dimer model is defined by spin values  $S = \{0, 1\}$  assigned to edges of a graph  $G = (V, E)$ . A set of edges  $M \subset E$  is a matching if no two edges in  $M$  are incident. Sometimes term partial matching is used to contrast with full matching, which is a matching with size  $|V|/2$  (namely every node is incident to an edge in the matching). The edges of  $M$  are called dimers and nodes in  $V$  which are not incident to any edge in  $M$  are called monomers. We set  $H(0, 0) = H(0, 1) = H(1, 0) = h(0) = 0, H(1, 1) = \infty, h(1) = \beta$ . The Gibbs measure is defined via (2). As in the case of hard-core model, it is convenient to introduce  $\lambda = \exp(-\beta) > 0$ . Similarly to the hard-core model we have for finite graphs  $\mathbb{G}$

$$Z_{\mathbb{G}} = \sum_M \lambda^{|M|} \tag{35}$$

were the summation is over all matchings in  $\mathbb{G}$ . The summation in (35) is called a matching polynomial in the combinatorics literature. We denote by  $\mathbf{M}$  a random matching chosen according to the Gibbs measure, when it is unique. In the case of finite graphs

$$\mathbb{P}_{\mathbb{G}}(\mathbf{M} = M) = Z_{\mathbb{G}}^{-1} \lambda^{|M|}.$$

The monomer-dimer model is a close relative of the hard-core model, even though its properties are substantially different. For example this model does not exhibit a phase transition for finite  $\lambda$  and is always in the uniqueness regime [19], though it does undergo phase transition in the pure dimer case  $\lambda = \infty$ . Moreover, it satisfies the SSM property for all activities  $\lambda$  as we shall shortly see. Corresponding analogues of Proposition 1 will be stated later once exponential SSM is asserted.

#### 5.1 Recursion, Sequential Cavity Algorithm and Correlation Decay

We now establish an analogue of (28) for the monomer-dimer model. The proof of this result can be found in [6] and is omitted. It is similar to the proof of (28). In the following, with a slight abuse of notation we write  $v \in M$  if matching  $M$  contains an edge incident to  $v$ .

**Theorem 6** [6] *For every finite graph  $\mathbb{G} = (V, E)$  and  $v \in V$*

$$\mathbb{P}_{\mathbb{G}}(v \notin \mathbf{M}) = \frac{1}{1 + \lambda \sum_{u \in N_{\mathbb{G}}(v)} \mathbb{P}_{\mathbb{G}_0}(u \notin \mathbf{M})} \tag{36}$$

where  $\mathbb{G}_0$  is induced by  $V \setminus \{v\}$  and  $\sum_{u \in N_{\mathbb{G}}(v)} = 0$  when  $v$  is an isolated node.

The further development in this subsection mirrors the one of Sect. 4.1, yet the conclusion will be different—the monomer-dimer model exhibits SSM for *all* values of  $\lambda$ . This will lead to an algorithm for computing the free energy and surface pressure for monomer-dimer model for every value  $\lambda > 0$ .

Given a finite graph  $\mathbb{G}$ , for every subgraph  $\hat{\mathbb{G}} = (\hat{V}, \hat{E})$  of  $\mathbb{G}$ , every node  $v \in \hat{\mathbb{G}}$  and every  $t \in \mathbb{Z}_+$  we introduce a quantity  $\Phi_{\hat{\mathbb{G}}}(v, t)$  defined inductively as follows. In the context of monomer-dimer model this quantity stands for (approximate) probability that  $v \notin \mathbf{M}$  in the subgraph  $\hat{\mathbb{G}}$ .

$$\Phi_{\hat{\mathbb{G}}}(v, t) = \begin{cases} 1, & t = 0 \text{ or } N(v) = \emptyset; \\ (1 + \lambda \sum_{1 \leq i \leq k} \Phi_{\mathbb{G}_0}(v_i, t - 1))^{-1}, & \\ t > 0 \text{ and } N(v) = \{v_1, \dots, v_k\} \neq \emptyset. \end{cases} \tag{37}$$

Here  $\hat{\mathbb{G}}_0$  is induced by  $\hat{V} \setminus \{v\}$ . If  $\Phi_{\mathbb{G}_0}(v_i, t - 1) = \mathbb{P}_{\mathbb{G}_0}(v_i \notin \mathbf{M})$  for all  $i$  then  $\Phi_{\mathbb{G}}(v, t) = \mathbb{P}_{\mathbb{G}}(v \notin \mathbf{M})$ .

Similarly, introduce  $\Psi_{\hat{\mathbb{G}}}(v, t)$  with the only exception that  $\Psi_{\hat{\mathbb{G}}}(v, 0) = 0$  for all  $\hat{\mathbb{G}}$  and  $v$ . The following proposition follows from Theorem 6 and the definitions of  $\Phi$  and  $\Psi$  using a simple induction argument.

**Lemma 3** *For every  $v \in V, t \in \mathbb{Z}_+$*

$$\begin{aligned} \Psi_{\mathbb{G}}(v, 2t) &\leq \mathbb{P}_{\mathbb{G}}(v \notin \mathbf{M}) \leq \Phi_{\mathbb{G}}(v, 2t), \\ \Phi_{\mathbb{G}}(v, 2t + 1) &\leq \mathbb{P}_{\mathbb{G}}(v \notin \mathbf{M}) \leq \Psi_{\mathbb{G}}(v, 2t + 1). \end{aligned}$$

Next we provide bounds on the computational effort required to compute  $\Phi$  and  $\Psi$ .

**Lemma 4** *For every finite graph  $\mathbb{G}$  with degree  $\Delta$ ,  $v \in \mathbb{G}$  and  $t$ , the values  $\Phi_{\mathbb{G}}(v, t)$ ,  $\Psi_{\mathbb{G}}(v, t)$  can be computed in time  $\exp(O(t \log \Delta))$ , where the constant in  $O(\cdot)$  is universal.*

*Proof* The result follows immediately from the recursive definitions of  $\Phi$  and  $\Psi$ . □

The correlation decay property is formulated in the following proposition which is proved in [6]. Let

$$\rho = \left( 1 - \frac{2}{\sqrt{1 + \lambda \Delta} + 1} \right)^{1/2}. \tag{38}$$

**Theorem 7** ([6]) *For every  $\Delta \geq 2, \lambda > 0$ , for every graph  $\mathbb{G}$  with degree at most  $\Delta$  and every node  $v$*

$$|\log \Phi_{\mathbb{G}}(v, t) - \log \Psi_{\mathbb{G}}(v, t)| \leq \rho^t \log(1 + \lambda \Delta). \tag{39}$$

*As a consequence, every graph  $\mathbb{G}$  satisfies exponential SSM for all  $\lambda > 0$ .*



We now state the analogues of Proposition 1 and Corollary 2. The proofs are very similar and omitted. Given any set  $W \subset E$ , let  $N(W) = W \cup \{e : \exists e' \in W, e \sim e'\}$ .

**Proposition 3** *Given a graph  $\mathbb{G} = (V, E)$ , for every mutually exclusive sets  $A, W_1, W_2 \subset E$  and spin assignment  $(s_e), e \in A$  on  $A$  the following identity holds with respect to the unique Gibbs measure.*

$$\begin{aligned} \mathbb{P}_{\mathbb{G}}(1\{e \in \mathbf{M}\} = s_e, \forall e \in A | W_1 \cap \mathbf{M} = \emptyset, W_2 \subset \mathbf{M}) \\ = \mathbb{P}_{\hat{\mathbb{G}}}(1\{e \in \mathbf{M}\} = s_e, \forall e \in A), \end{aligned} \tag{40}$$

where  $\hat{\mathbb{G}}$  is the subgraph obtained from  $\mathbb{G}$  by removing edges  $W_1 \cup N(W_2)$ .

We use notations  $\mathcal{P}(d, \lambda)$  and  $s\mathcal{P}(d, \lambda)$  for the free energy and the surface pressure for the monomer-dimer model on  $\mathbb{Z}^d$  as well. As a corollary of Theorem 3, and Proposition 3 we obtain

**Corollary 4** *For every  $\lambda > 0$  and  $d$*

$$\mathcal{P}(d, \lambda) = -\log \mathbb{P}_{\mathbb{Z}^d_{>0}}(0 \notin \mathbf{M}) = -\frac{1}{2} \log \mathbb{P}_{\mathbb{Z}^d_{>0, \text{even}}}(0 \notin \mathbf{M}). \tag{41}$$

### 5.2 Free Energy and Surface Pressure on $\mathbb{Z}^d$ . Numerical Results

We now obtain bounds on the free energy and surface pressure for the monomer-dimer model on  $\mathbb{Z}^d$ . Again denote by  $\Phi(t)$  and  $\Psi(t)$  the values of  $\Phi_{\mathbb{G}}(v, t)$ ,  $\Psi_{\mathbb{G}}(v, t)$  when applied to any graph  $\mathbb{G} = \mathbb{Z}^d_{>0} \cap B_n$  in the monomer-dimer context, for sufficiently large  $n$  and  $v = 0$ . The relations (33) and (34) hold as well and the proof is very similar.

Our algorithm for computing  $\mathcal{P}(d, \lambda)$  and  $s\mathcal{P}(\mathbb{Z}^d, \lambda)$  is again based on computing  $\Phi(t)$  and  $\Psi(t)$  and is again called *Sequential Cavity Algorithm* (SCA). We now report numerical results on computing  $\mathcal{P}(d, \lambda)$ . We have computed values  $\Phi(t)$ ,  $\Psi(t)$  for  $d = 2, 3, 4$  and a range of values  $\lambda$  using the chessboard pattern method. Our upper and lower bounds for free energy are presented in Table 1. The depth levels  $t = 14, 9, 7$  were used for the cases  $d = 2, 3, 4$ . As expected, our bounds are high quality for lower  $\lambda$  and then degrade as  $\lambda \rightarrow \infty$ . Each computation run took about 3 minutes on a workstation and we have not made an attempt to obtain very accurate bounds for each value  $\lambda$ . However for the case of interest  $\lambda = 1$  we ran our algorithm for larger depths. For the case  $d = 2$  a very accurate rigorous estimate  $0.6627989727 \pm 0.0000000001$  is due to Friedland and Peled [14], shown non-rigorously earlier by Baxter [2]. We have not made an attempt to improve this bound. However for the case  $d = 3$  we can significantly improve the best known bound  $0.7850 \leq \mathcal{P}(3, 1) \leq 0.7863$  (see introduction). At depth  $t = 19$  we obtained estimates  $0.78595 \leq \mathcal{P}(3, 1) \leq 0.78599$ , which is a two orders of magnitude improvement. We have also obtained bounds for  $d = 4$  for which no prior computations are available. We obtained  $0.8797 \leq \mathcal{P}(4, 1) \leq 0.8812$ . The computations were done at depth  $t = 14$ .

The following proposition gives a bound on the numerical complexity of SCA.

**Proposition 4** *For every  $d \geq 2, \lambda > 0, \epsilon > 0$  SCA produces an  $\epsilon$ -additive estimate of  $\mathcal{P}(d, \lambda)$  and  $s\mathcal{P}(d, \lambda, a)$  in time  $\log(1 + 2\lambda d)(1/\epsilon)^{O((\lambda d)^{\frac{1}{2}} \log d)}$ , where the constant in  $O(\cdot)$  is universal.*

**Table 1** Upper (U) and lower (L) bounds on free energy for  $d = 2, 3, 4$

$\lambda$	$d = 2$ L	$d = 2$ U	$d = 3$ L	$d = 3$ U	$d = 4$ L	$d = 4$ U
0.1000	2.3219	2.3219	2.3311	2.3311	2.3399	2.3399
0.2000	1.6802	1.6802	1.7096	1.7096	1.7363	1.7363
0.3000	1.3451	1.3451	1.3959	1.3959	1.4395	1.4395
0.4000	1.1361	1.1361	1.2050	1.2050	1.2621	1.2624
0.5000	0.9934	0.9934	1.0770	1.0770	1.1442	1.1453
0.6000	0.8902	0.8902	0.9853	0.9855	1.0599	1.0629
0.7000	0.8122	0.8122	0.9164	0.9171	0.9961	1.0025
0.8000	0.7513	0.7513	0.8627	0.8642	0.9457	0.9568
0.9000	0.7026	0.7026	0.8196	0.8224	0.9044	0.9215
1.0000	0.6628	0.6628	0.7840	0.7887	0.8695	0.8937
1.5000	0.5389	0.5392	0.6677	0.6890	0.7475	0.8163
2.0000	0.4742	0.4758	0.5982	0.6436	0.6671	0.7840
3.0000	0.4056	0.4139	0.5079	0.6055	0.5564	0.7586
4.0000	0.3665	0.3855	0.4455	0.5908	0.4793	0.7492
5.0000	0.3390	0.3704	0.3972	0.5836	0.4208	0.7448
6.0000	0.3174	0.3614	0.3575	0.5797	0.3740	0.7423
7.0000	0.2993	0.3558	0.3239	0.5772	0.3354	0.7408
8.0000	0.2837	0.3519	0.2947	0.5757	0.3026	0.7399
9.0000	0.2697	0.3493	0.2691	0.5746	0.2743	0.7392
10.0000	0.2570	0.3473	0.2465	0.5738	0.2496	0.7387
15.0000	0.2064	0.3426	0.1643	0.5719	0.1621	0.7376
20.0000	0.1685	0.3409	0.1147	0.5713	0.1110	0.7372
30.0000	0.1151	0.3397	0.0627	0.5708	0.0592	0.7369
40.0000	0.0811	0.3393	0.0386	0.5706	0.0359	0.7368
50.0000	0.0592	0.3391	0.0259	0.5705	0.0239	0.7368

Again for constant  $\lambda, d$  we obtain performance  $(1/\epsilon)^{O(1)}$ , which is a qualitative improvement over the numerical effort  $\exp(O((1/\epsilon)^{d-1}))$  of the transfer matrix method.

*Proof* We have  $\Delta = 2d$ . Applying Theorem 7, an additive error  $\epsilon$  is achieved provided that  $\rho^t \log(1 + 2\lambda d) < \epsilon$  or

$$t \geq (-\log \rho)^{-1} \left( \log \frac{1}{\epsilon} + \log \log(1 + 2\lambda d) \right).$$

Applying (38) we have  $\log \rho = O\left(\frac{1}{\sqrt{1+2\lambda d+1}}\right) = O\left(\frac{1}{\sqrt{\lambda d}}\right)$ . The result for  $\mathcal{P}(d, \lambda)$  then follows from this estimate and Lemma 4. The result for  $s\mathcal{P}(d, \lambda)$  is established using the same line of reasoning as for Proposition 2. □

### 6 Conclusions

Several statistical mechanics models besides hard-core and monomer-dimer models fit our framework, yet were not discussed in this paper. One such model is Ising model and its

generalization, Potts (coloring) model [31]. The Ising model satisfies our Assumption 1 by making  $s^* = 1$  or  $-1$ . Thus the representation Theorem 1 holds, provided (exponential) SSM holds. However, in order to turn it into a useful method for obtaining provably converging bounds, we need an analogue of Theorems 5 and 7, namely the correlation decay property on a computation tree. Such a result is indeed established in [16], but for an Ising model with very weak interactions. Thus it is of interest to strengthen the result in [16] and obtain some concrete estimates for the Ising model on  $\mathbb{Z}^d$ . We are not aware of earlier benchmark results for this model. The situation with the Potts model is similar with the exception of hard-core Potts model (proper coloring). In this case the required  $s^*$  does not exist, as for every color  $s$ ,  $H(s, s) = \infty$ . However, our method can be extended by considering for example a periodic coloring of nodes  $v > 0$  or using the chess-pattern version Theorem 2 of our main result. The required correlation decay result is established in [16] for the case  $q > 2.86\Delta$  and  $q, \Delta$  appropriately large constants. Thus in order to turn this result into a useful method for computing free energy and surface pressure for coloring model on  $\mathbb{Z}^d$ , one needs to deal with these constants explicitly. Also a convenient monotonicity present in the hard-core and monomer-dimer models is lost in the Potts model case, which makes application of Corollary 1 harder.

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