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FROM MESOSCALE BACK TO MICROSCALE: RECONSTRUCTION SCHEMES FOR COARSE-GRAINED STOCHASTIC LATTICE SYSTEMS

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Abstract. Starting from a microscopic stochastic lattice spin system and the corresponding coarse-grained model we introduce a mathematical strategy to recover microscopic information given the coarse-grained data. We define "reconstructed" microscopic measures satisfying two conditions: (i) they are close in specific relative entropy to the initial microscopic equilibrium measure conditioned on the coarse-grained data and (ii) their sampling is computationally advantageous when compared to sampling directly from the conditioned microscopic equilibrium measure. By using different techniques we consider the cases of both short and long range microscopic models.

Key words. Coarse-graining, microscopic reconstruction, Monte-Carlo simulation, parallel computing, lattice spin systems, Gibbs measure, cluster expansion.

AMS subject classifications. 65C05, 65C20, 82-08, 82B20, 82B80, 94A17.

1. Introduction. Problems in scientific disciplines ranging from materials science to the dynamics of macromolecules, to the spread of epidemics and climate modeling involve non-linear interactions within a vast disparity of scales ranging from the microscopic to the macroscopic. While microscopic simulation methods such as Molecular Dynamics and Monte Carlo (MC) algorithms can describe aspects of such complex systems, they are limited to short scales when compared to morphological features such as vortices, traveling waves or domain walls that typically involve much larger mesoscopic scales. In recent years there has been a growing interest in developing hierarchical coarse-graining (CG) methods to address this problem. The idea is to reduce the complexity of the microscopic system by lumping together degrees of freedom into appropriately chosen CG variables defining in this way a Coarse-Grained model. By focusing on the relevant order parameter (CG observable depending on the particular problem) one designs numerical methods of significantly reduced computational cost. Such CG models have been developed for the study and simulation of a number of applications, such as crystal growth, surface processes, polymers, proteins and complex fluids, among others ([1], [17], [21]). In particular, coarse-graining of polymeric chains and other macromolecular systems has attracted considerable attention. In this context the CG method consists in grouping together in a systematic manner several atoms on a macromolecule creating an effective new chain (see e.g. [7], [22], [2]).

In the present paper we are interested in the reconstruction of microscopic models given the CG data. The motivation for this is two-fold. First, the CG model being computationally advantageous, it is natural to approximate the microscopic model via the following multi-scale procedure:

1. *Coarse-Graining:* Derivation of a CG model from the original microscopic model.
2. CG simulation.
3. *Microscopic Reconstruction:* Being given a CG configuration η define a reconstructed microscopic model on the ground of η.
4. Simulation of the reconstructed microscopic model.

In short, the idea in this method is to reproduce the large scale structure by the CG model, and then to obtain microscopic information by appropriate microscopic reconstruction. It has been successfully followed in the multiscale treatment of various polycarbonates, as well as for a hierarchical approach to polystyrene allowing for important technological properties of the polymers to be calculated ([24], [25], [18], [8], [9]). This approach opens new perspectives for a mathematical investigation since the aforementioned applications were based on ad-hoc postulations for the definition of both the CG and reconstructed models. While the rigorous derivation of CG models in different contexts is addressed in e.g. [13], [10], [11] (see [12] for an up-to-date review) the present work constitutes the first systematical approach to the reconstruction problem. It is clear that reconstructed models should be such that on the one hand the four steps method described above is computationally advantageous when compared to running directly microscopic MC algorithms

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and on the other hand the information loss in the transition from the exact microscopic model to the overall reconstructed one is controlled (in order to avoid confusions we shall call *reconstructed model* the microscopic model depending on CG data η defined at the third stage of the procedure and *overall reconstructed model* the microscopic model resulting from all the four steps of the procedure). The second reason to investigate microscopic reconstruction lies on the fact that it often happens that only CG data is available to the experimenter: Microscopic details are beyond the reach of observation means (see e.g. [23]). In this case microscopic information should be derived from reconstructed models.

Here we investigate the reconstruction of microscopic models (Steps 3 and 4 above) in the context of equilibrium stochastic lattice systems of Ising type spins. Lattice systems for N particles are defined in terms of a microscopic lattice Hamiltonian $H_N(\sigma)$ with σ being the microscopic configuration. At inverse temperature $\beta > 0$ the system is in the configuration σ with probability

$$\mu_{N,\beta}(\sigma) = \frac{1}{Z_{N,\beta}} e^{-\beta H_N(\sigma)} P_N(\sigma)$$

where P_N stands for a prior distribution. In [13] a systematic approach for the Steps 1 and 2 above was proposed. There the coarse-graining is performed by subdividing the lattice into coarse cells and defining variables η on each coarse cell to be the total magnetization in the cell. The *exact* coarse-grained Hamiltonian $\bar{H}_M$ is obtained by means of the Kadanoff transform

$$e^{-\beta \bar{H}_M(\eta)} = \int e^{-\beta H_N(\sigma)} P_N(\sigma|\eta).$$

In [13] the authors found sufficient conditions under which $\bar{H}_M$ can be expanded in a series

$$\bar{H}_M(\eta) = \bar{H}_M^{(0)}(\eta) + \bar{H}_M^{(1)}(\eta) + \bar{H}_M^{(2)}(\eta) + \cdots + \bar{H}_M^{(p)}(\eta) + O(\varepsilon^{p+1})$$

where ε is a small parameter depending on the characteristics of the model and the level of coarse-graining. The CG models defined by truncated versions of this series expansions lead to numerical simulations that are of improving accuracy and less demanding than any direct microscopic simulation.

Regardless of computational constraints, being given a CG configuration η, a *perfect reconstructed model* is given by the conditioned microscopic equilibrium measure $\mu_{N,\beta}(\cdot|\eta)$. Our purpose in the present paper is to show how one can define a reconstructed microscopic model taking into account the following two conditions:

1. The reconstructed equilibrium measure lies within a controlled distance from $\mu_{N,\beta}(\cdot|\eta)$ uniformly in η.
2. Simulation of the reconstructed model is computationally advantageous when compared to running directly MC algorithms on the perfect reconstructed microscopic model.

The main feature of our reconstructed models is that they allow parallel computations. In this way, instead of running a *single* multi-constrained MC dynamic on a *huge state space* we are led to run in *parallel several* multi-constrained MC dynamics on *small state spaces*. This leads to a considerable speed-up of the simulations. As a result we can combine our methods with those proposed in [13] to define efficient overall reconstructed models.

The issue of microscopic reconstruction arose also in the mathematical analysis of the error resulting from the coarse-graining of stochastic particle dynamics ([15], [14]). The difficulty in carrying out the error estimates rests on the fact that the exact CG dynamic is not Markovian. To circumvent this obstacle in [15] it was suggested to define a reconstructed microscopic Markov process which is an approximation of the exact microscopic dynamic. The reconstructed dynamic was also used for the computation of weak errors in [14]. Notice however that the reconstruction methods presented here are much more involved and efficient that the uniform sampling employed there.

Let us mention that the problem of moving from a mesoscopic to a microscopic description is at the core of many other computational multi-scale methods (e.g. [16] and [6]) and it is usually

referred as reconstruction, or reverse mapping, or "lifting" operator. One of the common features in these approaches is the attempt to capture the macroscale behavior of a system using microscale models, without first deriving or obtaining the meso- (or macro-) scale models. An important step in this process is to specify the appropriate conditional (to the meso variables) distribution with respect to which one samples the microscopic configuration in the meso-to-micro mapping.

The paper is structured as follows: in Section 2.1 we present the model and fix the notation. Then, in Section 2.2 we present the results together with the subsequent numerical schemes distinguishing the cases of the coarse-grained boxes being smaller (Section 2.2.1) or larger (Section 2.2.2) than the interaction length. We also discuss the problem of overall reconstruction in Section 2.2.3. The proofs of the theorems are presented in Section 3. Finally, in Section 4 we give some numerical tests for our methods.

2. Main results and outline of the method.

2.1. The model.

The model at the microscopic scale. We consider as the physical domain for the system the d-dimensional torus $\mathbb{T}_d = [0,1)^d$ with periodic boundary conditions. There is no additional difficulty for the problem addressed here in considering other boundary conditions. The microscopic system is settled on the uniform lattice $\Lambda_N = (\frac{1}{n}\mathbb{Z})^d \cap \mathbb{T}_d$. The number of lattice sites $N = n^d$ is fixed, but arbitrary and finite. A microscopic configuration $\sigma = (\sigma(x))_{x\in\Lambda_N}$ is an element of $S_N = \{-1,1\}^{\Lambda_N}$ and its energy is given by the Hamiltonian

$$H_N(\sigma) = -\frac{1}{2}\sum_{x\in\Lambda_N}\sum_{\substack{y\in\Lambda_N\\ y\neq x}} J(x-y)\sigma(x)\sigma(y). \tag{2.1}$$

The potential J describes the interaction between individual spins and we will focus on the case of finite-range interactions, i.e., a spin at site x interacts with its neighbors which are at most L lattice points away from x. It will be useful to consider the range of the interaction L as a parameter of the model. To this end we introduce a C^1 map

$$V : \mathbb{R} \to \mathbb{R}, \quad \text{such that} \quad V(r) = 0 \quad \text{if } |r| \geq 1 \tag{2.2}$$

and we assume that the potential $J(x-y)$ has the form

$$J(x-y) = \frac{1}{L^d} V\left(\frac{n}{L+1}|x-y|\right) \quad x, y \in \Lambda_N. \tag{2.3}$$

The factor $1/L^d$ in (2.3) is a normalization which ensures that the strength of the potential J is essentially independent of L and we have $||J|| = \sum_{x\neq 0}|J(x)| \simeq \int |V(r)|dr$. The finite-volume equilibrium states of the system are weighted by the canonical Gibbs measure

$$\mu_{N,\beta}(\sigma) = \frac{1}{Z_{N,\beta}} e^{-\beta H_N(\sigma)} P_N(\sigma) \tag{2.4}$$

where β is the inverse temperature, $Z_{N,\beta}$ is the normalizing partition function and $P_N(\sigma)$ is a product measure

$$P_N(\sigma) = \bigotimes_{x\in\Lambda_N} \rho(\sigma(x)).$$

In order to simplify the notations we shall take without loss of generality $\rho(\pm 1) = 1/2$ and write μ_N and Z_N dropping the dependence on β. We shall denote by E_N the expectation with respect to P_N and for every $A \subset S_N$ we shall denote by $E_N[\,\cdot\,|A]$ the expectation with respect to P_N conditioned on the event A.

The coarse-graining map and the coarse-grained model. Next we consider two integers m and q such that $n = mq$. We partition the torus $\mathbb{T}_d$ into $M = m^d$ *coarse-cells*: For $k = (k_1, \dots, k_d) \in (\mathbb{Z} \cap [0, m-1])^d$ we define $C_k = [\frac{k_1}{m}, \frac{k_1+1}{m}) \times \cdots \times [\frac{k_d}{m}, \frac{k_d+1}{m})$ so $\mathbb{T}_d = \cup_k C_k$. We identify each cell C_k with a lattice point of the coarse lattice $\bar{\Lambda}_M = (\frac{1}{m}\mathbb{Z})^d \cap \mathbb{T}_d$. Each coarse cell contains $Q = q^d$ points of the microscopic lattice and we will refer to Q as the level of coarse-graining. The coarse-grained model is the image of the microscopic model through the following coarse-graining map:

$$F: \ \sigma \mapsto \eta = (\sum_{x \in C_k \cap \Lambda_N} \sigma(x))_{k \in \bar{\Lambda}_M}.$$

The coarse-grained configurations space is thus $\bar{S}_M = \{-Q, -Q+2, \dots, Q-2, Q\}^{\bar{\Lambda}_M}$. The prior distribution P_N on S_N induces a new prior distribution $\bar{P}_M$ on $\bar{S}_M$ given by

$$\bar{P}_M(\eta) = P_N(\sigma : F(\sigma) = \eta)$$

which is a product measure

$$\bar{P}_M(\eta) = \bigotimes_{k \in \bar{\Lambda}_M} \bar{\rho}(\eta(k))$$

with

$$\bar{\rho}(\eta(k)) = \binom{Q}{\frac{\eta(k)+Q}{2}} \left(\frac{1}{2}\right)^Q.$$

The distribution μ_N induces a new equilibrium distribution $\bar{\mu}_M$ on $\bar{S}_M$ given by

$$\bar{\mu}_M(\eta) = \mu_N(\sigma : F(\sigma) = \eta).$$

Actually

$$\bar{\mu}_M(\eta) = \frac{1}{\bar{Z}_M} e^{-\beta \bar{H}_M(\eta)} \bar{P}_M(\eta) \tag{2.5}$$

where $\bar{H}_M$ is defined via the Kadanoff transformation

$$e^{-\beta \bar{H}_M(\eta)} = E_N[e^{-\beta H_N(\sigma)} | F(\sigma) = \eta]. \tag{2.6}$$

It easily follows from the definition of $\bar{H}_M$ that $Z_N = \bar{Z}_M$. It is clear that the family of conditional probabilities $P_N(\cdot | F(\sigma) = \eta)$ defined on S_N and indexed by the $\eta \in \bar{S}_M$ will play a crucial role in the sequel. With a slight abuse of notation we shall write $P_N(\cdot|\eta), E_N[\cdot|\eta], \mu_N(\cdot|\eta)$, etc... For every $k \in \bar{\Lambda}_M$, every $\sigma \in S_N$ and $\eta \in \bar{S}_M$ such that $\eta = F(\sigma)$ the average $\eta(k)$ depends only on the $\sigma(x)$'s with $x \in C_k \cap \Lambda_N$. Hence the probability $P_N(\cdot|\eta)$ factorizes over the coarse cells:

$$P_N(\sigma|\eta) = \frac{P_N(\sigma \cap \{F(\sigma) = \eta\})}{\bar{P}_M(\eta)} = \bigotimes_{k \in \bar{\Lambda}_M} \tilde{\rho}_{k,\eta(k)}(\sigma) \tag{2.7}$$

where $\tilde{\rho}_{k,\eta(k)}(\sigma)$ stands for $P_N((\sigma(x))_{x \in C_k \cap \Lambda_N} | F(\sigma) = \eta)$. To simplify the notations and because for every $k \in \bar{\Lambda}_M$ our estimates are uniform in $\eta(k)$ we denote this measure simply by $\tilde{\rho}_k$. Finally let us introduce some more notations and definitions:

- Being given $\sigma \in S_N$ (resp. $\eta \in \bar{S}_M$), for any $D \subset \mathbb{T}_d$ we shall write $\sigma^D = (\sigma(x))_{x \in D \cap \Lambda_N}$ (resp. $\eta^D = (\eta(k))_{k \in D \cap \bar{\Lambda}_M}$). More generally, for every $B_1 \subset B_2 \subset \mathbb{T}_d$, being given $\alpha^{B_2} \in \{-1, 1\}^{\Lambda_N \cap B_2}$ we shall write $\alpha^{B_1} = (\alpha^{B_2}(x))_{x \in B_1 \cap \Lambda_N} \in \{-1, 1\}^{\Lambda_N \cap B_1}$.
- For any integer r, any partition $D_1, \dots, D_r$ of $\mathbb{T}_d$ into not necessarily connected parts and any $\sigma_1 \in \{-1, 1\}^{D_1 \cap \Lambda_N}, \dots, \sigma_r \in \{-1, 1\}^{D_r \cap \Lambda_N}$ (resp. $\eta_1 \in \{-Q, \dots, Q\}^{D_1 \cap \bar{\Lambda}_M}, \dots, \eta_r \in \{-Q, \dots, Q\}^{D_r \cap \bar{\Lambda}_M}$) we shall denote by $[\sigma_1, \dots, \sigma_r]$ (resp. $[\eta_1, \dots, \eta_r]$) the microscopic (resp. CG) configuration obtained by merging the partial configurations $\sigma_1, \dots, \sigma_r$ (resp. $\eta_1, \dots, \eta_r$).

- Let I be a subset of $(\mathbb{Z}\cap[0,m-1])^d$ and $\mathcal{I}=\cup_{i\in I}C_i$. Let η be a coarse-grained configuration and α be an element of $\{-1,1\}^{\mathcal{I}\cap\Lambda_N}$. We shall say that α and η are *compatible* if and only if for every $i\in I$ we have $\eta(i)=\sum_{x\in C_i\cap\Lambda_N}\alpha(x)$.
- For any two probability measures P,Q on a finite set Σ the relative entropy of P with respect to Q is defined by

$$H(P|Q)=\begin{cases}\sum_{x\in\Sigma}P(x)\log\frac{P(x)}{Q(x)} & \text{if } P\ll Q\\ \infty & \text{otherwise.}\end{cases}$$

  We will use this notation for both cases of Σ being S_N or $\bar{S}_M$. For a nice account on relative entropy see [5].

2.2. Reconstruction schemes. Our purpose in the present section is to describe numerical schemes for the sampling from probability measures defined on S_N and indexed by the $\eta\in\bar{S}_M$ that are approximations of the conditional probability measures $\mu_N(\cdot|\eta)$. More precisely we shall introduce probability kernels $\nu_N(\cdot;\cdot)$ (i.e. maps defined on $S_N\times\bar{S}_M$ such that for every $\eta\in\bar{S}_M$ the partial map $\nu_N(\cdot;\eta)$ is a probability measure defined on S_N) satisfying two conditions:

1. For every $\eta\in\bar{S}_M$ the probability measure $\nu_N(\cdot;\eta)$ lies within a controlled distance from $\mu_N(\cdot|\eta)$. The distance is measured in specific relative entropy.
2. We can design numerical schemes such that for every $\eta\in\bar{S}_M$ sampling from $\nu_N(\cdot;\eta)$ is computationally less demanding than any "direct" sampling from $\mu_N(\cdot|\eta)$.

In the sequel we will treat two cases:

1. If $q<L$ then a mean-field type approximation of the interaction potential (2.3) is justified since averaging the value of the spins over coarse cells of volume Q gives an error of the order $q/L<1$. This is the situation considered in Section 2.2.1.
2. If $q>L$ a mean-field approach is not a good approximation any more. We shall assume that μ_N satisfies a strong mixing condition and exploit this fact together with the conditioning in $\mu_N(\cdot|\eta)$. This is the situation considered in Section 2.2.2.

In the present paper we describe schemes designed for the reconstruction over the entire domain $\mathbb{T}_d$. However in most applications (see e.g. [18]) the reconstruction is performed over mesoscopic domains, i.e. not the whole $\mathbb{T}_d$ but parts of $\mathbb{T}_d$ containing a number of microscopic sites that is a large multiple of L^d. It should be clear to the reader how to adapt the analysis carried out here to these situations.

Finally, in Section 2.2.3, we introduce in the $q<L$ case computationally advantageous numerical schemes for the sampling from arbitrarily good approximations of the *unconditioned* measure μ_N. They rely on the following "separation of scales" property: A sample σ from μ_N is obtained by first getting a sample η from $\bar{\mu}_M$ and then a sample σ from $\mu_N(\cdot|\eta)$. Hence samples from approximations of μ_N are obtained by combining the schemes presented in Section 2.2.1 with the Coarse-Grained Monte-Carlo algorithm proposed in [13] which is tailored for the numerically efficient sampling from arbitrarily good approximations of $\bar{\mu}_M$ in the $q<L$ regime. In this way we propose, in the context of equilibrium stochastic lattice systems of Ising type spins, a complete derivation of the multi-scale approach presented in the Introduction. We shall give rigorous estimates on the information loss in the transition from the exact microscopic model to the overall reconstructed one and illustrate the accuracy of the approximation by numerical experiments detailed in Section 4.

2.2.1. Reconstruction schemes in the $q<L$ case. To simplify notations and without loss of generality we assume that there exist even numbers r and u such that $n=2uL$ and $L=rq$. A crucial quantity for the reconstruction schemes presented in this section is the so-called small parameter

$$\varepsilon=\beta\frac{q}{L}||\nabla V||_\infty \tag{2.8}$$

which measures how close to the high temperature and/or mean-field regime we are and how rough the coarsening of the microscopic model is. We shall also use $\delta=Q\varepsilon$ which represents the error per coarse-cell in the mean-field approximation while ε represents the error per microscopic lattice

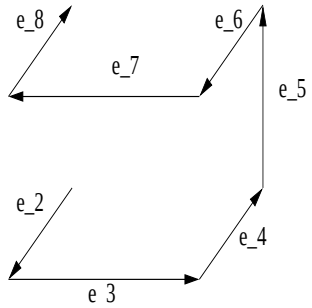

FIG. 2.1. *The vectors $e_2, \ldots, e_8$ connecting the cells in the sublattices $\mathcal{L}_i$, $i = 8, \ldots, 1$, for $d = 3$.*

site. First we show that due to the particular form of the Gibbs measure (2.4) the problem in hands reduces, from the computational point of view, to define a sequence of 2^d samplings. Then we propose several schemes designed to deal with this problem and give the corresponding rigorous error estimates.

We partition $\mathbb{T}_d$ into $2^d U$ ($U = u^d$) cells: For $l = (l_1, \ldots, l_d) \in (\mathbb{Z} \cap [0, 2u-1])^d$ we define $D_l = [\frac{l_1}{2u}, \frac{l_1+1}{2u}) \times \cdots \times [\frac{l_d}{2u}, \frac{l_d+1}{2u})$ so $\mathbb{T}_d = \cup_l D_l$ and every D_l contains L^d points of the microscopic lattice Λ_N. We call the D_l *reconstruction domains*. Next we partition $(\mathbb{Z} \cap [0, 2u-1])^d$ into 2^d subsets $\mathcal{L}_1, \ldots, \mathcal{L}_{2^d}$ in base of the parity of its elements. We get

$$\mathcal{L}_1 = \{l = (l_1, l_2, \ldots, l_d),\ 0 \le l_1, l_2, \ldots, l_d \le 2u-1,\ l_1, l_2, \ldots, l_d \text{ even}\}$$

and $\mathcal{L}_2 = \mathcal{L}_1 + e_2, \mathcal{L}_3 = \mathcal{L}_2 + e_3$ etc... where $(e_1, \ldots, e_{2^d})$ is a family of unit vectors parallel to the axis of $\mathbb{Z}^d$ as described in Figure 2.1. Proceeding this way we get an induced ordering of the sublattices $\mathcal{L}_1 < \mathcal{L}_2 < \mathcal{L}_3 < \cdots < \mathcal{L}_{2^d}$. For every integer i such that $1 \le i \le 2^d$ we further define

$$\mathcal{E}_i = \bigcup_{l \in \mathcal{L}_i} D_l \text{ and } S_{N,\mathcal{E}_i} = \{-1, 1\}^{\mathcal{E}_i \cap \Lambda_N}.$$

For every integer i such that $1 \le i \le 2^d$, every $\eta \in \bar{S}_M$ and every $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}$ compatible with η we shall denote by $\mu_{N,\mathcal{E}_i}(\cdot|\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta)$ the $\mathcal{E}_i \cap S_N$-marginal of

$$\mu_N(\cdot|\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \mu_N(\cdot|\sigma^{\mathcal{E}_1} = \alpha^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}} = \alpha^{\mathcal{E}_{i-1}}, F(\sigma) = \eta).$$

Let η be a fixed coarse-grained configuration and α be a microscopic configuration compatible with η. We have

$$\mu_N(\alpha|\eta) = \prod_{i=1}^{2^d} \mu_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_i}|\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta). \tag{2.9}$$

while naturally $\mu_N(\alpha|\eta) = 0$ if η and α are not compatible. In view of (2.9) we look for an approximation of $\mu_N(\alpha|\eta)$ expressed as

$$\nu_N(\alpha; \eta) = \prod_{i=1}^{2^d} \nu_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_i}; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) \tag{2.10}$$

where $\nu_{N,\mathcal{E}_i}(\cdot; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta)$ is a probability measure defined on $S_{N,\mathcal{E}_i}$. In words we shall successively sample the microscopic configuration on the different $\mathcal{E}_i$'s as i grows from 1 to 2^d. The main step is the definition of an approximation $\nu_{N,\mathcal{E}_1}(\cdot; \eta)$ of $\mu_{N,\mathcal{E}_1}(\cdot|\eta)$. Indeed, for every integer i such that $1 < i < 2^d$ the definition of the $\nu_{N,\mathcal{E}_i}$'s relies on the same ideas as for the definition of $\nu_{N,\mathcal{E}_1}$ with the difference that the CG data $\eta^{\mathcal{E}_1}, \ldots, \eta^{\mathcal{E}_{i-1}}$ is replaced by the microscopic data $\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}$.

Finally, assume for a while that we are given $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}} \in S_{N,\mathcal{E}_{2^d-1}}$ compatible with η. Since L is the range of interaction of μ_N the probability measure $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$ defined on $S_{N,\mathcal{E}_{2^d}}$ factorizes: for every $\varrho \in S_{N,\mathcal{E}_{2^d}}$

$$\mu_{N,\mathcal{E}_{2^d}}(\varrho|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta) = \bigotimes_{l \in \mathcal{L}_{2^d}} \mu_{N,D_l}(\varrho^{D_l}|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta) \tag{2.11}$$

where $\mu_{N,D_l}(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$ stands for the $D_l \cap \Lambda_N$-marginal of $\mu_N(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$. Each of the factors in the right hand side of the last display is a probability measure defined on $\{-1,1\}^{\Lambda_N \cap D_l}$ which is a set of cardinal 2^{L^d} i.e. a small set when compared to S_N. Furthermore, while sampling from $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$ the product structure in (2.11) allows to run parallel simulations resulting in a global speed-up of the computations and these simulations are perfect in the sense that we obtain samples from the *exact* $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$ and not from an approximation of it. Hence sampling with respect to $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$ does not represent a computational difficulty once we are given $\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}$ and we shall take $\nu_{N,\mathcal{E}_{2^d}}(\cdot; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta) = \mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$.

Now we focus on the definition of efficient numerical schemes in order to get samples from approximations of the conditional probability measures $\mu_{N,\mathcal{E}_1}$ defined on $S_{N,\mathcal{E}_1}$. Let η be a coarse-grained configuration and fix $\alpha \in S_{N,\mathcal{E}_1}$ compatible with η. We introduce $\bar{W}_{N,\mathcal{E}_1}(\alpha;\eta)$ by

$$e^{-\beta \bar{W}_{N,\mathcal{E}_1}(\alpha;\eta)} = E_N[e^{-\beta H_N(\sigma)}|\alpha, \eta] \tag{2.12}$$

the right hand side of the previous equality being a shortcut for $E_N[e^{-\beta H_N(\sigma)}|\sigma^{\mathcal{E}_1} = \alpha, F(\sigma) = \eta]$. It is easy to show that

$$\mu_{N,\mathcal{E}_1}(\alpha|\eta) = \frac{e^{-\beta \bar{W}_{N,\mathcal{E}_1}(\alpha;\eta)}}{e^{-\beta \bar{H}_M(\eta)}} \bigotimes_{k \in \mathcal{E}_1 \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}).$$

Notice that whenever α and η are not compatible we get $\mu_{N,\mathcal{E}_1}(\alpha|\eta) = 0$. Accordingly for every integer i such that $1 < i < 2^d$, *being given* $\eta \in \bar{S}_M$, and $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}$ compatibles with η, for every $\alpha \in S_{N,\mathcal{E}_i}$ compatible with η we have

$$\mu_{N,\mathcal{E}_i}(\alpha|\alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \frac{e^{-\beta \bar{W}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)}}{e^{-\beta \bar{W}_{N,\mathcal{E}_{i-1}}(\alpha^{\mathcal{E}_{i-1}};\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-2}},\eta)}} \bigotimes_{k \in \mathcal{E}_i \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \tag{2.13}$$

where $\bar{W}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta)$ is defined by

$$e^{-\beta \bar{W}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)} = E_N[e^{-\beta H_N(\sigma)}|\sigma^{\mathcal{E}_1} = \alpha^{\mathcal{E}_1}, \dots, \sigma^{\mathcal{E}_{i-1}} = \alpha^{\mathcal{E}_{i-1}}, \sigma^{\mathcal{E}_i} = \alpha, F(\sigma) = \eta]. \tag{2.14}$$

First approximation. A direct computation of $\bar{W}_{N,\mathcal{E}_1}$ is actually impractical so we proceed by introducing a first approximation

$$\bar{W}^{(0)}_{N,\mathcal{E}_1}(\alpha;\eta) = E_N[H_N(\sigma)|\alpha, \eta]. \tag{2.15}$$

We define a probability kernel $\nu^{(0)}_{N,\mathcal{E}_1}$ on $S_{N,\mathcal{E}_1} \times \bar{S}_M$ by

$$\nu^{(0)}_{N,\mathcal{E}_1}(\alpha;\eta) = \frac{e^{-\beta \bar{W}^{(0)}_{N,\mathcal{E}_1}(\alpha;\eta)}}{Z^{(0)}_{N,\mathcal{E}_1}(\eta)} \bigotimes_{k \in \mathcal{E}_1 \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \tag{2.16}$$

with

$$Z^{(0)}_{N,\mathcal{E}_1}(\eta)=\int_{S_{N,\mathcal{E}_1}} e^{-\beta\bar W^{(0)}_{N,\mathcal{E}_1}(\alpha;\eta)}\bigotimes_{k\in\mathcal{E}_1\cap\bar\Lambda_M}\tilde\rho_k(\alpha^{C_k}).$$

By elementary computations we get

$$\begin{aligned}\bar W^{(0)}_{N,\mathcal{E}_1}(\alpha;\eta)=&-\frac{1}{2}\sum_{l\in\mathcal{L}_1}\sum_{x\in D_l\cap\Lambda_N}\sum_{\substack{y\in D_l\cap\Lambda_N,\\ y\neq x}}J(x-y)\alpha(x)\alpha(y)\\ &-\frac{1}{2}\sum_{l,l'\in\mathcal{L}_2\cup\cdots\cup\mathcal{L}_{2^d}}\left(\sum_{k\in D_l\cap\bar\Lambda_M}\sum_{\substack{k'\in D_{l'}\cap\bar\Lambda_M,\\ k'\neq k}}\bar J(k,k')\eta(k)\eta(k')+\sum_{k\in D_l\cap\bar\Lambda_M}\bar J(0)(\eta^2(k)-Q)\right)\\ &-\sum_{l\in\mathcal{L}_1}\sum_{l'\in\mathcal{L}_2\cup\cdots\cup\mathcal{L}_{2^d}}\sum_{k\in D_{l'}\cap\bar\Lambda_M}\sum_{x\in D_l\cap\Lambda_N}\breve J(x,k)\alpha(x)\eta(k)\end{aligned}\tag{2.17}$$

where for every $k,k'\in\bar\Lambda_M, k\neq k'$ and $x\in\Lambda_N\setminus(C_k\cap\Lambda_N)$ we have

$$\bar J(k,k')=\frac{1}{Q^2}\sum_{x\in C_k\cap\Lambda_N}\sum_{y\in C_{k'}\cap\Lambda_N}J(x-y),\quad \bar J(0)=\frac{1}{Q(Q-1)}\sum_{x\in C_k\cap\Lambda_N}\sum_{\substack{y\in C_k\cap\Lambda_N,\\ y\neq x}}J(x-y),$$

and

$$\breve J(k,x)=\frac{1}{Q}\sum_{y\in C_k\cap\Lambda_N}J(x-y).$$

With a slight abuse of notation we shall write $\breve J(k,x)=\breve J(x,k)$ since J is even. Following the same idea for every integer i such that $1<i<2^d$, *being given* $\eta\in\bar S_M$, and $\alpha^{\mathcal{E}_1}\in S_{N,\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}}\in S_{N,\mathcal{E}_{i-1}}$ compatibles with η, for every $\alpha\in S_{N,\mathcal{E}_i}$ compatible with η one can built a first approximation of $\mu_{N,\mathcal{E}_i}(\alpha|\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)$ given at (2.13) of the form

$$\nu^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)=\frac{e^{-\beta\bar W^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)}}{Z^{(0)}_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)}\bigotimes_{k\in\mathcal{E}_i\cap\bar\Lambda_M}\tilde\rho_k(\alpha^{C_k})\tag{2.18}$$

with

$$\begin{aligned}\bar W^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}}\eta)&=E_N[H_N(\sigma)|\sigma^{\mathcal{E}_1}=\alpha^{\mathcal{E}_1},\dots,\sigma^{\mathcal{E}_{i-1}}=\alpha^{\mathcal{E}_{i-1}},\sigma^{\mathcal{E}_i}=\alpha,F(\sigma)=\eta]\\ &=-\frac{1}{2}\sum_{l,l'\in\mathcal{L}_1\cup\cdots\cup\mathcal{L}_i}\sum_{x\in D_l\cap\Lambda_N}\sum_{\substack{y\in D_{l'}\cap\Lambda_N,\\ y\neq x}}J(x-y)\alpha(x)\alpha(y)\\ &\quad-\frac{1}{2}\sum_{l,l'\in\mathcal{L}_{i+1}\cup\cdots\cup\mathcal{L}_{2^d}}\left(\sum_{k\in D_l\cap\bar\Lambda_M}\sum_{\substack{k'\in D_{l'}\cap\bar\Lambda_M,\\ k'\neq k}}\bar J(k,k')\eta(k)\eta(k')\right.\\ &\qquad\left.+\sum_{k\in D_l\cap\bar\Lambda_M}\bar J(0)(\eta^2(k)-Q)\right)\\ &\quad-\sum_{l\in(\mathcal{L}_1\cup\cdots\cup\mathcal{L}_i)}\sum_{l'\in\mathcal{L}_{i+1}\cup\cdots\cup\mathcal{L}_{2^d}}\sum_{k\in D_{l'}\cap\bar\Lambda_M}\sum_{x\in D_l\cap\Lambda_N}\breve J(x,k)\alpha(x)\eta(k)\end{aligned}\tag{2.19}$$

and

$$Z^{(0)}_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)=\int_{S_{N,\mathcal{E}_i}}e^{-\beta\bar W^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}}\eta)}\bigotimes_{k\in\mathcal{E}_i\cap\bar\Lambda_M}\tilde\rho_k(\alpha^{C_k}).$$

Our first result is the following

THEOREM 2.1. *There exists a constant δ_0 such that if $\delta = Q\varepsilon < \delta_0$ then for every integer i such that $1 \leq i < 2^d$, every $\eta \in \bar{S}_M$, every $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}, \alpha \in S_{N,\mathcal{E}_i}$ compatibles with η the following estimate holds*

$$\frac{\beta}{N}\left(\bar{W}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta) - \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta)\right) = O(\varepsilon^2) \tag{2.20}$$

where the O is uniform in η and $\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\alpha$.
For every $\eta \in \bar{S}_M$ we define a probability measure $\nu^{(0)}_N(\cdot;\eta)$ on S_N by

$$\nu^{(0)}_N(\sigma;\eta) = \left(\prod_{i=1}^{2^d-1} \nu^{(0)}_{N,\mathcal{E}_i}(\sigma^{\mathcal{E}_i};\sigma^{\mathcal{E}_1},\ldots,\sigma^{\mathcal{E}_{i-1}},\eta)\right)\mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}}|\sigma^{\mathcal{E}_1},\ldots,\sigma^{\mathcal{E}_{2^d-1}},\eta) \tag{2.21}$$

if σ and η are compatible and $\nu^{(0)}_N(\sigma;\eta) = 0$ otherwise. We prove in Section 3.1.2 the following consequence of Theorem 2.1 which states that the first approximation is actually a second order approximation in ε

COROLLARY 2.2. *If $\delta = Q\varepsilon < \delta_0$ then for every $\eta \in \bar{S}_M$ the following estimate holds*

$$\frac{1}{N}H\left(\nu^{(0)}_N(\cdot;\eta)|\mu_N(\cdot|\eta)\right) = O(\varepsilon^2) \tag{2.22}$$

where the O is uniform in $\eta \in \bar{S}_M$.
The particular form of each of the $\bar{W}^{(0)}_{N,\mathcal{E}_i}$'s makes for every $\eta \in \bar{S}_M$ every $\nu^{(0)}_{N,\mathcal{E}_i}$ a product measure. This leads to the following

Scheme A
1. We run in parallel U constrained simulations with CG boundary conditions given by η to get $\alpha^{\mathcal{E}_1}$ sampled from $\nu^{(0)}_{N,\mathcal{E}_1}(\cdot;\eta)$.
2. For every integer i starting from 2 and up to 2^d-1 we run in parallel U constrained simulations with mixed CG/microscopic boundary conditions given by $\eta,\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}}$ to get $\alpha^{\mathcal{E}_i} \in S_{N,\mathcal{E}_i}$ sampled from $\nu^{(0)}_{N,\mathcal{E}_i}(\cdot;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta)$.
3. We run in parallel U constrained simulations with microscopic boundary conditions given by $\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{2^d-1}}$ to obtain $\alpha^{\mathcal{E}_{2^d}} \in S_{N,\mathcal{E}_{2^d}}$ sampled from $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{2^d-1}},\eta)$.
4. We obtain a sample of $\nu^{(0)}_N(\cdot;\eta)$ by taking $[\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{2^d}}]$.

Numerical experiments following this scheme are presented in Section 4.

Higher order corrections. A natural question is to ask for schemes with higher order error estimates. Following [13] we notice that for every integer i such that $1 \leq i < 2^d$, being given any $\eta \in \bar{S}_M$, and $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}$ compatibles with η, for every $\alpha \in S_{N,\mathcal{E}_i}$ compatible with η we have

$$\bar{W}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta) - \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta) =$$

$$= -\frac{1}{\beta}\log E_N[e^{-\beta(H_N(\sigma)-\bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta))}|\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_i},\alpha,\eta]. \tag{2.23}$$

A high-temperature cluster expansion performed on the right hand side of the last display leads to:

THEOREM 2.3. *If $\delta = Q\varepsilon < \delta_0$ with δ_0 as in Theorem 2.1 then for every integer i such that $1 \leq i < 2^d$, being given any $\eta \in \bar{S}_M$, and $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}$ compatibles with η the*

function $\bar{W}_{N,\mathcal{E}_i}(\cdot;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)$ *defined on the elements of* $S_{N,\mathcal{E}_i}$ *that are compatible with* η *can be expanded into a convergent series*

$$\bar{W}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)=\sum_{p=0}^{+\infty}\bar{W}^{(p)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta) \tag{2.24}$$

where the $p=1,2$ *terms are given in Section 3.1.1. Furthermore, for every integer* i *such that* $1\leq i<2^d$ *and every integer* $p\geq 1$ *the following error bound holds uniformly in* α *and* $\eta,\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}}$

$$\frac{\beta}{N}\left(\bar{W}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)-\sum_{l=0}^{p}\bar{W}^{(l)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)\right)=O(\varepsilon^{p+1}). \tag{2.25}$$

For every integer $p\geq 1$ and every integer i such that $1\leq i<2^d$, being given any $\eta\in\bar{S}_M$ and $\alpha^{\mathcal{E}_1}\in S_{N,\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}}\in S_{N,\mathcal{E}_{i-1}}$ compatible with η we define on the elements of $S_{N,\mathcal{E}_i}$ that are compatible with η a probability measure $\nu^{(p)}_{N,\mathcal{E}_i}(\cdot;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)$ on $S_{N,\mathcal{E}_i}$ by

$$\nu^{(p)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)=\frac{e^{-\beta(\sum_{l=0}^{p}\bar{W}^{(l)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta))}}{\bar{Z}^{(p)}_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)}\bigotimes_{k\in\mathcal{E}_i\cap\bar{\Lambda}_M}\tilde{\rho}_k(\alpha^{C_k}).$$

The corresponding kernel defined on $S_N\times\bar{S}_M$ is

$$\nu^{(p)}_N(\sigma;\eta)=\left(\prod_{i=1}^{2^d-1}\nu^{(p)}_{N,\mathcal{E}_i}(\sigma^{\mathcal{E}_i};\sigma^{\mathcal{E}_1},\dots,\sigma^{\mathcal{E}_{i-1}},\eta)\right)\mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}}|\sigma^{\mathcal{E}_1},\dots,\sigma^{\mathcal{E}_{2^d-1}},\eta) \tag{2.26}$$

if σ and η are compatible and $\nu^{(0)}_N(\sigma;\eta)=0$ otherwise.

Corollary 2.4. *If* $\delta=Q\varepsilon<\delta_0$ *then for every* $\eta\in\bar{S}_M$ *and every integer* $p\geq 1$ *the following estimate holds*

$$\frac{1}{N}H\left(\nu^{(p)}_N(\cdot;\eta)|\mu_N(\cdot|\eta)\right)=O(\varepsilon^{p+1}) \tag{2.27}$$

where the O *is uniform in* $\eta\in\bar{S}_M$.

From the preceding result we derive the following

Scheme B

1. We run a multi-constrained simulation with CG boundary conditions given by η to get $\alpha^{\mathcal{E}_1}$ sampled from $\nu^{(p)}_{N,\mathcal{E}_1}(\cdot;\eta)$.

2. For every integer i starting from 2 and up to 2^d-1 we run a multi-constrained simulation with mixed CG/microscopic boundary conditions given by $\eta,\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}}$ to get $\alpha^{\mathcal{E}_i}\in S_{N,\mathcal{E}_i}$ sampled from $\nu^{(p)}_{N,\mathcal{E}_i}(\cdot;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta)$.

3. We run in parallel U constrained simulations with microscopic boundary conditions given by $\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{2^d-1}}$ to obtain $\alpha^{\mathcal{E}_{2^d}}\in S_{N,\mathcal{E}_{2^d}}$ sampled from $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{2^d-1}},\eta)$.

4. We obtain a sample of $\nu^{(p)}_N(\cdot;\eta)$ by taking $[\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{2^d}}]$.

Unfortunately steps **1.** and **2.** in this scheme are restrictive when compared to those in Scheme A. Indeed for every integer i such that $1\leq i<2^d$ the second order corrections $\bar{W}^{(1)}_{N,\mathcal{E}_i}+\bar{W}^{(2)}_{N,\mathcal{E}_i}$ already contain interactions across reconstruction domains D_l and $D_{l'}$ with $l,l'\in\mathcal{L}_i$ and $l\neq l'$ which make the sampling measures in **1.** and **2.** not product measures. As a consequence, these samplings are not reducible to sets of parallel computations. However, note that they correspond to sampling the values of the spins on lattices of $N/2^d$ points and thus remain advantageous when compared to a direct simulation over the entire domain. Numerical experiments following this scheme are presented in Section 4.

Higher order methods leading to parallel computations. A close look at the derivation of the corrections $\bar{W}^{(1)}_{N,\mathcal{E}_i}$ and $\bar{W}^{(2)}_{N,\mathcal{E}_i}$ from the cluster expansion performed in Section 3.1.1 shows how to partially overcome the difficulty in Scheme B pointed out above. Loosely speaking, the idea is that by increasing the size of the reconstruction domains the two bodies interactions that appear in $\nu^{(2)}_{N,\mathcal{E}_i}$ and couple different reconstruction domains $D_l \subset \mathcal{E}_i$ and $D_{l'} \subset \mathcal{E}_i$ necessarily vanish. Indeed, such two bodies interactions are the result of integrating over the values of three bodies interacting spins as found in the cluster expansion. Two of these spins are located in $D_l \subset \mathcal{E}_i$ and $D_{l'} \subset \mathcal{E}_i$ while the third one is located in $\mathcal{E}_j$ with $i < j \leq 2^d$. These three bodies interactions necessarily vanish as soon as one of the spins in $\mathcal{E}_i$ is located at more than L microscopic points away from the spin in $\mathcal{E}_j$. By taking reconstruction domains of $(2L)^d$ microscopic points we make sure that this cancellation condition is satisfied. More details are given in Section 3.1.1.

Now let us describe more precisely our setting. We partition $\mathbb{T}_d$ into $U = u^d$ cells: For $l = (l_1, \ldots, l_d) \in (\mathbb{Z} \cap [0, u-1])^d$ we define new reconstruction domains $D'_l = [\frac{l_1}{u}, \frac{l_1+1}{u}) \times \cdots \times [\frac{l_1}{u}, \frac{l_1+1}{u})$ so $\mathbb{T} = \bigcup_l D'_l$ and every D'_l contains $(2L)^d$ points of the microscopic lattice. The $\mathcal{L}'_i$'s, $\mathcal{E}'_i$'s, and $S_{N,\mathcal{E}'_i}$'s are defined on the ground of these D'_l's as in Section 2.2.1. For every $\eta \in \bar{S}_M$ and $\alpha \in S_N$ compatibles we have that

$$\mu_N(\alpha|\eta) = \prod_{i=1}^{2^d} \mu_{N,\mathcal{E}'_i}(\alpha^{\mathcal{E}'_i}|\alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta)$$

with

$$\mu_{N,\mathcal{E}'_{2^d}}(\varrho|\alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{2^d-1}}, \eta) = \bigotimes_{l \in \mathcal{L}'_{2^d}} \mu_{N,D'_l}(\varrho^{D'_l}|\alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{2^d-1}}, \eta).$$

The definition of the different probability measures involved here is clear by analogy with those employed so far. Again, our aim is to define efficient schemes for the sampling from probability measures that approximate the $\mu_{N,\mathcal{E}'_i}$'s. For every integer i such that $1 \leq i \leq 2^d - 1$, every $\eta \in \bar{S}_M$ and every $\alpha^{\mathcal{E}'_1} \in S_{N,\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}} \in S_{N,\mathcal{E}'_{i-1}}$ compatibles with η we define $\bar{V}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta)$ by

$$e^{-\beta \bar{V}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta)} = E_N[e^{-\beta H_N(\sigma)}|\alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \alpha, \eta] \tag{2.28}$$

and observe that

$$\mu_{N,\mathcal{E}'_i}(\alpha|\alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}\eta) = \frac{e^{-\beta \bar{V}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta)}}{e^{-\beta \bar{V}_{N,\mathcal{E}'_{i-1}}(\alpha^{\mathcal{E}'_{i-1}}; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-2}}, \eta)}} \bigotimes_{k \in \mathcal{E}'_i \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}). \tag{2.29}$$

A first approximation of $\bar{V}_{N,\mathcal{E}'_i}$ is obtained by

$$\bar{V}^{(0)}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta) = E_N[H_N(\sigma)|\alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \alpha, \eta] \tag{2.30}$$

as we did for the first approximation of $\bar{W}_{N,\mathcal{E}_i}$.

THEOREM 2.5. *If $\delta = Q\varepsilon < \delta_0$ with δ_0 as in Theorem 2.1 then for every integer i such that $1 \leq i < 2^d$, every $\eta \in \bar{S}_M$, $\alpha^{\mathcal{E}'_1} \in S_{N,\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}} \in S_{N,\mathcal{E}'_{i-1}}$ compatibles with η the function $\bar{V}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta)$ defined on the elements of $S_{N,\mathcal{E}'_i}$ that are compatibles with η can be expanded into a convergent series*

$$\bar{V}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta) = \sum_{p=0}^{+\infty} \bar{V}^{(p)}_{N,\mathcal{E}'_i}(\alpha; \alpha^{\mathcal{E}'_1}, \ldots, \alpha^{\mathcal{E}'_{i-1}}, \eta). \tag{2.31}$$

Furthermore, for every integer i such that $1 \leq i < 2^d$ and every integer $p \geq 1$ the following error bound holds uniformly in α and $\eta, \alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{i-1}'}$

$$\frac{\beta}{N}\left(\bar{V}_{N,\mathcal{E}_i'}(\alpha;\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{i-1}'},\eta)-\sum_{l=0}^{p}\bar{V}^{(l)}_{N,\mathcal{E}_i'}(\alpha;\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{i-1}'},\eta)\right)=O(\varepsilon^{p+1}). \tag{2.32}$$

We shall see in Section 3.1.1 that due to the definition of the D_l' for every $1 \leq i < 2^d$, every $\eta \in \bar{S}_M$ and every $\alpha^{\mathcal{E}_1'} \in S_{N,\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{i-1}'} \in S_{N,\mathcal{E}_{i-1}'}$ compatibles with η the probability measure defined on the elements of $S_{N,\mathcal{E}_i'}$ compatibles with η by

$$\gamma^{(2)}_{N,\mathcal{E}_i'}(\alpha;\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{i-1}'},\eta)=\frac{e^{-\beta(\sum_{p=0}^{2}\bar{V}^{(p)}_{N,\mathcal{E}_i'}(\alpha;\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{i-1}'}\eta))}}{\bar{Z}^{(2)}_{N,\mathcal{E}_i'}(\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{i-1}'},\eta)}\bigotimes_{k\in\mathcal{E}_i'\cap\bar{\Lambda}_M}\tilde{\rho}_k(\alpha^{C_k}) \tag{2.33}$$

is a product measure. Finally, for every $\eta \in \bar{S}_M$ we define a probability measure on S_N by

$$\gamma^{(2)}_N(\sigma;\eta)=\left(\prod_{i=1}^{2^d-1}\gamma^{(2)}_{N,\mathcal{E}_i'}(\sigma^{\mathcal{E}_i'};\sigma^{\mathcal{E}_1'},\ldots,\sigma^{\mathcal{E}_i'},\eta)\right)\mu_{N,\mathcal{E}_{2^d}'}(\sigma^{\mathcal{E}_{2^d}'}|\sigma^{\mathcal{E}_1'},\ldots,\sigma^{\mathcal{E}_{2^d-1}'},\eta) \tag{2.34}$$

if σ and η are compatible and $\gamma^{(2)}_N(\sigma;\eta)=0$ otherwise. We get

COROLLARY 2.6. *If $\delta = Q\varepsilon < \delta_0$ then for every $\eta \in \bar{S}_M$ the following estimate holds*

$$\frac{1}{N}H(\gamma^{(2)}_N(\cdot;\eta)|\mu_N(\cdot|\eta))=O(\delta^3) \tag{2.35}$$

where the O is uniform in $\eta \in \bar{S}_M$.

From the preceding result and the fact that for every $\eta \in \bar{S}_M$ the probability $\gamma^{(2)}_N(\cdot;\eta)$ is a product we derive the

Scheme C

1. We run in parallel $U/2^d$ constrained simulations with CG boundary conditions given by η to get $\alpha^{\mathcal{E}_1'}$ sampled from $\gamma^{(2)}_{N,\mathcal{E}_1'}(\cdot;\eta)$.

2. For every integer i starting from 2 and up to 2^d-1 we run in parallel $U/2^d$ constrained simulations with mixed CG/microscopic boundary conditions given by $\eta, \alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{i-1}'}$ to get $\alpha^{\mathcal{E}_i'} \in S_{N,\mathcal{E}_i'}$ sampled from $\gamma^{(2)}_{N,\mathcal{E}_i'}(\cdot;\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{i-1}'},\eta)$.

3. We run in parallel $U/2^d$ constrained simulations with microscopic boundary conditions given by $\alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{2^d-1}'}$ to obtain $\alpha^{\mathcal{E}_{2^d}'} \in S_{N,\mathcal{E}_{2^d}'}$ sampled from $\mu_{N,\mathcal{E}_{2^d}'}(\cdot|\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{2^d-1}'},\eta)$.

4. We obtain a sample of $\gamma^{(2)}_N(\cdot;\eta)$ by taking $[\alpha^{\mathcal{E}_1'},\ldots,\alpha^{\mathcal{E}_{2^d}'}]$.

Numerical experiments following Scheme C are presented in Section 4. Actually, as it is explained in Section 3.1.1, for every integer p up to $n/(L2^{(d+1/d)})$ one can define reconstruction schemes similar to Schemes A and C (i.e. consisting of 2^d steps of parallel computations) with global error $O(\delta^{p+1})$ in approximating $\mu_N(\cdot|\eta)$. For example, by taking reconstruction cells D_l'' with $(3L)^d$ microscopic lattice points one can define a scheme with 2^d steps of parallel computations and error $O(\delta^4)$ in approximating $\mu_N(\cdot|\eta)$.

2.2.2. Reconstruction schemes in the $q > L$ case. As in Section 2.2.1 in order to simplify notations and without loss of generality we assume that there exist two integers u and r such that $n = 2urq$. In the $q > L$ case the role of the small parameter is played by

$$\delta = \frac{L}{rq}.$$

Our result holds true as soon as the microscopic model satisfies a uniform strong mixing condition for multi-grand-canonical states (Condition MUSM given in Section 2.7 in [3]). By using Dobrushin's single site condition one can prove that there exists a constant ε_0 such that if $\beta||J|| < \varepsilon_0$ this strong mixing condition is satisfied.

We partition $\mathbb{T}_d$ into $2^d U$ ($U = u^d$) cells as in Section 2.2.1 and accordingly define reconstruction domains D_l that contain $R = r^d$ coarse-cells each. The $\mathcal{L}_i$'s, $\mathcal{E}_i$'s, and $S_{N,\mathcal{E}_i}$'s are defined on the ground of these D_l's as in Section 2.2.1. Again our starting point is the decomposition (2.9) and the corresponding "exact" reconstruction Hamiltonians (2.13). For every integer i such that $1 \leq i < 2^d$ we need to define a first approximation $\bar{W}^{(0)}_{N,\mathcal{E}_i}$ which is not the one given by (2.15). Indeed such an approximation would lead to an error of order $O(q/L)$ which is $O(1)$ since $q > L$. Before we give our result let us introduce one more notation. For every $l, l' \in (\mathbb{Z} \cap [0, 2u-1])^d$ and every $\sigma \in S_N$ we write

$$H_{l,l'}(\sigma^{D_l}, \sigma^{D_{l'}}) = \begin{cases} -\frac{1}{2} \sum_{x \in D_l \cap \Lambda_N} \sum_{\substack{y \in D_l \cap \Lambda_N, \\ x \neq y}} J(x-y)\sigma^{D_l}(x)\sigma^{D_l}(y) & \text{if} \quad l = l' \\ -\sum_{x \in D_l \cap \Lambda_N, y \in D_{l'} \cap \Lambda_N} J(x-y)\sigma^{D_l}(x)\sigma^{D_{l'}}(y) & \text{if} \quad l \neq l' \end{cases}$$

and we shall use the shortcut $H_{l,l}(\sigma^{D_l}) = H_{l,l}(\sigma^{D_l}, \sigma^{D_l})$.

THEOREM 2.7. *For every integer i such that $1 \leq i < 2^d$, every $\eta \in \bar{S}_M$ and $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}$ compatible with η and every $l \in (\mathbb{Z} \cap [0, 2u-1])^d$ such that $D_l \subset \mathcal{E}_i$ there exists a function $\bar{X}^{(0)}_{N,l}(\,\cdot\,; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta)$ defined on S_{N,D_l} such that*

$$\bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \sum_{l: D_l \subset \mathcal{E}_i} \Big(H_{l,l}(\alpha^{D_l}) + \bar{X}^{(0)}_{N,l}(\alpha^{D_l}; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) \Big) \tag{2.36}$$

satisfies

$$\frac{\beta}{N} \Big(\bar{W}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) - \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) \Big) = O(\frac{\delta}{N}) \tag{2.37}$$

uniformly in $\alpha \in S_{N,\mathcal{E}_i}$ and $\eta, \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}$.

The computation of the $\bar{X}^{(0)}_{N,l}$'s is described in Section 3.2. We propose as an approximation of the exact reconstruction measure on $\mathcal{E}_i$ the following

$$\nu^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \frac{e^{-\beta \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta)}}{Z^{(0)}_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta)} \bigotimes_{k \in \mathcal{E}_i \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \tag{2.38}$$

and define a reconstruction measure $\nu^{(0)}_N(\cdot; \eta)$ as in (2.21). We get

COROLLARY 2.8. *If $\beta||J|| < \varepsilon_0$ then for every $\eta \in \bar{S}_M$ the following estimate holds*

$$\frac{1}{N} H \Big(\nu^{(0)}_N(\cdot; \eta) | \mu_N(\cdot|\eta) \Big) = O(\frac{\delta}{N}) \tag{2.39}$$

where the O is uniform in $\eta \in \bar{S}_M$.

Due to the particular form of the the $\bar{X}^{(0)}_{N,l}$'s this first approximation factorizes over the reconstruction domains D_l belonging to $\mathcal{E}_i$. As a consequence we propose the following

Scheme D

1. We run in parallel U constrained simulations with CG boundary conditions given by η to get $\alpha^{\mathcal{E}_1}$ sampled from $\nu^{(0)}_{N,\mathcal{E}_1}(\cdot; \eta)$.

2. For every integer i starting from 2 and up to $2^d - 1$ we run in parallel U constrained simulations with mixed CG/microscopic boundary conditions given by $\eta, \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}$ to get $\alpha^{\mathcal{E}_i} \in S_{N,\mathcal{E}_i}$ sampled from $\nu^{(0)}_{N,\mathcal{E}_i}(\cdot; \alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{i-1}}, \eta)$.

3. We run in parallel U constrained simulations with microscopic boundary conditions given by $\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{2^d-1}}$ to obtain $\alpha^{\mathcal{E}_{2^d}} \in S_{N,\mathcal{E}_{2^d}}$ sampled from $\mu_{N,\mathcal{E}_{2^d}}(\cdot|\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{2^d-1}}, \eta)$.

4. We obtain a sample of $\nu^{(0)}_N(\cdot; \eta)$ by taking $[\alpha^{\mathcal{E}_1}, \ldots, \alpha^{\mathcal{E}_{2^d}}]$.

Numerical experiments following this scheme are presented in Section 4. Unlike the $q < L$ case we are not able here to propose parallel computation schemes with higher order error estimates.

2.2.3. Overall reconstruction schemes. Combining the methods presented in Section (2.2.1) in the $q < L$ case with the Coarse-Grained Monte Carlo (CGMC) algorithm described in [13] gives a numerically advantageous method to get samples from a measure $\mathcal{G}_N$ defined on S_N that approximates μ_N arbitrarily well. Indeed, for every integer $p \geq 0$ the CGMC method consists on a direct Monte Carlo Markov Chain sampling from a Gibbs measure $\bar{\mu}_M^{(p)}$ defined on $\bar{S}_M$ and such that

$$\frac{1}{N} H(\bar{\mu}_M^{(0)} | \bar{\mu}_M) = O(\varepsilon^2)$$

and for every $p \geq 1$

$$\frac{1}{N} H(\bar{\mu}_M^{(p)} | \bar{\mu}_M) = O(\varepsilon^{p+1})$$

with ε defined in (2.8). Notice that for every $\eta \in \bar{S}_M$ and every $\sigma \in S_N$ such that $F(\sigma) = \eta$ we have

$$\mu_N(\sigma) = \mu_N(\sigma|\eta)\bar{\mu}_M(\eta). \tag{2.40}$$

By defining e.g. $\mathcal{G}_N^{(2)}$ on S_N by

$$\mathcal{G}_N^{(2)}(\sigma) = \gamma_N^{(2)}(\sigma;\eta)\bar{\mu}_M^{(2)}(\eta) \tag{2.41}$$

with $\gamma_N^{(2)}(\sigma;\eta)$ as defined in (2.34) the separation of scales in both (2.40) and (2.41) leads to

$$\begin{aligned} \frac{1}{N} H(\mathcal{G}_N^{(2)} | \mu_N) &= \frac{1}{N} H(\bar{\mu}_M^{(2)} | \bar{\mu}_M) + \frac{1}{N} \sum_{\eta \in \bar{S}_M} \bar{\mu}_M^{(2)}(\eta)\, H(\gamma_N^{(2)}(\cdot;\eta) | \mu_N(\cdot|\eta)) \\ &= O(\varepsilon^3). \end{aligned}$$

In view of the latter result we propose the following algorithm

Scheme E
1. We run a CGMC simulation and obtain $\eta \in \bar{S}_M$ sampled from $\bar{\mu}_M^{(2)}$.
2. We run in parallel $N/(4L)^d$ constrained simulations with CG boundary conditions given by η to get $\alpha^{\mathcal{E}_1'}$ sampled from $\gamma_{N,\mathcal{E}_1'}^{(2)}(\cdot;\eta)$.
3. For every integer i starting from 2 and up to $2^d - 1$ we run in parallel $N/(4L)^d$ constrained simulations with mixed CG/microscopic boundary conditions given by $\eta, \alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{i-1}'}$ to get $\alpha^{\mathcal{E}_i'} \in S_{N,\mathcal{E}_i'}$ sampled from $\gamma_{N,\mathcal{E}_i'}^{(2)}(\cdot; \alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{i-1}'}, \eta)$.
4. We run in parallel $N/(4L)^d$ constrained simulations with microscopic boundary conditions given by $\alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{2^d-1}'}$ to obtain $\alpha^{\mathcal{E}_{2^d}'} \in S_{N,\mathcal{E}_{2^d}'}$ sampled from $\mu_{N,\mathcal{E}_{2^d}'}(\cdot|\alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{2^d-1}'}, \eta)$.
5. We obtain a sample of $\mathcal{G}_N^{(2)}$ by taking $[\alpha^{\mathcal{E}_1'}, \ldots, \alpha^{\mathcal{E}_{2^d}'}]$.

Numerical experiments following this scheme are presented in Section 4.

3. Proofs.

3.1. The $q < L$ case. The main content of this section is the identification of the higher order corrections to the first approximation Scheme A. This is achieved in Section 3.1.1. There we further show that the error estimates (2.20, 2.25, 2.32) are simple consequences of this higher-order computation. The estimation of the errors measured in specific relative entropy (2.22, 2.27, 2.35) is carried out in Section 3.1.2.

3.1.1. The series expansion. We want to construct corrections for the initial choices (2.15, 2.19). For this one would like to expand the exponential in (2.23), but the exponent is not small: It is of the order of the volume times some small parameter. Cluster expansions are tools which allow to expand such quantities in convergent power series using the independence properties of product measures. Let i be an integer such that $1 \leq i < 2^d$, $\eta \in \bar{S}_M$ and $\alpha^{\mathcal{E}_1} \in S_{N,\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}} \in S_{N,\mathcal{E}_{i-1}}$ compatibles with η. For every $\alpha \in S_{N,\mathcal{E}_i}$ compatible with η and every $\sigma \in S_N$ such that $\sigma^{\mathcal{E}_1} = \alpha^{\mathcal{E}_1}, \dots, \sigma^{\mathcal{E}_{i-1}} = \alpha^{\mathcal{E}_{i-1}}, \sigma^{\mathcal{E}_i} = \alpha$ we have

$$H_N(\sigma) - \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \sum_{\substack{(k,k') \in \bar{\Lambda}_M, \\ k \leq k'}} \bar{\Delta}_{k,k'} J(\sigma; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \alpha)$$

where " $\leq$ " stands for the lexicographical order on $\mathbb{Z}^d$ and

$$\bar{\Delta}_{k,k'} J(\sigma) = \begin{cases} \Delta_{k,k'} J(\sigma) & \text{if there is } l \in \mathcal{L}_{i+1} \cup \dots \cup \mathcal{L}_{2^d} \text{ s.t. } k, k' \in D_l \\ \breve{\Delta}_{k,k'} J(\sigma) & \text{if there is } l \in \mathcal{L}_{i+1} \cup \dots \cup \mathcal{L}_{2^d} \text{ and } l' \in \mathcal{L}_i \text{ s.t. } k \in D_l, k' \in D_{l'} \\ \tilde{\Delta}_{k,k'} J(\sigma) & \text{if there is } l \in \mathcal{L}_i \text{ and } l' \in \mathcal{L}_{i+1} \cup \dots \cup \mathcal{L}_{2^d} \text{ s.t. } k \in D_l, k' \in D_{l'} \\ 0 & \text{otherwise} \end{cases}$$

with

$$\Delta_{k,k'} J(\sigma; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \alpha) = -\frac{1}{2} \sum_{\substack{x \in C_k \\ y \in C_{k'}, y \neq x}} (J(x-y) - \bar{J}(k,k'))\sigma(x)\sigma(y)(2 - \delta_{k,k'}),$$

$$\breve{\Delta}_{k,k'} J(\sigma; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \alpha) = - \sum_{\substack{x \in C_k \\ y \in C_{k'}}} (J(x-y) - \breve{J}(k,y))\sigma(x)\alpha^{C_{k'}}(y),$$

and

$$\tilde{\Delta}_{k,k'} J(\sigma; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \alpha) = - \sum_{\substack{x \in C_k \\ y \in C_{k'}}} (J(x-y) - \breve{J}(k',y))\alpha^{C_k}(x)\sigma(y).$$

In order to shorten the notations and since $\eta, \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}$ are given we shall simply write $\bar{\Delta}_{k,k'} J(\sigma)$. These terms are connected to the small parameter δ since it follows from a simple Taylor expansion that for every $k, k' \in \bar{\Lambda}_M$

$$\sup_{\eta \in \bar{S}_M} \sup_{j:1 \leq j \leq i-1} \sup_{\alpha^{\mathcal{E}_j} \in S_{N,\mathcal{E}_j}} \sup_{\alpha \in S_{N,\mathcal{E}_i}} \sup_{\sigma \in S_N} |\bar{\Delta}_{k,k'} J(\sigma)| \leq 2 \frac{q^{2d+1}}{L^{d+1}} ||\nabla V||_\infty.$$

By letting

$$\bar{f}_{k,k'}(\sigma) = e^{-\beta \bar{\Delta}_{k,k'} J(\sigma)} - 1 \tag{3.1}$$

we get

$$E_N[e^{-\beta(H_N(\sigma) - \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta))} | \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \alpha, \eta] =$$

$$= \int \prod_{\substack{k,l \in \bar{\Lambda}_M \\ k \leq l}} (1 + \bar{f}_{k,l}) \left(\prod_{j=1}^{i-1} 1_{\{\sigma:\ \sigma^{\mathcal{E}_j} = \alpha^{\mathcal{E}_j}\}} \right) 1_{\{\sigma:\ \sigma^{\mathcal{E}_i} = \alpha\}} \bigotimes_{k \in \bar{\Lambda}_M \cap \mathcal{E}_{i+1} \cup \dots \cup \mathcal{E}_{2^d}} \tilde{\rho}_k(\sigma).$$

The polymer model is as in [13] with the only difference that we are integrating over the domain $\mathcal{E}_{i+1} \cup \dots \cup \mathcal{E}_{2^d}$ keeping fixed the variables $\sigma^{\mathcal{E}_j}$ for $1 \leq j \leq i$. In order to benefit from the analysis carried out in [13] we introduce the following notation:

$$\hat\rho_k(\sigma) = \begin{cases} \tilde\rho_k(\sigma) & \text{if } k \in \bar\Lambda_M \cap (\mathcal{E}_{i+1} \cup \cdots \cup \mathcal{E}_{2^d}) \\ 1_{\{\sigma^{C_k} = \alpha^{C_k}\}} & \text{if } k \in \bar\Lambda_M \cap (\mathcal{E}_1 \cup \cdots \cup \mathcal{E}_i) \end{cases}$$

so

$$E_N[e^{-\beta(H_N(\sigma) - \bar W^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta))}|a^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\alpha,\eta] = \int_{S_N} \prod_{k,l\in\bar\Lambda_{M,\le}} (1+\bar f_{k,l}) \bigotimes_{k\in\bar\Lambda_M} \hat\rho_k(\sigma).$$

We shall simply write $\int$ for $\int_{S_N}$ when no confusion can occur. By expanding and arranging the terms in the sum into a cluster representation we obtain

$$E_N[e^{-\beta(H_N(\sigma) - \bar W^{(0)}_{N,\mathcal{E}}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta))}|a^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\alpha,\eta] = \sum_{n\ge 0}\frac{1}{n!} \sum_{\substack{(R_1,\ldots,R_n)\in\mathcal{R}^n \\ i\ne j \Rightarrow R_i\cap R_j=\emptyset,}} \prod_{i=1}^n \zeta(R_i) \tag{3.2}$$

where $\mathcal{R}$ is the set of non-empty subsets of $\bar\Lambda_M$. For every $R \in \mathcal{R}$ the activity $\zeta(R)$ of the cluster R is

$$\zeta(R) = \int \sum_{g\in G_R} \prod_{\{k,l\}\in g} \bar f_{kl}(\sigma) \bigotimes_{\{k\}\in R} \hat\rho_k(\sigma) \tag{3.3}$$

where G_R stands for the set of generalized connected graphs on the set R. The activities of the polymers are functions of η and α. By a straightforward adaptation of the proof of Lemma 2.3 in [13] (see also Theorem 2 in [4]) one can prove that there exists a $\delta_0 > 0$ such that if $\delta = Q\varepsilon < \delta_0$ then we have

$$\sup_{j:1\le j\le i-1} \sup_{\alpha^{\mathcal{E}_j}\in S_{N,\mathcal{E}_j}} \sup_{\alpha\in S_{N,\mathcal{E}_i}} \sup_{\eta\in\bar S_M} \sup_{k\in\bar\Lambda_M} \sum_{\substack{R\in\mathcal{R}, R\supset\{k\} \\ |R|=1}} |\zeta(R)| \le \delta$$

and for every $r \ge 2$

$$\sup_{j:1\le j\le i-1} \sup_{\alpha^{\mathcal{E}_j}\in S_{N,\mathcal{E}_j}} \sup_{\alpha\in S_{N,\mathcal{E}_i}} \sup_{\eta\in\bar S_M} \sup_{k\in\bar\Lambda_M} \sum_{\substack{R\in\mathcal{R}, R\supset\{k\} \\ |R|=r}} |\zeta(R)| \le \delta^{r-1}.$$

Then, according to Theorem 2 in [4] if $\delta = Q\varepsilon < \delta_0$ we get

$$\bar W_{N,\mathcal{E}}(\alpha,\eta) = \bar W^{(0)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\ldots,\alpha^{\mathcal{E}_{i-1}},\eta) - \frac{1}{\beta}\sum_{n\ge 1}\frac{1}{n!} \sum_{\substack{(R_1,\ldots,R_n)\in\mathcal{R}^n \\ R_i\subset\bar\Lambda_M}} \phi(R_1,\ldots,R_n)\prod_{i=1}^n \zeta(R_i) \tag{3.4}$$

with

$$\phi(R_1,\ldots,R_n) = \begin{cases} 1 & \text{if } n = 1 \\ \sum_{g\in G_n}\prod_{\{i,j\}\in g}(1(R_i,R_j)-1) & \text{if } n > 1 \end{cases}$$

where G_n is the set of the generalized, connected graphs on $\{1,\ldots,n\}$ and

$$1(R_i,R_j) = \begin{cases} 0 & \text{if } \{R_i\cap R_j \ne \emptyset\} \\ 1 & \text{if } \{R_i\cap R_j = \emptyset\}. \end{cases}$$

Again a straightforward adaptation of the proof of Lemma 2.1 in [13] shows that

$$\sum_{R\in\mathcal{R}, R\subset\bar\Lambda_M} |\zeta(R)| \le M(\delta + \sum_{r\ge 2}\delta^{r-1}) \tag{3.5}$$

and that for every $n \geq 2$

$$\frac{1}{n!} \sum_{\substack{(R_1,\dots,R_n)\in\mathcal{R}^n \\ R_i\subset\bar\Lambda_M}} |\phi(R_1,\dots,R_n)| \prod_{i=1}^{n} \zeta(R_i)| \leq \frac{M}{2(n-1)} \left(2e\frac{5}{4}\frac{\delta}{1-\delta}\right)^{n-1} \left(\delta e + \sum_{r\geq 2} r(\delta e)^{r-1}\right). \tag{3.6}$$

The inequalities (3.5) and (3.6) allow to identify in (3.4) the terms of the series expansion of Theorem 2.3. Now notice that all the controls depend on δ, M, Q and L but *not on the size of the reconstruction domains*: The same computations give formally the same corrections to the $\bar V^{(0)}_{N,\mathcal{E}'_i}$ under the same condition on δ. Hence the series expansion of Theorem 2.5 is also shown to hold. Now we are left to prove that Theorem 2.1 holds and that the sampling measures in scheme C are product measures. First we observe that

$$\begin{aligned}\bar W^{(1)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta) &= -\frac{1}{\beta}\sum_{R:|R|=1,2}\zeta(R)\\ &= O(M\delta)\end{aligned}$$

and

$$\begin{aligned}\bar W^{(2)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta) &= -\frac{1}{2\beta}\sum_{\substack{R_1,R_2\\|R_i|=1,2}}\phi(R_1,R_2)\zeta(R_1)\zeta(R_2) - \frac{1}{\beta}\sum_{R:|R|=3}\zeta(R)\\ &= O(M\delta^2).\end{aligned}$$

Actually, in the sums defining $\bar W^{(1)}_{N,\mathcal{E}_i}$ and $\bar W^{(2)}_{N,\mathcal{E}_i}$ some terms are already of order 4 or higher. Indeed

$$\begin{aligned}\bar W^{(1)}_{N,\mathcal{E}}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta) = &-\frac{1}{\beta}\sum_{k\in\bar\Lambda_M}\int \bar f_{kk}\hat\rho_k(\sigma)\\ &-\frac{1}{\beta}\sum_{(k,l)\in\bar\Lambda_{M,\leq}}\int(\bar f_{kl}+\bar f_{kl}\bar f_{kk}+\bar f_{kl}\bar f_{ll}+\bar f_{kl}\bar f_{kk}\bar f_{ll})\hat\rho_k(\sigma)\hat\rho_l(\sigma)\end{aligned} \tag{3.7}$$

and

$$\begin{aligned}\bar W^{(2)}_{N,\mathcal{E}_i}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{i-1}},\eta) = &\frac{1}{2\beta}\sum_{k\in\bar\Lambda_M}\left(\int \bar f_{kk}\hat\rho_k(\sigma)\right)^2 +\\ &+\frac{1}{2\beta}\sum_{(k,l)\in\bar\Lambda_{M,\leq}}\int \bar f_{kk}\hat\rho_k(\sigma)\int(\bar f_{kl}+\bar f_{kl}\bar f_{kk}+\bar f_{kl}\bar f_{ll}+\bar f_{kl}\bar f_{kk}\bar f_{ll})\hat\rho_k(\sigma)\hat\rho_l(\sigma)+\\ &+\frac{1}{2\beta}\sum_{k\in\{0,\dots,M-1\}}\ \sum_{l_1:(k,l_1)\in\bar\Lambda_{M,\leq}}\ \sum_{l_2:(k,l_2)\in\bar\Lambda_{M,\leq}}\\ &\int(\bar f_{kl_1}+\bar f_{kk}\bar f_{kl_1}+\bar f_{kl_1}\bar f_{l_1l_1}+\bar f_{kk}\bar f_{kl_1}\bar f_{l_1l_1})\hat\rho_k(\sigma)\hat\rho_{l_1}(\sigma)\times\\ &\times\int(\bar f_{kl_2}+\bar f_{kk}\bar f_{kl_2}+\bar f_{kl_2}\bar f_{l_2l_2}+\bar f_{kk}\bar f_{kl_2}\bar f_{l_2l_2})\hat\rho_k(\sigma)\hat\rho_{l_2}(\sigma)+\\ &-\frac{1}{\beta}\sum_{k\in\{0,\dots,M-1\}}\ \sum_{l_1:(k,l_1)\in\bar\Lambda_{M,\leq}}\ \sum_{l_2:(l_1,l_2)\in\bar\Lambda_{M,\leq}\text{ or }(k,l_2)\in\bar\Lambda_{M,\leq}}\\ &\int(\bar f_{kl_1}\bar f_{l_1l_2}+\bar f_{kl_1}\bar f_{kl_2}+\bar f_{kl_2}\bar f_{l_1l_2}+[\dots])\hat\rho_k(\sigma)\hat\rho_{l_1}(\sigma)\hat\rho_{l_2}(\sigma)\end{aligned} \tag{3.8}$$

where $[\dots]$ means the previous three terms with all possible combinations of loops. Combining (3.7) and (3.8) with the facts that

$$\bar f_{k,l}(\sigma) = e^{-\beta\bar\Delta_{kl}J(\sigma)}-1 = \sum_{p=1}^{\infty}\frac{1}{p!}(-\beta\bar\Delta_{kl}J(\sigma))^p \text{ with } \bar\Delta_{kl}J(\sigma)\sim O(q^{2d}\frac{q}{L^{2d+1}}\|\nabla V\|_\infty) \tag{3.9}$$

uniformly in $\sigma \in S_N, \alpha \in S_{N,\mathcal{E}}$ and $\eta \in \bar{S}_M$ and that for every $k, l \in \bar{\Lambda}_M$

$$\int \bar{\Delta}_{k,l} J(\sigma) \hat{\rho}_k(\sigma) \hat{\rho}_l(\sigma) = 0$$

we get an improved estimate on $\bar{W}^{(1)}_{N,\mathcal{E}}$

$$\begin{aligned} -\bar{W}^{(1)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \beta \sum_k \int \frac{1}{2} (\bar{\Delta}_{kk} J(\sigma))^2 \hat{\rho}_k(\sigma) + \beta \sum_{k<l} \int \frac{1}{2} (\bar{\Delta}_{kl} J(\sigma))^2 \hat{\rho}_k(\sigma) \hat{\rho}_l(\sigma) + \\ + \beta \sum_{k<l} \int \bar{\Delta}_{kk} J(\sigma) \bar{\Delta}_{kl} J(\sigma) \hat{\rho}_k(\sigma) \hat{\rho}_l(\sigma) + \\ + \beta \sum_{k<l} \int \bar{\Delta}_{kl} J(\sigma) \bar{\Delta}_{ll} J(\sigma) \hat{\rho}_k(\sigma) \hat{\rho}_l(\sigma) \\ = O(M\delta^2) \end{aligned} \tag{3.10}$$

and

$$\begin{aligned} -\bar{W}^{(2)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta) = \beta \sum_{k_1} \sum_{k_2 > k_1} \sum_{k_3 > k_2} \int \bar{\Delta}_{k_1 k_2} J(\sigma) \bar{\Delta}_{k_2 k_3} J(\sigma) \hat{\rho}_{k_1}(\sigma) \hat{\rho}_{k_2}(\sigma) \hat{\rho}_{k_3}(\sigma) + \\ + \int \bar{\Delta}_{k_2 k_3} J(\sigma) \bar{\Delta}_{k_1 k_3} J(\sigma) \hat{\rho}_{k_2}(\sigma) \hat{\rho}_{k_3}(\sigma) \hat{\rho}_{k_1}(\sigma) + \\ + \int \bar{\Delta}_{k_1 k_3} J(\sigma) \bar{\Delta}_{k_1 k_2} J(\sigma) \hat{\rho}_{k_3}(\sigma) \hat{\rho}_{k_1}(d\sigma) \hat{\rho}_{k_2}(\sigma) \\ = O(M\delta^2) \end{aligned} \tag{3.11}$$

the other terms from (3.7) and (3.8) being higher order. In particular this proves that as soon as $\delta < \delta_0$ we have

$$\frac{\beta}{N} \left(\bar{W}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta) - \bar{W}^{(0)}_{N,\mathcal{E}_i}(\alpha; \alpha^{\mathcal{E}_1}, \dots, \alpha^{\mathcal{E}_{i-1}}, \eta) \right) = O(\varepsilon^2)$$

uniformly in η, α and σ and Theorem 2.1 is thus established.

In the $p = 2$ case the obtained reconstruction kernel is not a product measure only because of the presence of terms like e.g. $\bar{\Delta}_{k_1 k_2} J(\sigma) \bar{\Delta}_{k_2 k_3} J(\sigma)$ with $k_1 \in D_l \subset \mathcal{E}_i$, $k_3 \in D_{l'} \subset \mathcal{E}_i$, $l \neq l'$ and $k_2 \in \mathcal{E}_2 \cap \bar{\Lambda}_M$ for some integer j such that $i < j \leq 2^d$. Should we have reconstructed over domains with $(2L)^d$ microscopic points we would have got formally the same expression with the difference that if say $\bar{\Delta}_{k_1 k_2} J(\sigma) \neq 0$ then necessarily C_{k_1} and C_{k_2} are less than L microscopic points away which implies that C_{k_2} and C_{k_3} are at least L microscopic points away hence $\bar{\Delta}_{k_2 k_3} J(\sigma) = 0$ (remember that due to the definition of the reconstruction domains $D_l^{'}$ the coarse-cells C_{k_1} and C_{k_3} are at least $2L$ microscopic points away). It follows from this observation that for every $\eta \in \bar{S}_M$ the measure $\gamma^{(2)}_{N,\mathcal{E}'}(\cdot; \eta)$ is product.

Finally, it is clear from (3.6) that in the definition of a reconstruction scheme with $O(\delta^4)$ error one has to consider terms like $\bar{\Delta}_{k_1,k_2} J(\sigma) \bar{\Delta}_{k_2,k_3} J(\sigma) \bar{\Delta}_{k_3,k_4} J(\sigma)$. The previous observation applies once again and we see that by choosing reconstruction domains $D_l^{''}$ including $(3L)^d$ microscopic points, for every $\sigma \in S_N$ at least one of the 3 factors in the previous expression cancels making the kernel in the first step of the reconstruction algorithm a product measure.

3.1.2. Specific relative entropy estimate. In this section we prove (2.27). The proof of all specific relative entropy estimates given in this paper, including those of Section 2.2.2 and 2.2.3

work the same way. For every integer $p \geq 1$ and every $\eta \in \bar{S}_M$ we have:

$$
\begin{aligned}
&\frac{1}{N} H(\nu_N^{(p)}(\cdot;\eta)|\mu_N(\cdot|\eta)) \\
&= \frac{1}{N} \sum_{\sigma \in S_N} \nu_N^{(p)}(\sigma;\eta) \log \frac{\nu_N^{(p)}(\sigma;\eta)}{\mu_N(\sigma|\eta)} \\
&= \frac{1}{N} \sum_{\sigma \in S_N} \left[\left(\prod_{i=1}^{2^d-1} \nu_{N,\mathcal{E}_i}^{(p)}(\sigma^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta) \right) \mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}} | \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{2^d-1}}, \eta) \times \right. \\
&\qquad \left. \times \log \frac{(\prod_{i=1}^{2^d-1} \nu_{N,\mathcal{E}_i}^{(p)}(\sigma^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)) \mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}} | \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{2^d-1}}, \eta)}{\prod_{i=1}^{2^d} \mu_{N,\mathcal{E}_i}(\sigma^{\mathcal{E}_i} | \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)} \right] \\
&= \frac{1}{N} \sum_{\sigma \in S_N} \left(\prod_{i=1}^{2^d-1} \nu_{N,\mathcal{E}_i}^{(p)}(\sigma^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta) \right) \mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}} | \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{2^d-1}}, \eta) \times \\
&\quad \times \left[\sum_{i=1}^{2^d} \left(-\beta(\bar{W}_{N,\mathcal{E}_i}^{(p)}(\sigma^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta) - \bar{W}_{N,\mathcal{E}_i}(\sigma^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)) + \right. \right. \\
&\qquad \left. \left. + \log \frac{\bar{Z}_{N,\mathcal{E}_i}(\sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)}{\bar{Z}_{N,\mathcal{E}_i}^{(p)}(\sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)} \right) \right] \qquad (3.12)
\end{aligned}
$$

and for every integer i such that $1 \leq i < 2^d - 1$ we have

$$
\begin{aligned}
&Z_{N,\mathcal{E}_i}^{(p)}(\sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta) \\
&= \int_{S_{N,\mathcal{E}_i}} e^{-\beta \bar{W}_{N,\mathcal{E}_i}^{(p)}(\alpha^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)} \bigotimes_{k \in \mathcal{E}_i \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \\
&= \int_{S_{N,\mathcal{E}_i}} e^{-\beta(\bar{W}_{N,\mathcal{E}_i}^{(p)}(\alpha^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta) - \bar{W}_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)) - \beta \bar{W}_{N,\mathcal{E}_i}(\alpha^{\mathcal{E}_i}; \sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)} \bigotimes_{k \in \mathcal{E}_i \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \\
&= e^{NO(\varepsilon^{p+1})} \bar{Z}_{N,\mathcal{E}_i}(\sigma^{\mathcal{E}_1}, \ldots, \sigma^{\mathcal{E}_{i-1}}, \eta)
\end{aligned}
$$

which combined with (2.25) and (3.12) proves the announced result.

3.2. The $q > L$ case. The main content of this section is the computation of the $\bar{X}_{N,l}^{(0)}$'s in Theorem 2.7. In order to simplify notations and without loss of generality we shall take $r = 1$. The $\bar{X}_{N,l}^{(0)}$'s are obtained through a "backward" induction procedure, from indices l such that $D_l \subset \mathcal{L}_{2^d}$ to indices l such that $D_l \subset \mathcal{L}_1$. We shall detail one step of this induction. Unlike the $q < L$ case here we work out a *rewriting* of $\mu_N(\cdot|\eta)$ based on a backward procedure aimed at taking profit of the strong mixing condition satisfied by the microscopic model. Once this is done we easily obtain approximations as in (2.10), the "0-th order" of which are the ones that appear in (2.38). The difficulty in order to determine the terms that correspond to the reconstruction measure over $\mathcal{E}_i$ is to control how the extra terms which appear in each integration in the previous sublattices indexed by $2^d, \ldots, i+1$ get accommodated into the current sublattice of integration. To this end we follow the strategy presented in [20] for the factorization of finite-volume Gibbs measures.

Let us introduce some more notations. For every $l \in (\mathbb{Z} \cap [0, 2u-1])^d$ we shall denote by $p(l)$ the unique $i \in \{1, \ldots, 2^d\}$ such that $D_l \subset \mathcal{E}_i$. For every integer $i \in \{1, \ldots, 2^d\}$ and every $\sigma \in S_N$ we shall write $\sigma^{<i} = \sigma^{\cup_{j<i} \mathcal{E}_j}$. We split the Hamiltonian as follows:

$$
H_N(\sigma) = \sum_{i=1}^{2^d} \sum_{l:\, p(l)=i} H_{l,l}(\sigma^{D_l}) + \sum_{i=1}^{2^d} \sum_{l:\, p(l)=i} W_{l,i}(\sigma^{D_l}, \sigma^{<i}) \qquad (3.13)
$$

where

$$
W_{l,i}(\sigma^{D_l},\, \sigma^{<i}) := \sum_{\{l':\, \|l'-l\|=1,\, p(l')<i\}} H_{l,l'}(\sigma^{D_l}, \sigma^{D_{l'}})
$$

is the energy due to the interaction of D_l with the neighboring reconstruction domains ($\|l'-l\| := \max_{i=1,\dots,d}|l'_i - l_i|$). Given a reconstruction domain D_l we define the set of neighboring reconstruction domains by $\partial D_l := \cup_{\{l' :\, \|l'-l\|=1\}} D_{l'}$, and $\partial D_l^< := \cup_{\{l' :\, \|l'-l\|=1,\, p(l')<p(l)\}} D_{l'}$. Finally for every $k \in \mathcal{L}_{2^d}$ we write $A_{2^d}(k) = D_k$ and for every integer i such that $1 \le i \le 2^d - 1$ and every $k \in \mathcal{L}_i$ we take $A_i(k) = D_{k-e_{i+1}} \cup D_k \cup D_{k+e_{i+1}}$.

Reconstruction measure on $\mathcal{E}_{2^d}$. We first define the reconstruction measure on all $D_l \subset \mathcal{E}_{2^d}$. As noticed in (2.11) we naturally have

$$\bar{X}^{(0)}_{N,l}(\alpha^{D_l};\, \alpha^{<2^d}, \eta) = W_{l,2^d}(\alpha^{D_l};\, \alpha^{<2^d})$$

and no error results from reconstructing over $\mathcal{E}_{2^d}$ once $\sigma^{<2^d}$ is given. However we shall detail how this can be obtained as the initial step of our backward induction scheme in order to show how extra couplings on the $\sigma^{<2^d}$ appear. We rewrite $\mu_N(\sigma|\eta)$ as a measure over $S_{N,\mathcal{E}_{2^d}}$ with $\sigma^{<2^d}$ as a fixed boundary conditions

$$e^{-\beta H_N(\sigma)} \prod_{k\in\bar\Lambda_M} \tilde\rho_k(\sigma^{D_k}) = \prod_{i=1}^{2^d-1} \prod_{k\in\mathcal{E}_i\cap\bar\Lambda_M} \Big(e^{-\beta H_{k,k}(\sigma^{D_k},\sigma^{D_k})} e^{-\beta W_{k,i}(\sigma^{D_k},\sigma^{<i})} \tilde\rho_k(\sigma^{D_k})\Big) \times \prod_{k\in\mathcal{E}_{2^d}\cap\bar\Lambda_M} Z(A_{2^d}(k);\sigma^{<2^d};\eta(k))\;\; \mu_{N,D_k}(\sigma^{D_k}|\,\sigma^{<2^d},\eta) \tag{3.14}$$

where we obtain the following reconstruction measure over $\mathcal{E}_{2^d}$:

$$\mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}}|\,\sigma^{<2^d},\eta) := \prod_{k\in\mathcal{E}_{2^d}\cap\bar\Lambda_M} \left[\frac{1}{Z(A_{2^d}(k);\sigma^{<2^d};\eta(k))} e^{-\beta W_{k,2^d}(\sigma^{D_k};\sigma^{<2^d})} e^{-\beta H_{k,k}(\sigma^{D_k})} \tilde\rho_k(\sigma^{D_k})\right]. \tag{3.15}$$

Note that $\mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}}|\,\sigma^{<2^d},\eta)$ is normalized for all fixed boundary conditions $\sigma^{<2^d}$ and canonical constraints $\eta(k)$, $k \in \mathcal{E}_{2^d}\cap\bar\Lambda_M$. The point is that in order to write a product measure over $k \in \mathcal{E}_{2^d}\cap\bar\Lambda_M$ we introduced through $Z(A_{2^d}(k);\sigma^{<2^d};\eta(k))$ extra couplings between (among others) the variables $\sigma^{\mathcal{E}_{2^d-1}} \in S_{N,\mathcal{E}_{2^d-1}}$ that we want to accommodate into a new "product" structure as we proceed with the definition of the reconstruction measure on $\mathcal{E}_{2^d-1}$. This is the context of the next paragraph.

Reconstruction measure on $\mathcal{E}_{2^d-1}$. As mentioned before for every $k \in \mathcal{L}_{2^d}$ the partition function

$$Z(A_{2^d}(k);\sigma^{<2^d};\eta(k)) = \int_{S_{N,A_{2^d}(k)}} e^{-\beta W_{k,2^d}(\sigma^{D_k};\sigma^{<2^d})} e^{-\beta H_{k,k}(\sigma^{D_k})} \tilde\rho_k(\sigma^{D_k})$$

depending on the boundary conditions $\sigma^{<2^d}$ on the set ∂D_k couples the configurations in $\partial D_k^<$. In particular, it couples the configurations $\sigma^{\mathcal{E}_{2^d-1}}$ and gives rise to an effective interaction between them. To define the measure on $\mathcal{E}_{2^d-1}$ we move along the vector e_{2^d} and we denote by $S^+_{k,e_{2^d}}Z$ the partition function on D_k with the same boundary conditions as $Z(A_{2^d}(k);\sigma^{<2^d};\eta)$ in the $+e_{2^d}$ direction of D_k, free boundary conditions in the $-e_{2^d}$ direction and unchanged in the other directions. Similarly, we denote by $S^-_{k,e_{2^d}}Z$ the partition function with free boundary conditions in the direction $+e_{2^d}$ and by $S^0_{k,e_{2^d}}Z$ with free in both $\pm e_{2^d}$ directions. Doing this we split the induced interaction between $D_{k-e_{2^d}}$ and $D_{k+e_{2^d}}$ into a factorized part and an error part:

$$Z(A_{2^d}(k);\sigma^{<2^d};\eta(k)) = \frac{(S^+_{k,e_{2^d}}Z)(S^-_{k,e_{2^d}}Z)}{(S^0_{k,e_{2^d}}Z)}(1+\Phi^1_k), \text{where } \Phi^1_k := \frac{Z(A_{2^d}(k);\sigma^{<2^d};\eta(k))(S^0_{k,e_{2^d}}Z)}{(S^+_{k,e_{2^d}}Z)(S^-_{k,e_{2^d}}Z)} - 1. \tag{3.16}$$

To follow the terminology in [20] this action is called *unfolding* in the direction e_{2^d}. According to Proposition 5.1 in [3] the assumptions on Theorem 2.7 imply that Φ^1_k is uniformly small: $\sup_\eta \sup_\sigma |\Phi^1_k| \le \delta$.

The new partition functions $(S^+_{k,e_{2^d}}Z)$ and $(S^-_{k,e_{2^d}}Z)$ are functions of $\sigma^{\mathcal{E}_{2^d-1}}$ indexed by $k \in \mathcal{L}_{2^d}$ and we want to index them with respect to $k \in \mathcal{L}_{2^d-1}$. Following [20] we call this action *splitting* in the direction e_{2^d}. We have:

$$\prod_{k\in\mathcal{L}_{2^d}} (S^+_{k,e_{2^d}}Z)(S^-_{k,e_{2^d}}Z) = \prod_{k\in\mathcal{L}_{2^d-1}} (S^+_{k-e_{2^d},e_{2^d}}Z)(S^-_{k+e_{2^d},e_{2^d}}Z). \tag{3.17}$$

Then, if we neglect for the moment the error term $(1+\Phi^1_k)$ in (3.16), we see (by plugging (3.16) into (3.14)) that in order to define $\mu_{N,\mathcal{E}_{2^d-1}}$ we have to deal with the following

$$\prod_{k\in\mathcal{L}_{2^d}} (S^0_{k,e_{2^d}}Z)^{-1} \prod_{k\in\mathcal{L}_{2^d-1}} \left[e^{-\beta H_k(\sigma^{D_k})} e^{-\beta W_{k,2^d-1}(\sigma^{D_k};\sigma^{<2^d-1})} (S^+_{k-e_{2^d},e_{2^d}}Z)(S^-_{k+e_{2^d},e_{2^d}}Z)\tilde{\rho}_k(\sigma^{D_k}) \right].$$

We obtain a quantity viewed as a partition function on $A_{2^d-1}(k), k \in \mathcal{L}_{2^d-1}$ by

$$Z(A_{2^d-1}(k);\sigma^{<2^d-1};\eta(k)) =$$

$$= \int_{S_{N,D_k}} e^{-\beta H_{k,k}(\sigma^{D_k})} e^{-\beta W_{k,2^d-1}(\sigma^{D_k};\sigma^{<2^d-1})} (S^+_{k-e_{2^d},e_{2^d}}Z)(S^-_{k+e_{2^d},e_{2^d}}Z)\tilde{\rho}_k(\sigma^{D_k})$$

that depends on $\sigma^{<2^d-2}$. By normalizing with this function we have

$$\begin{aligned} e^{-H_N(\sigma)} \prod_{k\in\mathcal{L}} \tilde{\rho}_k(\sigma) = \prod_{i\le 2^d-2} \prod_{k\in\mathcal{L}_i} \left(e^{-\beta H_{k,k}(\sigma^{D_k})} e^{-\beta W_{k,i}(\sigma^{D_k};\sigma^{<i})} \tilde{\rho}_k(\sigma^{D_k}) \right) \prod_{k\in\mathcal{L}_{2^d}} (S^0_{k,e_{2^d}}Z)^{-1} \times \\ \times \prod_{k\in\mathcal{L}_{2^d-1}} Z(A_{2^d-1}(k);\sigma^{<2^d-1};\eta(k)) \prod_{k\in\mathcal{L}_{2^d}} (1+\Phi^1_k) \times \\ \times \nu^{(0)}_{N,\mathcal{E}_{2^d-1}}(\sigma^{\mathcal{E}_{2^d-1}} |\, \sigma^{<2^d-1},\eta)\, \mu_{N,\mathcal{E}_{2^d}}(\sigma^{\mathcal{E}_{2^d}} |\, \sigma^{<2^d},\eta) \end{aligned} \tag{3.18}$$

where $\mu_{N,\mathcal{E}_{2^d-1}}$ is given by:

$$\begin{aligned} \nu^{(0)}_{N,\mathcal{E}_{2^d-1}}(\sigma^{\mathcal{E}_{2^d-1}} |\, \sigma^{<2^d-1},\eta) = \prod_{k\in\mathcal{L}_{2^d-1}} \left[\frac{1}{Z_{D_k}(\sigma^{<2^d-1};\eta(k))} e^{-\beta H_{k,k}(\sigma^{D_k})} e^{-\beta W_{k,2^d-1}(\sigma^{D_k};\sigma^{<2^d-1})} \times \right. \\ \left. \times\, (S^+_{k-e_{2^d},e_{2^d}}Z)(S^-_{k+e_{2^d},e_{2^d}}Z)\tilde{\rho}_k(\sigma^{D_k}) \right]. \end{aligned} \tag{3.19}$$

From (3.14), (3.16) and (3.17) we have:

$$\bar{W}_{N,\mathcal{E}_{2^d-1}}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{2^d-1}},\eta) = \frac{1}{\beta}\sum_{k\in\mathcal{L}_{2^d}} \log(S^{(0)}_{k,e_{2^d}}Z) - \frac{1}{\beta}\log\left[\prod_{k\in\mathcal{L}_{2^d}}(1+\Phi^1_k)\right]$$
$$-\frac{1}{\beta}\sum_{k\in\mathcal{L}_{2^d-1}} \left(-\beta H_{k,k}(\alpha^{D_k},\alpha^{D_k}) - \beta W_{k,2^d-1}(\alpha^{D_k},\alpha^{<2^d-1}) + \log\left[(S^+_{l-e_{2^d},e_{2^d}}Z)(S^-_{l+e_{2^d},e_{2^d}}Z) \right] \right).$$

Neglecting the terms that depend on η alone this leads us to propose

$$\bar{X}^{(0)}_{N,l}(\alpha^{D_l};\,\alpha^{<2^d-1},\eta) := W_{l,2^d-1}(\alpha^{D_l};\,\alpha^{<2^d-1}) - \frac{1}{\beta}\log\left[(S^+_{l-e_{2^d},e_{2^d}}Z)(S^-_{l+e_{2^d},e_{2^d}}Z) \right]$$

with error:

$$\frac{\beta}{N}\left(\bar{W}_{N,\mathcal{E}_{2^d-1}}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{2^d-2}},\eta) - \bar{W}^{(0)}_{N,\mathcal{E}_{2^d-1}}(\alpha;\alpha^{\mathcal{E}_1},\dots,\alpha^{\mathcal{E}_{2^d-2}},\eta) \right) = O(\frac{\delta}{N}).$$

For higher dimensions we proceed by repeating the above steps (unfolding and splitting). By introducing the notation

$$Z(A_i(k)/D_k;\sigma^{<i};\eta(k)) = (S^+_{k-e_{i+1},e_{i+1}}Z)(S^-_{l+e_{i+1},e_{i+1}}Z)$$

we get a general expression for $\nu^{(0)}_{N,\mathcal{E}_i}$ given by

$$\nu^{(0)}_{N,\mathcal{E}_i}(\sigma^{D_i}|\,\sigma^{<i},\eta) = \prod_{k\in\mathcal{L}_i} \nu^{(0)}_{N,D_k}(\sigma^{D_k}|\,\sigma^{<i},\eta) \tag{3.20}$$

where

$$\nu^{(0)}_{N,D_k}(\sigma^{D_k}|\,\sigma^{<i},\eta) = \frac{e^{-\beta H_{k,k}(\sigma^{D_k})}e^{-\beta W_{k,i}(\sigma^{D_k};\sigma^{<i})}}{Z(A_i(k);\sigma^{<i};\eta(k))} Z(A_i(k)/D_k;\sigma^{<i};\eta(k))\tilde{\rho}_k(\sigma^{D_k}) \tag{3.21}$$

hence

$$\bar{X}^{(0)}_{N,l}(\alpha^{D_l};\,\alpha^{<i},\eta) := W_{l,i}(\alpha^{D_l};\,\alpha^{<i}) - \frac{1}{\beta}\log Z(A_i(k)/D_k;\sigma^{<i};\eta(k)).$$

4. Numerical experiments. In this section we illustrate the accuracy and efficiency of the schemes we introduced by giving the results of some numerical experiments in the $d = 1$ case. We consider a microscopic lattice of size $N = 512$ and a microscopic coupling defined by $V(x) = 1$ when $|x| \le L/L + 1$ and $V(x) = 0$ when $|x| \ge 1$. The definition of V on $(L/L + 1, 1)$ does not play any role in the numerical simulation of our finite size model. The mean-field approximation for this model undergoes a phase transition at temperature $\beta_c = 1$. In our numerical experiments we consider different values for Q, L and β in order to illustrate their interplay in the problems addressed here.

4.1. Accuracy. To evaluate the accuracy of the schemes we made MC computations of

$$< H_N(\sigma)|\eta >_{\varrho_\beta} = \int_{S_N} H_N(\sigma)\varrho_\beta(\sigma|\eta) \tag{4.1}$$

with η being a CG configuration and the microscopic measure $\varrho_\beta(\sigma|\eta)$ being either $\mu_{N,\beta}(\sigma|\eta)$ or one of its approximations. We distinguish between two cases for η:

1. η is sampled from $\bar{\mu}_{M,\beta}$ and we call it a "typical" η.
2. η is sampled from $\bar{P}_M$ and we call it a "deviant" η.

Due to the existence of a phase transition, $\bar{\mu}_{M,\beta}$ has two different qualititive behaviors depending on the relative values of β and β_c. Roughly, when $\beta < \beta_c$ the p.m. $\bar{\mu}_{M,\beta}$ is close to $\bar{P}_M$ and the obtained "typical" and "deviant" η's are similar. Furthermore, in this regime and for these coarse-grained configurations $\bar{\mu}_{M,\beta}(\cdot|\eta)$ is close to $\bar{P}_M(\cdot|\eta)$ which is also the case for $\nu^{(0)}(\cdot;\eta)$. This explains why, when $\beta < \beta_c$, the observed results of first approximation schemes A and D are satisfactory independently of Q/L.

When $\beta > \beta_c$ most of the coarse-cells in typical η's get covered: $\eta(k) = \pm Q$. In this case most of the information on the microscopic configuration is already given by η and again the observed result of first approximation schemes A and D are satisfactory. In order to fully illustrate the accuracy of our reconstruction schemes we choose to numerically investigate their behavior at low-temperature with deviant η's i.e. *coarse-grained configurations where almost all information on the microscopic configurations is lost in the transition micro-CG*. In particular we show that in situations where Scheme A do not work well the corrected algorithms B and C significantly improve upon its results *even at very low temperatures*. These simulations confirm the importance of the ratio $\beta Q/L$ in the measure of the performance of these algorithms.

In the Tables 5.1-5.6 below we first give the value of (4.1) with $\varrho_\beta(\cdot|\eta) = \mu_\beta(\cdot|\eta)$ computed by a Direct MCMC algorithm which is a straightforward adaptation of the algorithm proposed in Chapter 5 in [19] to get samples from the Conserved Order Parameter (COP) Ising model. Then we give the value of (4.1) where $\varrho_\beta(\cdot|\eta)$ is one of the approximating measures suggested in Scheme A-D. This value is obtained by taking the mean over independent and identically distributed samples from the corresponding $\varrho_\beta(\cdot|\eta)$. We further give the relative error when compared to the reference value obtained by the Direct MC simulation. Finally in Table 4.7 we compare the result of the MC computation of $\int_{S_N} H_N(\sigma)\mu_N(\sigma)$ and $\int_{S_N} H_N(\sigma)\mathcal{G}^{(2)}_N(\sigma)$ with $\mathcal{G}^{(2)}_N$ given in Section 2.2.3.

4.2. Efficiency. It is an intrinsic feature of the direct MCMC reconstruction algorithm that it must be run on a single processor since it requires to simulate the configuration of the system over the entire lattice at once. As a consequence (i) each step of the MCMC simulation involves huge computations and (ii) the relaxation time of the dynamic is expected to be important as it depends on the size of the configuration space (among other things).

In contrast with this situation our reconstruction schemes allow to distribute the computations in two ways. First, we only need to simultaneously simulate the configuration of the system on the sublattices $\mathcal{L}_i$. Second, each of these simulations can be spread over several processors running in parallel (one per reconstruction domain in Schemes A, C, D, E). In short, we propose to replace one costly computation by a cascade of comparatively simple computations. More precisely, we observe that

(i) taking (as in [13]) as a reference for the computational complexity of the direct MCMC reconstruction algorithm the number of operations for evaluation of the microscopic Hamiltonian H_N we obtain $O((nL)^d)$ while the computation of its analogous over the reconstruction domains in Scheme A requires $O(L^{2d})$ operations and the computation of its analogous over the reconstruction domains in Scheme C requires $O(L^{3d})$ operations. The computational complexity of Scheme B is of the same order of that of a direct MCMC reconstruction. This is due to the coupling of the reconstruction domains present in that particular scheme. In the $q > L$ case the computation of the local microscopic Hamiltonian in Scheme D requires $O(Rq^dL^d)$ operations. Note that in the latter case a prior computation of the boundary terms $\bar{X}^{(0)}_{N,l}$ is required.

(ii) the number of microscopic configurations compatible with a CG configuration on the entire domain $\mathbb{T}$ can be as large as $O\left(\left(\frac{2^{q^d}}{\sqrt{q^d}}\right)^{m^d}\right)$. In comparison the number of microscopic configurations compatible with a CG configuration on a reconstruction domain in Scheme A can not exceed $O\left(\frac{2^{q^d}}{\sqrt{q^d}}\right)$, $O\left(\left(\frac{2^{q^d}}{\sqrt{q^d}}\right)^2\right)$ in Scheme C and $O\left(\left(\frac{2^{q^d}}{\sqrt{q^d}}\right)^{r^d}\right)$ in Scheme D. As a consequence of this size reduction the number of MC steps required to reach equilibrium on a reconstruction domain for any of our approximation algorithm is much smaller than the relaxation time of the direct MCMC simulation on the whole $\mathbb{T}$. Table 5.8 and 5.9 below gives the corresponding observed quantities for $\beta = 5$ and deviant η's.

5. Conclusions. Starting from a microscopic stochastic system and the corresponding coarse-grained model we introduced a mathematical strategy to recover microscopic information given the coarse-grained data. We defined "reconstructed" microscopic measures satisfying two conditions: (i) they are close in specific relative entropy to the initial microscopic equilibrium measure conditioned on the coarse-grained data and (ii) their sampling is computationally advantageous when compared to sampling directly from the conditioned microscopic equilibrium measure. We worked out these questions in the context of equilibrium stochastic lattice systems of Ising type spins. We met condition (i) by defining reconstructed Hamiltonians that are uniformly close to the original microscopic one. We met condition (ii) by defining reconstructed models fitted for parallel computations. We employed different tools depending on whether the coarse-graining is performed over or below the interaction length of the microscopic Hamiltonian. In the latter case we used a high-temperature cluster expansion while in the former we exploited the factorization properties of high-temperature multi-canonical constrained Gibbs measures.

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REFERENCES

[1] Chatterjee A. and Vlachos D. An overview of spatial microscopic and accelerated kinetic monte carlo simulations for materials' simulations. *J. Computer-Aided Materials Design*, 14(2):253, 2007.

[2] Reinier L. C. Akkermans and W. J. Briels. Coarse-grained interactions in polymer melts: A variational approach. *J. Chem. Phys.*, 115(13):6210–6219, 2001.

[3] Lorenzo Bertini, Emilio N. M. Cirillo, and Enzo Olivieri. Renormalization-group transformations under strong mixing conditions: Gibbsianness and convergence of renormalized interactions. *J. Statist. Phys.*, 97(5-6):831–915, 1999.
[4] C. Cammarota. Decay of correlations for infinite range interactions in unbounded spin systems. *Comm. Math. Phys.*, 85(4):517–528, 1982.
[5] T. M. Cover and J. A. Thomas. *Elements of Information Theory.* John Wiley and Sons, Inc., 1991.
[6] Weinan E and Bjorn Engquist. The heterogeneous multiscale methods. *Commun. Math. Sci.*, 1(1):87–132, 2003.
[7] Fukunaga H., Takimoto J., and Doi M. A coarse-graining procedure for flexible polymer chains with bonded and nonbonded interactions. *Journal of Chemical Physics*, 116(18):8183–8190, 2002.
[8] V.A. Harmandaris, N.P. Adhikari, N.F.A. van der Vegt, and K. Kremer. Hierarchical modeling of polystyrene: From atomistic to coarse-grained simulations. *Macromolecules*, 39:6708–6719, 2006.
[9] V.A. Harmandaris, N.P. Adhikari, N.F.A. van der Vegt, K. Kremer B.A. Mann, R. Voelkel, H. Weiss, and C.C.Liew. Ethylbenzene diffusion in polystyrene: United atom atomistic/ coarse grained simulations and experiments. *Macromolecules*, 40:7026–7035, 2007.
[10] V.A. Harmandaris, Markos A. Katsoulakis, Petr Plecháč. Coarse-Graining schemes for off-lattice interacting particles with internal degrees of freedom. In progress.
[11] Markos A. Katsoulakis, Andrew J. Majda and Dionisos G. Vlachos. Coarse-grained stochastic processes and and monte-Carlo simulations in lattice systems. *J. Comput. Phys.* 186:250–278, 2003.
[12] Markos A. Katsoulakis, Petr Plecháč and Luc Rey-Bellet. Mathematical and Statistical methods for the coarse-graining of many particles stochastic systems. *J. Sci. Comp.*, 37:43-71, 2008.
[13] Markos A. Katsoulakis, Petr Plecháč, Luc Rey-Bellet, and Dimitrios K. Tsagkarogiannis. Coarse-graining schemes and a posteriori error estimates for stochastic lattice systems. *M2AN Math. Model. Numer. Anal.*, 41(3):627–660, 2007.
[14] Markos A. Katsoulakis, Petr Plecháč, and Alexandros Sopasakis. Error analysis of coarse-graining for stochastic lattice dynamics. *SIAM J. Numer. Anal.*, 44(6):2270–2296 (electronic), 2006.
[15] Markos A. Katsoulakis and José Trashorras. Information loss in coarse-graining of stochastic particle dynamics. *J. Stat. Phys.*, 122(1):115–135, 2006.
[16] Ioannis G. Kevrekidis, C. William Gear, James M. Hyman, Panagiotis G. Kevrekidis, Olof Runborg, and Constantinos Theodoropoulos. Equation-free, coarse-grained multiscale computation: enabling microscopic simulators to perform system-level analysis. *Commun. Math. Sci.*, 1(4):715–762, 2003.
[17] K. Kremer and F. Müller-Plathe. Multiscale problems in polymer science: simulation approaches. *MRS Bull.*, page 205, March 2001.
[18] F. Müller-Plathe. Coarse-graining in polymer simulation: from the atomistic to the mesoscale and back. *Chem. Phys. Chem.*, 3:754, 2002.
[19] M. E. J. Newman and G. T. Barkema. *Monte Carlo methods in statistical physics.* The Clarendon Press Oxford University Press, New York, 1999.
[20] E. Olivieri and P. Picco. Cluster expansion for d-dimensional lattice systems and finite-volume factorization properties *J. Stat. Phys.*, 59(1-2):221-256, 1990.
[21] I. Pivkin and G. Karniadakis. Coarse-graining limits in open and wall-bounded dissipative particle dynamics systems. *J. Chem. Phys.*, 124:184101, 2006.
[22] Dirk Reith, Hendrik Meyer, and Florian Müller-Plathe. Mapping atomistic to coarse-grained polymer models using automatic simplex optimization to fit structural properties. *Macromolecules*, 34:2335–2345, 2001.
[23] Sabine Rosenfeldt, Elena Karpuk, Matthias Lehmann, Herbert Meier, Peter Lindner, Ludger Harnau, and Matthias Ballauff. The Solution Structure of Stilbenoid Dendrimers: A Small-Angle Scattering Study *Chem. Phys. Chem.*, 7:2097, 2006.
[24] W. Tschöp, K. Kremer, O. Hahn, J. Batoulis, and T. J., Bürger. Simulation of polymer melts. i. coarse-graining procedure for polycarbonates. *Acta Polymer.*, 49:61–74, 1998.
[25] W. Tschöp, K. Kremer, O. Hahn, J. Batoulis, and T. J., Bürger. Simulation of polymer melts. ii. from coarse-grained models back to atomistic description. *Acta Polymer.*, 49:75–79, 1998.

TABLE 5.1
N=512, L=16, Q=4.

		Direct MC	Scheme A		Scheme B		Scheme C	
Typical η	$\beta = 0.5$	-0.0018	-0.0018	0 %	-0.0018	0 %	-0.0018	0 %
	$\beta = 1$	-0.1001	-0.1001	0 %	-0.1001	0 %	-0.1001	0 %
	$\beta = 1.5$	-0.3513	-0.3513	0 %	-0.3513	0 %	-0.3513	0 %
	$\beta = 2$	-0.4382	-0.4382	0 %	-0.4382	0 %	-0.4382	0 %
Deviant η	$\beta = 0.5$	-0.0047	-0.0047	0 %	-0.0047	0 %	-0.0047	0 %
	$\beta = 1$	-0.0043	-0.0043	0 %	-0.0043	0 %	-0.0043	0 %
	$\beta = 1.5$	-0.0086	-0.0086	0 %	-0.0086	0 %	-0.0086	0 %
	$\beta = 2$	-0.0035	-0.0035	0 %	-0.0035	0 %	-0.0035	0 %
	$\beta = 5$	-0.0060	-0.0059	2 %	-0.0060	0 %	-0.0060	0 %
	$\beta = 10$	-0.0099	-0.0093	6 %	-0.099	0 %	-0.0096	3 %

TABLE 5.2
N=512, L=16, Q=8.

		Direct MC	Scheme A		Scheme B		Scheme C	
Typical η	$\beta = 0.5$	-0.0235	-0.0235	0 %	-0.0235	0 %	-0.0235	0 %
	$\beta = 1$	-0.0244	-0.0244	0 %	-0.0244	0 %	-0.0244	0 %
	$\beta = 1.5$	-0.3765	-0.3765	0 %	-0.3765	0 %	-0.3765	0 %
	$\beta = 2$	-0.4695	-0.4695	0 %	-0.4695	0 %	-0.4695	0 %
Deviant η	$\beta = 0.5$	-0.00048	-0.00048	0 %	-0.00048	0 %	-0.00048	0 %
	$\beta = 1$	0.0039	0.0039	0 %	0.0039	0 %	0.0039	0 %
	$\beta = 1.5$	0.0010	0.0010	0 %	0.0010	0 %	0.0010	0 %
	$\beta = 2$	-0.0016	-0.0016	0 %	-0.0016	0 %	-0.016	0 %
	$\beta = 5$	-0.0068	-0.0062	9 %	-0.0068	0 %	-0.0064	6 %
	$\beta = 10$	-0.0167	-0.0129	23 %	-0.0174	4 %	-0.0155	7 %

TABLE 5.3
N=512, L=16, Q=16.

		Direct MC	Scheme A		Scheme B		Scheme C	
Typical η	$\beta = 0.5$	-0.0036	-0.0036	0 %	-0.0036	0 %	-0.0036	0 %
	$\beta = 1$	-0.0666	-0.0666	0 %	-0.0666	0 %	-0.0666	0 %
	$\beta = 1.5$	-0.3387	-0.3387	0 %	-0.3387	0 %	-0.3387	0 %
	$\beta = 2$	-0.4136	-0.4136	0 %	-0.4136	0 %	-0.4136	0 %
Deviant η	$\beta = 0.5$	-0.0096	-0.0096	0 %	-0.0096	0 %	-0.0096	0 %
	$\beta = 1$	-0.0058	-0.0058	0 %	-0.0058	0 %	-0.0058	0 %
	$\beta = 1.5$	-0.0042	-0.0040	5 %	-0.0042	0 %	-0.0042	0 %
	$\beta = 2$	-0.0100	-0.0095	5 %	-0.0100	0 %	-0.0099	1 %
	$\beta = 5$	-0.0286	-0.0204	29 %	-0.0303	6 %	-0.0269	6 %
	$\beta = 10$	-0.0616	-0.0340	45 %	-0.0675	10 %	-0.0600	3 %

TABLE 5.4
N=512, L=4, Q=4.

		Direct MC	Scheme D, R=1		Scheme D, R=2	
Typical η	$\beta = 0.5$	-0.0605	-0.0605	0 %	-0.0605	0 %
	$\beta = 1$	-0.1944	-0.1944	0 %	-0.1944	0 %
	$\beta = 1.5$	-0.2957	-0.2956	0 %	-0.2957	0 %
	$\beta = 2$	-0.4129	-0.4129	0 %	-0.4129	0 %
Deviant η	$\beta = 0.5$	0.0046	0.0046	0 %	0.0046	0 %
	$\beta = 1$	-0.0155	-0.0154	0 %	-0.0155	0 %
	$\beta = 1.5$	-0.0135	-0.0129	4 %	-0.0134	1 %
	$\beta = 2$	-0.0474	-0.0464	2 %	-0.0474	0 %
	$\beta = 5$	-0.0774	-0.0712	8 %	-0.0769	1 %
	$\beta = 10$	-0.0942	-0.0844	10 %	-0.0929	1 %

TABLE 5.5
N=512, L=4, Q=8.

		Direct MC	Scheme D, R=1		Scheme D, R=2	
Typical η	$\beta = 0.5$	-0.0380	-0.0379	0 %	-0.0380	0 %
	$\beta = 1$	-0.1608	-0.1605	0 %	-0.1608	0 %
	$\beta = 1.5$	-0.3192	-0.3183	0 %	-0.3192	0 %
	$\beta = 2$	-0.4120	-0.4119	0 %	-0.4120	0 %
Deviant η	$\beta = 0.5$	-0.0219	-0.0218	0 %	-0.0219	0 %
	$\beta = 1$	-0.0413	-0.0407	2 %	-0.0413	0 %
	$\beta = 1.5$	-0.0547	-0.0513	6 %	-0.0543	1 %
	$\beta = 2$	-0.0784	-0.0679	13 %	-0.0761	3 %
	$\beta = 5$	-0.1779	-0.1330	25 %	-0.1589	10 %
	$\beta = 10$	-0.1878	-0.1427	25 %	-0.1679	10 %

TABLE 5.6
N=512, L=4, Q=16.

		Direct MC	Scheme D, R=1		Scheme D, R=2	
Typical η	$\beta = 0.5$	-0.0599	-0.0599	0 %	-0.0599	0 %
	$\beta = 1$	-0.1202	-0.1196	0 %	-0.1203	0 %
	$\beta = 1.5$	-0.2600	-0.2558	2 %	-0.2598	0 %
	$\beta = 2$	-0.4200	-0.4205	0 %	-0.4199	0 %
Deviant η	$\beta = 0.5$	-0.0321	-0.0320	0 %	-0.0321	0 %
	$\beta = 1$	-0.0768	-0.0761	1 %	-0.0768	0 %
	$\beta = 1.5$	-0.1603	-0.1518	5 %	-0.1592	1 %
	$\beta = 2$	-0.2592	-0.0229	12 %	-0.2431	6 %
	$\beta = 5$	-0.3400	-0.2995	12 %	-0.3068	10 %
	$\beta = 10$	-0.3435	-0.3005	12 %	-0.3096	10 %

TABLE 5.7
N=512, L=16.

	β=0.5		β=1		β=1.5		β=2	
Direct MC	-0.0124		-0.0659		-0.3579		-0.4574	
Scheme E, Q=4	-0.0124	0 %	-0.0659	0 %	-0.3579	0 %	-0.4574	0 %
Scheme E, Q=8	-0.0124	0 %	-0.0659	0 %	-0.3579	0 %	-0.4574	0 %
Scheme E, Q=16	-0.0124	0 %	-0.0659	0 %	-0.3579	0 %	-0.4574	0 %

TABLE 5.8
N=512, L=16, β=5, deviant η.

	Direct MCMC	Scheme A	Scheme C
Q=4	1000	50	100
Q=8	1500	100	200
Q=16	3000	200	300

TABLE 5.9
N=512, L=4, β=5, deviant η.

	Direct MCMC	Scheme D, R=1	Scheme D, R=2
Q=4	4000	20	50
Q=8	1500000	150	300
Q=16	10000000	500	3000