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

JOSÉ TRASHORRAS* AND DIMITRIOS K. TSAGKAROGIANNIS†

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.

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], [18], [21]). In particular, coarse-graining of polymeric chains and other macromolecular systems has attracted considerable attention. In this particular 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. [8], [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], [19], [9], [10]). 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. [14], [11], [12] (see [13] 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 [14] 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 [14] the authors found sufficient conditions under which \bar{H}_M can be expanded in a series

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

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 simulations.

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 - i.e. a reconstructed Hamiltonian $\bar{W}_N(\cdot, \eta)$ defined on the space of microscopic configurations - 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 exact reconstructed microscopic model.

The main feature of our reconstructed models is that they allow parallel computations. In this way, instead of running a 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 [14] 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 ([16], [15]). The difficulty in carrying out the error estimates rests on the fact that the CG dynamic is not Markovian. To circumvent this obstacle in [16] 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 [15]. Notice however that the reconstruction methods presented here are much more involved and efficient than 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. [17] 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 torus $\mathbb{T} = [0, 1)$ with periodic boundary conditions. There is no real additional difficulty for the problem addressed here in considering the d -dimensional torus and/or other boundary conditions. The microscopic system is settled on the uniform lattice $\Lambda_N = (\frac{1}{N}\mathbb{Z}) \cap \mathbb{T}$. The number of lattice sites N 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

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

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

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

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

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

The factor $1/L$ 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

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

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} into M coarse cells: For $k \in \mathbb{Z}$ with $0 \leq k \leq M-1$ we define $C_k = [\frac{k}{M}, \frac{k+1}{M})$ so $\mathbb{T} = \cup_{0 \leq k \leq M-1} C_k$. For convenience in latter use we also define $C_M = C_0 = [0, \frac{1}{M})$. We identify each cell C_k with a lattice point of the coarse lattice $\bar{\Lambda}_M = (\frac{1}{M}\mathbb{Z}) \cap \mathbb{T}$. Each coarse cell contains Q 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:

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

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

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

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

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

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:

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

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 $D \subset \mathbb{T}$ 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 $B_1 \subset B_2 \subset \mathbb{T}$, 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} 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. η_1, \dots, η_r).

- Let I be a subset of $\{0, \dots, M-1\}$ 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 on \mathcal{I}* 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 length 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 mixing condition and exploit the fact that this property is enforced by the conditioning in $\mu_N(\cdot|\eta)$ since spins located in a coarse-cell do not interact with spins located in the next to nearest neighbor coarse-cell. 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} . However in most applications (see e.g. [19]) the reconstruction is performed over mesoscopic domains, i.e. not the whole \mathbb{T} but parts of \mathbb{T} containing a number of microscopic sites that is a large multiple of L . 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 and developed in [14] 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

$$\varepsilon = \beta \frac{Q}{L} \|\nabla V\|_\infty \quad (2.8)$$

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 site.

First we show that due to the particular form of the Gibbs measure (2.4) the problem in hands essentially reduces, from the computational point of view, to sampling the value of the spins on half of the microscopic lattice points. Then we propose several schemes designed to deal with this problem and give the corresponding rigorous error estimates.

We partition \mathbb{T} into $2U$ cells: For $l \in \mathbb{Z}$ with $0 \leq l \leq 2U - 1$ we define $D_l = [\frac{l}{2U}, \frac{l+1}{2U})$ so $\mathbb{T} = \bigcup_{0 \leq l \leq 2U-1} D_l$ and every D_l contains L points of the microscopic lattice Λ_N . For convenience in latter use we also define $D_{2U} = D_0$. We call the D_l *reconstruction domains* and define

$$\mathcal{E} = \bigcup_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} D_l, \quad S_{N,\mathcal{E}} = \{-1, 1\}^{\mathcal{E} \cap \Lambda_N}, \quad \mathcal{O} = \bigcup_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} D_l, \quad \text{and} \quad S_{N,\mathcal{O}} = \{-1, 1\}^{\mathcal{O} \cap \Lambda_N}.$$

Let η be a fixed coarse-grained configuration and α be a microscopic configuration compatible with η on \mathbb{T} . We shall denote by $\mu_{N,\mathcal{O}}(\cdot | \alpha^\mathcal{E}, \eta)$ (resp. $\mu_{N,\mathcal{E}}(\cdot | \eta)$) the $\mathcal{O} \cap \Lambda_N$ -marginal of

$$\mu_N(\cdot | \alpha^\mathcal{E}, \eta) = \mu_N(\cdot | \sigma^\mathcal{E} = \alpha^\mathcal{E}, F(\sigma) = \eta)$$

(resp. the $\mathcal{E} \cap \Lambda_N$ -marginal of $\mu_N(\cdot | \eta)$). We have

$$\mu_N(\alpha | \eta) = \mu_{N,\mathcal{E}}(\alpha^\mathcal{E} | \eta) \mu_{N,\mathcal{O}}(\alpha^\mathcal{O} | \alpha^\mathcal{E}, \eta) \quad (2.9)$$

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

$$\nu_N(\alpha; \eta) = \nu_{N,\mathcal{E}}(\alpha^\mathcal{E}; \eta) \nu_{N,\mathcal{O}}(\alpha^\mathcal{O}; \alpha^\mathcal{E}, \eta).$$

Assume for a while that we are given $\alpha^\mathcal{E} \in S_{N,\mathcal{E}}$. Since L is the range of interaction of μ_N the probability measure $\mu_{N,\mathcal{O}}(\cdot | \alpha^\mathcal{E}, \eta)$ defined on $S_{N,\mathcal{O}}$ factorizes: for every $\varrho \in S_{N,\mathcal{O}}$

$$\mu_{N,\mathcal{O}}(\varrho | \alpha^\mathcal{E}, \eta) = \bigotimes_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} \mu_{N,D_l}(\varrho^{D_l} | \alpha^\mathcal{E}, \eta) \quad (2.10)$$

where $\mu_{N,D_l}(\cdot | \alpha^\mathcal{E}, \eta)$ stands for the $D_l \cap \Lambda_N$ -marginal of $\mu_N(\cdot | \alpha^\mathcal{E}, \eta)$. 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 i.e. a small set when compared to S_N . Furthermore, while sampling from $\mu_{N,\mathcal{O}}(\cdot | \alpha^\mathcal{E}, \eta)$ the product structure in (2.10) 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* $\mu_{N,\mathcal{O}}(\cdot | \alpha^\mathcal{E}, \eta)$ and not from an approximation of it. Hence sampling with respect to $\mu_{N,\mathcal{O}}(\cdot | \alpha^\mathcal{E}, \eta)$ does not represent a computational difficulty once we are given $\alpha^\mathcal{E}$ and we shall take $\nu_{N,\mathcal{O}}(\cdot; \alpha^\mathcal{E}, \eta) = \mu_{N,\mathcal{O}}(\cdot | \alpha^\mathcal{E}, \eta)$.

Our task is thus reduced to define efficient numerical schemes in order to get samples from an approximation of the probability measure $\mu_{N,\mathcal{E}}(\cdot | \eta)$ defined on $S_{N,\mathcal{E}}$. Let η be a coarse-grained configuration and fix $\alpha \in S_{N,\mathcal{E}}$ compatible with η on \mathcal{E} . We introduce $\bar{W}_{N,\mathcal{E}}(\alpha, \eta)$ by

$$e^{-\beta \bar{W}_{N,\mathcal{E}}(\alpha, \eta)} = E_N[e^{-\beta H_N(\sigma)} | \alpha, \eta] \quad (2.11)$$

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

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

Notice that whenever α and η are not compatible over \mathcal{E} we get $\mu_{N,\mathcal{E}}(\alpha | \eta) = 0$.

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

$$\bar{W}_{N,\mathcal{E}}^{(0)}(\alpha; \eta) = E_N[H_N(\sigma)|\alpha, \eta]. \quad (2.12)$$

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

$$\nu_{N,\mathcal{E}}^{(0)}(\alpha; \eta) = \frac{e^{-\beta \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta)}}{Z_{N,\mathcal{E}}^{(0)}(\eta)} \bigotimes_{k \in \mathcal{E} \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \quad (2.13)$$

with

$$Z_{N,\mathcal{E}}^{(0)}(\eta) = \int_{S_{N,\mathcal{E}}} e^{-\beta \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta)} \bigotimes_{k \in \mathcal{E} \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}).$$

By elementary computations we get

$$\begin{aligned} \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) &= -\frac{1}{2} \sum_{l: \text{even}} \sum_{x \in D_l \cap \Lambda_N} \sum_{\substack{y \in D_l \cap \Lambda_N \\ y \neq x}} J(x-y) \alpha(x) \alpha(y) \\ &\quad -\frac{1}{2} \sum_{l: \text{odd}} \left(\sum_{k \in D_l \cap \bar{\Lambda}_M} \sum_{\substack{k' \in D_l \cap \bar{\Lambda}_M \\ k' \neq k}} \bar{J}(k, k') \eta(k) \eta(k') + \sum_{k \in D_l \cap \bar{\Lambda}_M} \bar{J}(0) (\eta^2(k) - Q) \right) \\ &\quad - \sum_{l: \text{even}} \sum_{k \in (D_{l-1} \cup D_{l+1}) \cap \bar{\Lambda}_M} \sum_{x \in D_l \cap \Lambda_N} \check{J}(x, k) \alpha(x) \eta(k) \end{aligned} \quad (2.14)$$

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

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

With a slight abuse of notation we shall write $\check{J}(k, x) = \check{J}(x, k)$ since J is even. For every $\eta \in \bar{S}_M$ we define a probability measure $\nu_N^{(0)}(\cdot; \eta)$ on S_N by

$$\nu_N^{(0)}(\sigma; \eta) = \begin{cases} \nu_{N,\mathcal{E}}^{(0)}(\sigma^\mathcal{E}; \eta) \mu_{N,\mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta) & \text{if } \sigma \text{ and } \eta \text{ are compatible over } \mathbb{T} \\ 0 & \text{otherwise.} \end{cases} \quad (2.15)$$

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 $\eta \in \bar{S}_M$ and every $\alpha \in S_{N,\mathcal{E}}$ compatible with η on \mathcal{E} the following estimate holds*

$$\frac{\beta}{N} \left(\bar{W}_{N,\mathcal{E}}(\alpha, \eta) - \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) \right) = O(\varepsilon^2) \quad (2.16)$$

where the O is uniform in η and α .

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*

$$\frac{1}{N}H\left(\nu_N^{(0)}(\cdot; \eta) | \mu_N(\cdot | \eta)\right) = O(\varepsilon^2) \quad (2.17)$$

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

The particular form of $\bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta)$ makes $\nu_{N,\mathcal{E}}^{(0)}(\cdot; \eta)$ a product measure for every $\eta \in \bar{S}_M$. This leads to the following

Scheme A

Step 1 We run in parallel U constrained simulations with coarse-grained boundary conditions given by $\eta^\mathcal{O}$ to obtain $\alpha_1 \in S_{N,\mathcal{E}}$ sampled from $\nu_{N,\mathcal{E}}^{(0)}(\cdot; \eta)$.

Step 2 We run in parallel U constrained simulations with microscopic boundary conditions given by α_1 to obtain $\alpha_2 \in S_{N,\mathcal{O}}$ sampled from $\mu_{N,\mathcal{O}}(\cdot | \alpha_1, \eta)$.

Step 3 We obtain a sample of $\nu_N^{(0)}(\cdot; \eta)$ by taking $[\alpha_1, \alpha_2]$.

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 [14] we notice that for every η and every $\alpha \in S_{N,\mathcal{E}}$ compatible with η on \mathcal{E} we have

$$\bar{W}_{N,\mathcal{E}}(\alpha, \eta) - \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) = -\frac{1}{\beta} \log E_N[e^{-\beta(H_N(\sigma) - W_{N,\mathcal{E}}^{(0)}(\alpha, \eta))} | \alpha, \eta]. \quad (2.18)$$

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 $\eta \in \bar{S}_M$ and $\alpha \in S_{N,\mathcal{E}}$ compatible over \mathcal{E} the function $\bar{W}_{N,\mathcal{E}}(\alpha, \eta)$ can be expanded into a convergent series*

$$\bar{W}_{N,\mathcal{E}}(\alpha, \eta) = \sum_{p=0}^{+\infty} \bar{W}_{N,\mathcal{E}}^{(p)}(\alpha, \eta) \quad (2.19)$$

where the $p = 1, 2$ terms are explicitly given in Section 3.1.1. Furthermore, for every integer $p \geq 1$ the following error bound holds uniformly in α and η

$$\frac{\beta}{N} \left(\bar{W}_{N,\mathcal{E}}(\alpha, \eta) - \sum_{l=0}^p \bar{W}_{N,\mathcal{E}}^{(l)}(\alpha, \eta) \right) = O(\varepsilon^{p+1}). \quad (2.20)$$

For every integer $p \geq 1$ we define a kernel $\nu_{N,\mathcal{E}}^{(p)}(\cdot; \cdot)$ on $S_{N,\mathcal{E}} \times \bar{S}_M$ by

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

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

$$\nu_N^{(p)}(\sigma; \eta) = \begin{cases} \nu_{N,\mathcal{E}}^{(p)}(\sigma^\mathcal{E}; \eta) \mu_{N,\mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta) & \text{if } \sigma \text{ and } \eta \text{ are compatible over } \mathbb{T} \\ 0 & \text{otherwise.} \end{cases} \quad (2.21)$$

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*

$$\frac{1}{N}H\left(\nu_N^{(p)}(\cdot; \eta) | \mu_N(\cdot | \eta)\right) = O(\varepsilon^{p+1}) \quad (2.22)$$

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

From the preceding result we derive the following

Scheme B

Step 1 We run a multi-constrained simulation with coarse-grained boundary conditions given by $\eta^{\mathcal{O}}$ to obtain $\alpha_1 \in S_{N,\mathcal{E}}$ sampled from $\nu_{N,\mathcal{E}}^{(p)}(\cdot; \eta)$.

Step 2 We run in parallel U constrained simulations with microscopic boundary conditions given by α_1 to obtain $\alpha_2 \in S_{N,\mathcal{O}}$ sampled from $\mu_{N,\mathcal{O}}(\cdot | \alpha_1, \eta)$.

Step 3 We obtain a sample of $\nu_N^{(p)}(\cdot; \eta)$, where $p = 1, 2, \dots$ by taking $[\alpha_1, \alpha_2]$.

Unfortunately the first step in this scheme is restrictive when compared to Step 1 in Scheme A. Indeed the second order corrections $\bar{W}_{N,\mathcal{E}}^{(1)}(\alpha, \eta) + \bar{W}_{N,\mathcal{E}}^{(2)}(\alpha, \eta)$ already contain interactions across reconstruction domains D_l and D_{l+2} with l even which make the sampling measure in Step 1 not a product measure. As a consequence, Step 1 is not reducible to a set of parallel computations. However, note that Step 1 corresponds to sampling the values of the spins on a lattice of $N/2$ points and thus remains 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 $\bar{W}_N^{(1)}$ and $\bar{W}_N^{(2)}$ 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 $\nu_{N,\mathcal{E}}^{(2)}$ and couple D_l and D_{l+2} for every l even 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, each spin being located in a coarse cell contained in D_l, D_{l+1} and D_{l+2} . This three bodies interaction vanish as soon as two adjacent spins are located at more than L microscopic points away from each other. By taking reconstruction domains of $2L$ 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} into U cells: For $l \in \mathbb{Z}$ with $0 \leq l \leq U-1$ we define new reconstruction domains $D'_l = [\frac{l}{U}, \frac{l+1}{U})$ and $D'_U = D'_0$ so $\mathbb{T} = \bigcup_{0 \leq l \leq U-1} D'_l$ and every D'_l contains $2L$ points of the microscopic lattice. Again we define

$$\mathcal{E}' = \bigcup_{\substack{0 \leq l \leq U-1 \\ l \text{ even}}} D'_l, \quad S_{N,\mathcal{E}'} = \{-1, 1\}^{\mathcal{E}' \cap \Lambda_N}, \quad \mathcal{O}' = \bigcup_{\substack{0 \leq l \leq U-1 \\ l \text{ odd}}} D'_l, \quad \text{and} \quad S_{N,\mathcal{O}'} = \{-1, 1\}^{\mathcal{O}' \cap \Lambda_N}.$$

For every $\eta \in \bar{S}_M$ and $\alpha \in S_N$ compatible over \mathbb{T} we have that

$$\mu_N(\alpha | \eta) = \mu_{N,\mathcal{E}'}(\alpha^{\mathcal{E}'} | \eta) \mu_{N,\mathcal{O}'}(\alpha^{\mathcal{O}'} | \alpha^{\mathcal{E}'}, \eta),$$

with

$$\mu_{N,\mathcal{O}'}(\alpha^{\mathcal{O}'} | \alpha^{\mathcal{E}'}, \eta) = \bigotimes_{l \text{ odd}} \mu_{N,D'_l}(\alpha^{D'_l} | \alpha^{\mathcal{E}'}, \eta).$$

The definition of the different probability measures involved here is clear by analogy with those employed so far. Again, from a computational point of view, the main task is to define efficient schemes for the sampling from a probability measure that approximates $\mu_{N,\mathcal{E}'}(\cdot | \eta)$ on $S_{N,\mathcal{E}'}$. A perfect sampling from this measure is obtained through the function $\bar{V}_{N,\mathcal{E}'}(\alpha, \eta)$ defined on $S_{N,\mathcal{E}'} \times \bar{S}_M$ by

$$e^{-\beta \bar{V}_{N,\mathcal{E}'}(\alpha, \eta)} = E_N[e^{-\beta H_N(\sigma)} | \alpha, \eta] \quad (2.23)$$

since

$$\mu_{N,\mathcal{E}'}(\alpha | \eta) = \frac{e^{-\beta \bar{V}_{N,\mathcal{E}'}(\alpha, \eta)}}{e^{-\beta \bar{H}_M(\eta)}} \bigotimes_{k \in \mathcal{E}' \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}). \quad (2.24)$$

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

$$\bar{V}_{N,\mathcal{E}'}^{(0)}(\alpha, \eta) = E_N[H_N(\sigma)|\alpha, \eta] \quad (2.25)$$

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

THEOREM 2.5. *If $\delta = Q\varepsilon < \delta_0$ with δ_0 given in Theorem 2.1 then for every $\eta \in \bar{S}_M$ and $\alpha \in S_{N,\mathcal{E}'}$ compatible over \mathcal{E}' the function $\bar{V}_{N,\mathcal{E}'}(\alpha, \eta)$ can be expanded into a convergent series*

$$\bar{V}_{N,\mathcal{E}'}(\alpha, \eta) = \sum_{p=0}^{+\infty} \bar{V}_{N,\mathcal{E}'}^{(p)}(\alpha, \eta). \quad (2.26)$$

Furthermore, for every integer $p \geq 1$ the following error bound holds uniformly in α and η

$$\frac{\beta}{N} \left(\bar{V}_{N,\mathcal{E}'}(\alpha, \eta) - \sum_{l=0}^p \bar{V}_{N,\mathcal{E}'}^{(l)}(\alpha, \eta) \right) = O(\varepsilon^{p+1}). \quad (2.27)$$

We shall see in Section 3.1.1 that due to the definition of the D_l' for every $\eta \in \bar{S}_M$ the measure on $S_{N,\mathcal{E}'}$

$$\gamma_{N,\mathcal{E}'}^{(2)}(\alpha; \eta) = \frac{e^{-\beta(\sum_{p=0}^2 \bar{V}_{N,\mathcal{E}'}^{(p)}(\alpha, \eta))}}{\bar{Z}_{N,\mathcal{E}'}^{(2)}(\eta)} \bigotimes_{k \in \mathcal{E}' \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \quad (2.28)$$

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

$$\gamma_N^{(2)}(\sigma; \eta) = \begin{cases} \gamma_{N,\mathcal{E}'}^{(2)}(\sigma^{\mathcal{E}'}; \eta) \mu_{N,\mathcal{O}'}(\sigma^{\mathcal{O}'} | \sigma^{\mathcal{E}'}, \eta) & \text{if } \sigma \text{ and } \eta \text{ are compatible over } \mathbb{T} \\ 0 & \text{otherwise} \end{cases} \quad (2.29)$$

and get

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

$$\frac{1}{N} H(\gamma_N^{(2)}(\cdot; \eta) | \mu_N(\cdot | \eta)) = O(\delta^3) \quad (2.30)$$

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 $\gamma_N^{(2)}(\cdot; \eta)$ is product we derive the

Scheme C

Step 1 We run in parallel $U/2$ constrained simulations with coarse-grained boundary conditions given by $\eta^{\mathcal{O}'}$ to obtain α_1 sampled from $\gamma_{N,\mathcal{E}'}^{(2)}(\cdot; \eta)$.

Step 2 We run in parallel $U/2$ constrained simulations with microscopic boundary conditions given by α_1 to obtain α_2 sampled from $\mu_{N,\mathcal{O}'}(\cdot | \alpha_1, \eta)$.

Step 3 We obtain a sample of $\gamma_N^{(2)}(\cdot, \eta)$ by taking $[\alpha_1, \alpha_2]$.

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 $N/4L$ one can define reconstruction schemes similar to Schemes A and C (i.e. consisting of two 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 $3L$ microscopic lattice points one can define a scheme with 2 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

$$\delta = \frac{1}{RQ}.$$

According to Proposition 5.1 in [3] this quantity partially measures the mixing properties of $\mu_N(\cdot|\eta)$ uniformly in $\eta \in \bar{S}_M$ as soon as μ_N satisfies suitable conditions to be given below.

We partition \mathbb{T} into $2U$ cells: For $l \in \mathbb{Z}$ with $0 \leq l \leq 2U - 1$ we define $D_l = [\frac{l}{2U}, \frac{l+1}{2U})$ and $D_{2U} = D_0$ so $\mathbb{T} = \bigcup_{0 \leq l \leq 2U-1} D_l$ and every D_l contains R coarse-cells hence RQ points of the microscopic lattice. We write

$$\mathcal{E} = \bigcup_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} D_l, \quad S_{N,\mathcal{E}} = \{-1, 1\}^{\mathcal{E} \cap \Lambda_N}, \quad \mathcal{O} = \bigcup_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} D_l, \quad \text{and} \quad S_{N,\mathcal{O}} = \{-1, 1\}^{\mathcal{O} \cap \Lambda_N}.$$

Again, for every $\eta \in \bar{S}_M$ and every σ compatible with η on \mathbb{T} we have

$$\mu_N(\sigma|\eta) = \mu_{N,\mathcal{E}}(\sigma^{\mathcal{E}}|\eta) \mu_{N,\mathcal{O}}(\sigma^{\mathcal{O}}|\sigma^{\mathcal{E}}, \eta).$$

For the same reason as detailed in Section 2.2.1 we focus on defining schemes for the sampling from approximations of $\mu_{N,\mathcal{E}}(\cdot|\eta)$. Let η be a coarse-grained configuration and fix $\alpha \in S_{N,\mathcal{E}}$ compatible with η on \mathcal{E} . We introduce $\bar{W}_{N,\mathcal{E}}(\alpha, \eta)$ by

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

and observe that

$$\mu_{N,\mathcal{E}}(\alpha|\eta) = \frac{e^{-\beta \bar{W}_{N,\mathcal{E}}(\alpha, \eta)}}{e^{-\beta \bar{H}_M(\eta)}} \bigotimes_{k \in \mathcal{E} \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}). \quad (2.31)$$

First approximation. Again a direct computation of $\bar{W}_{N,\mathcal{E}}$ is impractical and we proceed by introducing a first approximation $\bar{W}_{N,\mathcal{E}}^{(0)}$. The Hamiltonian proposed in (2.12) is not a good approximation anymore since it leads to an error of order $O(Q/L)$ which is $O(1)$ in the $Q > L$ case. Rather, our approach is based on a rewriting of $\mu_{N,\mathcal{E}}(\cdot|\eta)$ in order to take profit as much as possible of its mixing properties. For every $\sigma \in S_N$ we have

$$H_N(\sigma) = \sum_{(l,l') \in \mathcal{D}_{\leq}} H_{l,l'}(\sigma^{D_l}, \sigma^{D_{l'}})$$

where

$$\mathcal{D}_{\leq} = \{(l, l') \in \{0, \dots, 2U - 1\} \times \{1, \dots, 2U\} \text{ such that } l \leq l'\} \quad (2.32)$$

and

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

Let η be a fixed coarse-grained configuration. For every l such that $0 \leq l \leq 2U - 1$, every $\sigma_1 \in \{-1, 1\}^{\Lambda_N \cap D_{l-1}}$ and every $\sigma_2 \in \{-1, 1\}^{\Lambda_N \cap D_{l+1}}$ we define:

$$Z_l(\sigma_1, \sigma_2; \eta) = \int_{\{-1,1\}^{D_l \cap \Lambda_N}} e^{-\beta H_{l,l+1}(\sigma^{D_l}, \sigma_2)} e^{-\beta H_{l-1,l}(\sigma_1, \sigma^{D_l})} e^{-\beta H_{l,l}(\sigma^{D_l}, \sigma^{D_l})} \bar{\rho}_l(\sigma^{D_l}), \quad (2.33)$$

where $\bar{\rho}_l(\sigma^{D_l}) = \bigotimes_{k \in \bar{\Lambda}_M \cap D_l} \tilde{\rho}_k(\sigma^{C_k})$ and

$$Z_l(\sigma_1, 0; \eta) = \int_{\{-1,1\}^{D_l \cap \Lambda_N}} e^{-\beta H_{l-1,l}(\sigma_1, \sigma^{D_l})} e^{-\beta H_{l,l}(\sigma^{D_l}, \sigma^{D_l})} \bar{\rho}_l(\sigma^{D_l}). \quad (2.34)$$

We further define $Z_l(0, \sigma_2; \eta)$ and $Z_l(0, 0; \eta)$ by analogy with (2.34). For every $\alpha \in S_{N,\mathcal{E}}$ compatible with η on \mathcal{E} we write

$$f_{l-1,l+1}(\alpha, \eta) = \frac{Z_l(\alpha^{D_{l-1}}, \alpha^{D_{l+1}}; \eta) Z_l(0, 0; \eta)}{Z_l(0, \alpha^{D_{l+1}}; \eta) Z_l(\alpha^{D_{l-1}}, 0; \eta)} - 1. \quad (2.35)$$

Finally, for every l such that $0 \leq l \leq 2U - 1$, we introduce

$$A_{l-1,l,l+1}(\eta) = \int_{\{-1,1\}^{(D_{l-1} \cup D_l \cup D_{l+1}) \cap \Lambda_N}} e^{-\beta H_{l,l+1}(\sigma^{D_l}, \sigma^{D_{l+1}})} e^{-\beta H_{l-1,l}(\sigma^{D_{l-1}}, \sigma^{D_l})} \times \\ \times e^{-\beta H_{l+1,l+1}(\sigma^{D_{l+1}}, \sigma^{D_{l+1}})} e^{-\beta H_{l,l}(\sigma^{D_l}, \sigma^{D_l})} e^{-\beta H_{l-1,l-1}(\sigma^{D_{l-1}}, \sigma^{D_{l-1}})} \bigotimes_{k \in \{l-1, l, l+1\}} \bar{\rho}_k(\sigma^{D_k}),$$

$$f_l^*(\alpha^{D_l}, \eta) = \frac{1}{A_{l-1,l,l+1}(\eta)} Z_{l+1}(\alpha^{D_l}, 0; \eta) Z_{l-1}(0, \alpha^{D_l}; \eta), \quad (2.36)$$

$$B_l(\eta) = Z_l(0, 0; \eta), \quad (2.37)$$

and

$$\rho_l^*(\alpha^{D_l}) = f_l^*(\alpha^{D_l}, \eta) e^{-\beta H_{l,l}(\alpha^{D_l}, \alpha^{D_l})} \bar{\rho}_l(\alpha^{D_l}). \quad (2.38)$$

The quantities $A_{l-1,l,l+1}(\eta)$ and $B_l(\eta)$ only depend on η while ρ_l^* and f_l^* only depend on α^{D_l} and η . The following rewriting of $\mu_{N,\mathcal{E}}(\cdot|\eta)$ is proved in Section 3.2.1.

LEMMA 2.7. *For every $\eta \in \bar{S}_M$ and every $\alpha \in S_{N,\mathcal{E}}$ compatible with η on \mathcal{E} we have*

$$\mu_{N,\mathcal{E}}(\alpha|\eta) = \frac{1}{e^{-\bar{H}_M(\eta)}} \prod_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} A_{l-1,l,l+1}(\eta) \prod_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} B_l^{-1}(\eta) \prod_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} (1 + f_{l-1,l+1}(\alpha, \eta)) \prod_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} \rho_l^*(\alpha^{D_l}). \quad (2.39)$$

Notice that $\mu_{N,\mathcal{E}}(\alpha|\eta)$ fails to be a product measure due to the presence of the $f_{l-1,l+1}$ terms. However according to Proposition 5.1 in [3] as soon as μ_N satisfies e.g. Dobrushin's uniqueness condition (see Chapter 8 in [7]) we have

LEMMA 2.8. [**Proposition 5.1 in [3]**] *There exists a constant C depending on N, Q and L such that*

$$\sup_{l \in \mathcal{O}} \sup_{\eta \in \bar{S}_M} \sup_{\alpha \in S_{N,\mathcal{E}}} |f_{l-1,l+1}(\alpha, \eta)| \leq C\delta.$$

From the decomposition of $\mu_{N,\mathcal{E}}(\cdot|\eta)$ given in (2.39) we propose as a zero order approximation to $\bar{W}_{N,\mathcal{E}}$ the Hamiltonian

$$\bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) = \sum_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} H_{l,l}(\alpha^{D_l}, \alpha^{D_l}) - \frac{1}{\beta} \sum_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} \log f_l^*(\alpha^{D_l}, \eta). \quad (2.40)$$

The corresponding zero order measure turns out to be a product measure and is given by:

$$\nu_{N,\mathcal{E}}^{(0)}(\alpha; \eta) = \frac{1}{Z_{N,\mathcal{E}}^{(0)}} e^{-\beta \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta)} \bigotimes_{\substack{0 \leq l \leq 2U-1 \\ l \text{ even}}} \bar{\rho}_l(\alpha^{D_l}).$$

In the same fashion as in (2.15) the corresponding reconstruction kernel defined on $S_N \times \bar{S}_M$ is given by

$$\nu_N^{(0)}(\sigma; \eta) = \begin{cases} \nu_{N,\mathcal{E}}^{(0)}(\sigma^\mathcal{E}; \eta) \mu_{N,\mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta) & \text{if } \sigma \text{ and } \eta \text{ are compatible over } \mathbb{T} \\ 0 & \text{otherwise.} \end{cases} \quad (2.41)$$

From now on we assume that μ_N satisfies Dobrushin's uniqueness condition or any of the sufficient conditions given in [3] for Proposition 5.1 there to hold.

THEOREM 2.9. *There is a constant C such that*

$$\frac{1}{N} H(\nu_N^{(0)}(\cdot; \eta) | \mu_N(\cdot | \eta)) \leq \frac{C\delta}{N}. \quad (2.42)$$

We remark that for every $\eta \in \bar{S}_M$ the measure $\nu_N^{(0)}(\cdot; \eta)$ is product. This leads to the following

Scheme D

Step 1 We run in parallel U constrained simulations with coarse-grained boundary conditions and obtain α_1 sampled from $\nu_{N,\mathcal{E}}^{(0)}(\cdot; \eta)$.

Step 2 We run in parallel U constrained simulations with microscopic boundary conditions given by α_1 and we get α_2 sampled from $\mu_{N,\mathcal{O}}(\cdot | \alpha_1, \eta)$.

Step 3 We obtain a sample of $\nu_N^{(0)}(\cdot | \eta)$ by taking $\sigma = [\alpha_1, \alpha_2]$.

Numerical experiments following this scheme are presented in Section 4.

Higher order corrections. According to Lemma 2.7 $\bar{W}_{N,\mathcal{E}}(\alpha, \eta)$ can be splitted into an order one part (zero order approximation) and to higher order terms:

$$\beta \bar{W}_{N,\mathcal{E}}(\alpha, \eta) = \beta \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) - \sum_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} \log(1 + f_{l-1, l+1}(\alpha^{D_{l-1}}, \alpha^{D_{l+1}})). \quad (2.43)$$

When we can make $C\delta$ small enough (e.g. by taking large values for R) we obtain higher order corrections by expanding the logarithm in (2.43):

$$\beta \bar{W}_{N,\mathcal{E}}(\alpha, \eta) = \beta \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) - \sum_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} (f_{l-1, l+1}(\alpha^{D_{l-1}}, \alpha^{D_{l+1}}))^n.$$

For every $p \geq 1$ we propose the following reconstruction kernel on $S_{N,\mathcal{E}} \times \bar{S}_M$

$$\nu_{N,\mathcal{E}}^{(p)}(\alpha; \eta) = \frac{1}{Z_{N,\mathcal{E}}^{(p)}(\eta)} e^{-\beta \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) + \sum_{\substack{0 \leq l \leq 2U-1 \\ l \text{ odd}}} \sum_{n=1}^p \frac{(-1)^{n+1}}{n} (f_{l-1, l+1})^n} \bigotimes_{l \in \mathcal{E}} \bar{\rho}_l(\alpha^{D_l}) \quad (2.44)$$

and the corresponding reconstruction kernel on $S_N \times \bar{S}_M$ defined by analogy with (2.41) satisfies

THEOREM 2.10. *There is a constant C such that for every $\eta \in \bar{S}_M$ and every $p \geq 1$ the following error estimate holds*

$$\frac{1}{N} H(\nu_N^{(p)}(\cdot; \eta) | \mu_N(\cdot | \eta)) \leq \frac{C^p \delta^p}{N}. \quad (2.45)$$

Subsequently we suggest Scheme E.

Scheme E

Step 1 We run a multi-constrained simulation with coarse-grained boundary conditions given by $\eta^{\mathcal{O}}$ to obtain $\alpha_1 \in S_{N,\mathcal{E}}$ sampled from $\nu_{N,\mathcal{E}}^{(p)}(\cdot; \eta)$.

Step 2 We run in parallel U constrained simulations with microscopic boundary conditions given by α_1 to obtain $\alpha_2 \in S_{N,\mathcal{O}}$ sampled from $\mu_{N,\mathcal{O}}(\cdot | \alpha^{\mathcal{E}}, \eta)$.

Step 3 We obtain a sample of $\nu_N^{(p)}(\cdot, \eta)$, where $p = 1, 2, \dots$ by taking $[\alpha_1, \alpha_2]$.

Unfortunately the first step in this scheme is restrictive when compared to Step 1 in Scheme D. Indeed, the terms $f_{l-1,l+1}$ couple reconstruction domains making the sampling measure in Step 1 not a product measure. Furthermore, unlike Step 1 in Scheme B, there is in general no simple closed expression for the coupling $f_{l-1,l+1}(\alpha^{D_{l-1}}, \alpha^{D_{l+1}})$ in terms of $\alpha^{D_{l-1}}, \alpha^{D_{l+1}}$ and $\eta(l)$. Finally, let us also mention that the constant C depends on Q, β, L and $\|J\|$ (for a detailed analysis see Section 4 in [3]). Hence, the advantage of running Scheme E rather than a direct MC simulation needs to be discussed on a case-by-case basis.

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 [14] 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

$$\mu_N(\sigma) = \mu_N(\sigma | \eta) \bar{\mu}_M(\eta). \quad (2.46)$$

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

$$\mathcal{G}_N^{(2)}(\sigma) = \gamma_N^{(2)}(\sigma; \eta) \bar{\mu}_M^{(2)}(\eta) \quad (2.47)$$

with $\gamma_N^{(2)}(\sigma; \eta)$ as defined in (2.29) the separation of scales in both (2.46) and (2.47) 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 F

Step 1 We run a CGMC simulation and obtain $\eta \in \bar{S}_M$ sampled from $\bar{\mu}_M^{(2)}$.

Step 2 We run in parallel $N/4L$ simulations with coarse-grained boundary conditions given by $\eta^{\mathcal{O}'}$ to obtain $\alpha_1 \in S_{N,\mathcal{E}'}$ sampled from $\gamma_N^{(2)}(\cdot; \eta)$.

Step 3 We run in parallel $N/4L$ constrained simulations with microscopic boundary conditions given by α_1 to obtain $\alpha_2 \in S_{N,\mathcal{O}}$ sampled from $\mu_{N,\mathcal{O}}(\cdot | \alpha^{\mathcal{E}'}, \eta)$.

Step 4 We obtain a sample of $\mathcal{G}_N^{(2)}$ by taking $[\alpha_1, \alpha_2]$.

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 (2.16, 2.20, 2.27) are simple consequences of this higher-order computation. The estimation of the errors measured in specific relative entropy (2.17, 2.22, 2.30) is carried out in Section 3.1.2.

3.1.1. The series expansion. We want to construct corrections for the initial choice (2.12). For this one would like to expand the exponential in (2.18), 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 $\eta \in \bar{S}_M$ and $\alpha \in S_{N,\mathcal{E}}$ be compatible over \mathcal{E} . For every $\sigma \in S_N$ compatible with η over \mathbb{T} and such that $\sigma^\mathcal{E} = \alpha$ we have

$$H_N(\sigma) - \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) = \sum_{(k,k') \in \bar{\Lambda}_{M,\leq}} \bar{\Delta}_{k,k'} J(\sigma)$$

where

$$\bar{\Lambda}_{M,\leq} = \{(k, k') \in \{0, \dots, M-1\} \times \{1, \dots, M\} \text{ such that } k \leq k'\}$$

and

$$\bar{\Delta}_{k,k'} J(\sigma) = \begin{cases} \Delta_{k,k'} J(\sigma) & \text{if there is } l \text{ odd s.t. } k, k' \in D_l \\ \check{\Delta}_{k,k'} J(\sigma) & \text{if there is } l \text{ odd s.t. } k \in D_l, k' \in D_{l+1} \\ \tilde{\Delta}_{k,k'} J(\sigma) & \text{if there is } l \text{ odd s.t. } k \in D_{l-1}, k' \in D_l \\ 0 & \text{otherwise} \end{cases}$$

with

$$\Delta_{k,k'} J(\sigma) = -\frac{1}{2} \sum_{\substack{x \in C_k \\ y \in C_{k'}, y \neq x}} (J(x-y) - \bar{J}(k, k')) \sigma(x) \sigma(y) (2 - \delta_{k,k'}),$$

$$\check{\Delta}_{k,k'} J(\sigma) = - \sum_{\substack{x \in C_k \\ y \in C_{k'}}} (J(x-y) - \check{J}(k, y)) \sigma(x) \alpha(y),$$

and

$$\tilde{\Delta}_{k,k'} J(\sigma) = - \sum_{\substack{x \in C_k \\ y \in C_{k'}}} (J(x-y) - \check{J}(k', y)) \alpha(x) \sigma(y).$$

These terms are connected to the small parameter δ since it follows from a simple Taylor expansion that for every $k, k' \in \bar{\Lambda}_M$

$$\sup_{\eta \in \bar{S}_M} \sup_{\alpha \in S_{N,\mathcal{E}}} \sup_{\sigma \in S_N} |\bar{\Delta}_{k,k'} J(\sigma)| \leq 2 \frac{Q^3}{L^2} \|\nabla V\|_\infty.$$

By letting

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

we get

$$E_N[e^{-\beta(H_N(\sigma) - \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta))} | \alpha, \eta] = \int_{\{\sigma: \sigma^\mathcal{E} = \alpha\}} \prod_{k,l \in \bar{\Lambda}_{M,\leq}} (1 + \bar{f}_{k,l}) \bigotimes_{k \in \bar{\Lambda}_M \cap \mathcal{O}} \tilde{\rho}_k(\sigma).$$

The polymer model is as in [14] with the only difference that we are integrating over the half space \mathcal{O} keeping fixed the variables $\sigma^\mathcal{E} = \alpha$. In order to benefit from the analysis carried out in [14] we introduce the following notation:

$$\hat{\rho}_k(\sigma) = \begin{cases} \tilde{\rho}_k(\sigma) & \text{if } k \in \bar{\Lambda}_M \cap \mathcal{O} \\ 1_{\{\sigma^{C_k} = \alpha^{C_k}\}} & \text{if } k \in \bar{\Lambda}_M \cap \mathcal{E} \end{cases}$$

so

$$E_N[e^{-\beta(H_N(\sigma) - \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta))} | \alpha, \eta] = \int_{S_N} \prod_{k,l \in \bar{\Lambda}_M, \leq} (1 + \bar{f}_{k,l}) \bigotimes_{k \in \bar{\Lambda}_M} \hat{\rho}_k(\sigma).$$

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

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

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

$$\zeta(R) = \int \sum_{g \in G_R} \prod_{\{k,l\} \in g} \bar{f}_{kl}(\sigma) \bigotimes_{\{k\} \in R} \hat{\rho}_k(\sigma) \quad (3.3)$$

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 [14] (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

$$\sup_{\alpha \in S_{N,\mathcal{E}}} \sup_{\eta \in \bar{S}_M} \sup_{k \in \bar{\Lambda}_M} \sum_{\substack{R \in \mathcal{R}, R \supset \{k\} \\ |R|=1}} |\zeta(R)| \leq \delta$$

and for every $r \geq 2$

$$\sup_{\alpha \in S_{N,\mathcal{E}}} \sup_{\eta \in \bar{S}_M} \sup_{k \in \bar{\Lambda}_M} \sum_{\substack{R \in \mathcal{R}, R \supset \{k\} \\ |R|=r}} |\zeta(R)| \leq \delta^{r-1}.$$

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

$$\bar{W}_{N,\mathcal{E}}(\alpha, \eta) = \bar{W}_{N,\mathcal{E}}^{(0)}(\alpha, \eta) - \frac{1}{\beta} \sum_{n \geq 1} \frac{1}{n!} \sum_{\substack{(R_1, \dots, R_n) \in \mathcal{R}^n \\ R_i \subset \bar{\Lambda}_M}} \phi(R_1, \dots, R_n) \prod_{i=1}^n \zeta(R_i) \quad (3.4)$$

with

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

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

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

Again a straightforward adaptation of the proof of Lemma 2.1 in [14] shows that

$$\sum_{R \in \mathcal{R}, R \subset \bar{\Lambda}_M} |\zeta(R)| \leq M(\delta + \sum_{r \geq 2} \delta^{r-1}) \quad (3.5)$$

and that for every $n \geq 2$

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

The inequalities (3.5) and (3.6) allow to identify in (3.4) the terms of the series expansion of Theorem 2.3. In particular

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

and

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

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

$$\begin{aligned} \bar{W}_{N,\mathcal{E}}^{(1)}(\alpha, \eta) &= -\frac{1}{\beta} \sum_{k \in \bar{\Lambda}_M} \int \bar{f}_{kk} \hat{\rho}_k(\sigma) \\ &\quad - \frac{1}{\beta} \sum_{(k,l) \in \bar{\Lambda}_{M,\leq}} \int (\bar{f}_{kl} + \bar{f}_{kl} \bar{f}_{kk} + \bar{f}_{kl} \bar{f}_{ll} + \bar{f}_{kl} \bar{f}_{kk} \bar{f}_{ll}) \hat{\rho}_k(\sigma) \hat{\rho}_l(\sigma) \end{aligned} \quad (3.7)$$

and

$$\begin{aligned} \bar{W}_{N,\mathcal{E}}^{(2)}(\alpha, \eta) &= \frac{1}{2\beta} \sum_{k \in \bar{\Lambda}_M} \left(\int \bar{f}_{kk} \hat{\rho}_k(\sigma) \right)^2 + \\ &\quad + \frac{1}{2\beta} \sum_{(k,l) \in \bar{\Lambda}_{M,\leq}} \int \bar{f}_{kk} \hat{\rho}_k(\sigma) \int (\bar{f}_{kl} + \bar{f}_{kl} \bar{f}_{kk} + \bar{f}_{kl} \bar{f}_{ll} + \bar{f}_{kl} \bar{f}_{kk} \bar{f}_{ll}) \hat{\rho}_k(\sigma) \hat{\rho}_l(\sigma) + \\ &\quad + \frac{1}{2\beta} \sum_{k \in \{0, \dots, M-1\}} \sum_{l_1: (k, l_1) \in \bar{\Lambda}_{M,\leq}} \sum_{l_2: (k, l_2) \in \bar{\Lambda}_{M,\leq}} \\ &\quad \int (\bar{f}_{kl_1} + \bar{f}_{kk} \bar{f}_{kl_1} + \bar{f}_{kl_1} \bar{f}_{l_1 l_1} + \bar{f}_{kk} \bar{f}_{kl_1} \bar{f}_{l_1 l_1}) \hat{\rho}_k(\sigma) \hat{\rho}_{l_1}(\sigma) \times \\ &\quad \times \int (\bar{f}_{kl_2} + \bar{f}_{kk} \bar{f}_{kl_2} + \bar{f}_{kl_2} \bar{f}_{l_2 l_2} + \bar{f}_{kk} \bar{f}_{kl_2} \bar{f}_{l_2 l_2}) \hat{\rho}_k(\sigma) \hat{\rho}_{l_2}(\sigma) + \\ &\quad - \frac{1}{\beta} \sum_{k \in \{0, \dots, M-1\}} \sum_{l_1: (k, l_1) \in \bar{\Lambda}_{M,\leq}} \sum_{l_2: (l_1, l_2) \in \bar{\Lambda}_{M,\leq} \text{ or } (k, l_2) \in \bar{\Lambda}_{M,\leq}} \\ &\quad \int (\bar{f}_{kl_1} \bar{f}_{l_1 l_2} + \bar{f}_{kl_1} \bar{f}_{kl_2} + \bar{f}_{kl_2} \bar{f}_{l_1 l_2} + [\dots]) \hat{\rho}_k(\sigma) \hat{\rho}_{l_1}(\sigma) \hat{\rho}_{l_2}(\sigma) \end{aligned} \quad (3.8)$$

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

$$\bar{f}_{k,l}(\sigma) = e^{-\beta \bar{\Delta}_{kl} J(\sigma)} - 1 = \sum_{p=1}^{\infty} \frac{1}{p!} (-\beta \bar{\Delta}_{kl} J(\sigma))^p \text{ with } \bar{\Delta}_{kl} J(\sigma) \sim O(Q^2 \frac{Q}{L^2} \|\nabla V\|_{\infty}) \quad (3.9)$$

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 $\bar{W}_{N,\mathcal{E}}^{(1)}$

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

and

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

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

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

uniformly in η, α and σ and Theorem 1 is thus established.

In order to compute the interactions that enter into play in Step 1 of Scheme B with $p = 2$ we discard terms like e.g. $\int (\bar{\Delta}_{kk} J(\sigma))^2 \hat{\rho}_k(\sigma)$ since they are either 0 ($k \in \bar{\Lambda}_M \cap \mathcal{E}$) or functions of η alone ($k \in \bar{\Lambda}_M \cap \mathcal{O}$). After simple but long computations we get

$$-\bar{W}_{N,\mathcal{E}}^{(1)}(\alpha, \eta) = \beta \sum_{m: \text{even}} \sum_{k \in \bar{\Lambda}_M \cap D_m} \left(\sum_{x, y \in C_k} \Theta_1(m, x, y, \eta) \alpha(x) \alpha(y) + \sum_{y \in C_k} \Theta_2(m, y, \eta) \alpha(y) \right)$$

where

$$\Theta_1(m, x, y, \eta) = \frac{1}{2} \sum_{l \in \bar{\Lambda}_M \cap (D_{m-1} \cup D_{m+1})} C_1(l, x, y) (1 - e_2(\eta(l)))$$

with

$$C_1(l, x, y) = \sum_{u \in C_l} (J(u-x) - \check{J}(l, x))(J(u-y) - \check{J}(l, y)) \quad \text{and} \quad e_2(\eta(l)) = \frac{\eta^2(l) - Q}{Q(Q-1)},$$

and

$$\Theta_2(m, y, \eta) = \sum_{l \in \bar{\Lambda}_M \cap (D_{m-1} \cup D_{m+1})} (C_2(l, y) e_3(\eta(l)) + C_3(l, y) e_1(\eta(l)))$$

with

$$C_2(l, y) = \sum_{\substack{u, v, w \in C_l \\ u \neq v, v \neq w, w \neq u}} (J(u - v) - \bar{J}(0))(J(w - y) - \check{J}(l, y)),$$

$$C_3(l, y) = 2 \sum_{\substack{u, v \in C_l \\ u \neq v}} (J(u - v) - \bar{J}(0))(J(u - y) - \check{J}(l, y)),$$

$$e_1(\eta(l)) = \frac{\eta(l)}{Q} \quad \text{and} \quad e_3(\eta(l)) = \frac{4\eta^3(l) + 4\eta(l)Q^2 - 24\eta(l)Q + 16\eta(l)}{8Q(Q-1)(Q-2)}.$$

Notice that Θ_1 couples spins that are inside the same coarse cell while Θ_2 acts like an external magnetic field. We further have

$$\begin{aligned} -\bar{W}_{N, \mathcal{E}}^{(2)}(\alpha, \eta) &= \beta \sum_{m: \text{even}} \sum_{k \in \bar{\Lambda}_M \cap D_m} \left(\sum_{y \in C_k} \Theta_3(m, y, \eta) \alpha(y) \right) + \\ &+ \beta \sum_{m: \text{even}} \sum_{\substack{k, l \in \bar{\Lambda}_M \cap D_m \\ k < l}} \sum_{x \in C_k, y \in C_l} \Theta_4(m, x, y, \eta) \alpha(x) \alpha(y) + \\ &+ \beta \sum_{m: \text{odd}} \sum_{k \in \bar{\Lambda}_M \cap D_{m-1}} \sum_{k' \in \bar{\Lambda}_M \cap D_{m+1}} \sum_{x \in C_k, y \in C_{k'}} \Theta_5(m, x, y, \eta) \alpha(x) \alpha(y) \end{aligned}$$

with

$$\Theta_4(m, x, y, \eta) = \sum_{j \in \bar{\Lambda}_M \cap (D_{m+1} \cup D_{m-1})} C_4(x, y, j) (1 - e_2(\eta(j))),$$

where

$$C_4(x, y, j) = \sum_{u \in C_j} (J(x - u) - \check{J}(x, j))(J(y - u) - \check{J}(y, j)),$$

$$\begin{aligned} \Theta_3(m, y, \eta) &= \sum_{\substack{(k, k') \in (\bar{\Lambda}_M \cap D_{m-1})^2 \cup (\bar{\Lambda}_M \cap D_{m+1})^2 \\ k < k'}} C_5(y, k, k') e_1(\eta(k')) (1 - e_2(\eta(k))) \\ &+ \sum_{\substack{(k, k') \in (\bar{\Lambda}_M \cap D_{m-1})^2 \cup (\bar{\Lambda}_M \cap D_{m+1})^2 \\ k < k'}} C_5(y, k', k) e_1(\eta(k)) (1 - e_2(\eta(k'))) \\ &+ \sum_{\substack{k \in \bar{\Lambda}_M \cap D_{m-1} \\ k' \in \bar{\Lambda}_M \cap D_{m+1}}} C_6(y, k, k') e_1(\eta(k)) (1 - e_2(\eta(k'))) \\ &+ \sum_{\substack{k \in \bar{\Lambda}_M \cap D_{m-1} \\ k' \in \bar{\Lambda}_M \cap D_{m+1}}} C_6(y, k', k) e_1(\eta(k')) (1 - e_2(\eta(k))). \end{aligned}$$

where

$$C_5(y, k, k') = \sum_{u \in C_k, v \in C_{k'}} (J(y - u) - \check{J}(y, k))(J(u - v) - \bar{J}(k, k'))$$

$$C_6(y, k, k') = \sum_{u \in C_k, v \in C_{k'}} (J(y - v) - \check{J}(y, k'))(J(u - v) - \bar{J}(k, k'))$$

and finally

$$\Theta_5(m, x, y, \eta) = \sum_{j \in \bar{\Lambda}_M \cap D_m} C_7(x, y, j)(1 - e_2(\eta(j)))$$

where

$$C_7(x, y, j) = \sum_{u \in C_j} (J(x - u) - \check{J}(x, j))(J(u - y) - \check{J}(j, y)).$$

Notice that Θ_3 acts like an external magnetic field, Θ_4 couples spin that are in different coarse cells within the same reconstruction domains and Θ_5 couples spins that are in different reconstruction domains.

In the $p = 2$ case the obtained reconstruction kernel is not a product measure because of the presence of the Θ_5 coupling. Now notice that all the computations we performed are based on controls that depend on M, Q and L , *but not on the size of the reconstruction domains* D_l . Should we have reconstructed over domains D'_l with $2L$ microscopic points we would have get formally the same expression with the difference that in this case for every m odd, every $k \in \bar{\Lambda}_M \cap D_{m-1}$, $k' \in \bar{\Lambda}_M \cap D_{m+1}$ and every $x \in C_k, y \in C_{k'}$ we necessarily have $\Theta_5(m, x, y, \eta) = 0$. Indeed, for every $j \in \bar{\Lambda}_M \cap D_m$ and every $u \in C_j$ we necessarily have either $J(x - u) - \check{J}(x, j) = 0$ or $J(u - y) - \check{J}(j, y) = 0$ since the interaction range of the potential J is L . It follows from this observation that for every $\eta \in \bar{S}_M$ the measure $\gamma_{N, \mathcal{E}}^{(2)}(\cdot; \eta)$ 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 $3L$ 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 (2.22). 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:

$$\begin{aligned} \frac{1}{N} H(\nu_N^{(p)}(\cdot, \eta) | \mu_N(\cdot | \eta)) &= \frac{1}{N} \sum_{\sigma \in S_N} \nu_N^{(p)}(\sigma, \eta) \log \frac{\nu_N^{(p)}(\sigma, \eta)}{\mu_N(\sigma | \eta)} \\ &= \frac{1}{N} \sum_{\sigma \in S_N} \nu_{N, \mathcal{E}}^{(p)}(\sigma^\mathcal{E}, \eta) \mu_{N, \mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta) \log \frac{\nu_{N, \mathcal{E}}^{(p)}(\sigma^\mathcal{E}, \eta) \mu_{N, \mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta)}{\mu_{N, \mathcal{E}}(\sigma^\mathcal{E} | \eta) \mu_{N, \mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta)} \\ &= \frac{1}{N} \sum_{\sigma \in S_N} \nu_{N, \mathcal{E}}^{(p)}(\sigma^\mathcal{E}, \eta) \mu_{N, \mathcal{O}}(\sigma^\mathcal{O} | \sigma^\mathcal{E}, \eta) \times \\ &\quad \times \left[-\beta(\bar{W}_{N, \mathcal{E}}^{(p)}(\sigma^\mathcal{E}, \eta) - \bar{W}_{N, \mathcal{E}}(\sigma^\mathcal{E}, \eta)) + \log \frac{\bar{Z}_{N, \mathcal{E}}(\eta)}{Z_{N, \mathcal{E}}^{(p)}(\eta)} \right] \end{aligned} \quad (3.12)$$

and

$$\begin{aligned} Z_{N, \mathcal{E}}^{(p)}(\eta) &= \int_{S_{N, \mathcal{E}}} e^{-\beta \bar{W}_{N, \mathcal{E}}^{(p)}(\alpha, \eta)} \bigotimes_{k \in \mathcal{E} \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \\ &= \int_{S_{N, \mathcal{E}}} e^{-\beta(\bar{W}_{N, \mathcal{E}}^{(p)}(\alpha, \eta) - \bar{W}_{N, \mathcal{E}}(\alpha, \eta)) - \beta \bar{W}_{N, \mathcal{E}}(\alpha, \eta)} \bigotimes_{k \in \mathcal{E} \cap \bar{\Lambda}_M} \tilde{\rho}_k(\alpha^{C_k}) \\ &= e^{N\mathcal{O}(\varepsilon^{p+1})} \bar{Z}_{N, \mathcal{E}}(\eta) \end{aligned}$$

which combined with (2.20) and (3.12) proves the announced result.

3.2. The $Q > L$ case. In this Section we prove Lemma 2.7. Theorem 2.9 and 2.10 are straightforward consequences of Lemmas 2.7 and 2.8 that are obtained by adapting the computations of Section 3.1.2

3.2.1. Proof of Lemma 2.7. As before, the effective interaction $\bar{W}_{N,\varepsilon}(\alpha, \eta)$ for $\alpha \in S_{N,\varepsilon}$ is given after integrating over $\sigma^{\mathcal{O}} \in S_{N,\mathcal{O}}$ compatible with η over \mathcal{O} :

$$\begin{aligned} e^{-\beta \bar{W}_{N,\varepsilon}(\alpha, \eta)} &= \int_{\{-1,1\}^{\Lambda_N \cap \mathcal{O}}} e^{-\beta H_N([\sigma^{\mathcal{O}}, \alpha])} \prod_{k \in \bar{\Lambda}_M \cap \mathcal{O}} \tilde{\rho}_k(\sigma^{C_k}) \\ &= e^{-\beta \sum_{l \in \mathcal{E}} H_{l,l}(\alpha^{D_l}, \alpha^{D_l})} \times \\ &\quad \times \prod_{l \in \mathcal{O}} \left[\int_{\{-1,1\}^{\Lambda_N \cap \mathcal{O}}} e^{-\beta H_{l,l}(\sigma^{D_l}, \sigma^{D_l})} e^{-\beta H_{l-1,l}(\alpha^{D_{l-1}}, \sigma^{D_l})} e^{-\beta H_{l,l+1}(\sigma^{D_l}, \alpha^{D_{l+1}})} \bar{\rho}_l(\sigma^{D_l}) \right] \end{aligned}$$

Note that the term in brackets in the last display $[\dots] = Z_l(\alpha^{D_{l-1}}, \alpha^{D_{l+1}}; \eta)$, couples the configurations $\alpha^{D_{l-1}}$ and $\alpha^{D_{l+1}}$. To proceed with our calculation we want to decouple them, so we decompose $[\dots]$ as follows:

$$[\dots] = \frac{Z_l(0, \alpha^{D_{l+1}}; \eta) Z_l(\alpha^{D_{l-1}}, 0; \eta)}{Z_l(0, 0; \eta)} (f_{l-1,l+1}(\alpha) + 1).$$

By changing indices we have that

$$\prod_{l \in \mathcal{O}} Z_l(0, \alpha^{D_{l+1}}; \eta) Z_l(\alpha^{D_{l-1}}, 0; \eta) = \prod_{l \in \mathcal{E}} Z_{l+1}(\alpha^{D_l}, 0; \eta) Z_{l-1}(0, \alpha^{D_l}; \eta)$$

We multiply and divide by $A_{l-1,l,l+1}(\eta)$ and finally obtain the announced formulation.

4. Numerical experiments. In this section we illustrate the efficiency of the schemes we introduced by giving the results of some numerical experiments. We consider a microscopic lattice of size $N = 512$ and a microscopic coupling defined by $J(x) = 1/2L$ when $|x| \leq L/N$ and $J(x) = 0$ otherwise. We consider different values for Q, L and β in order to illustrate their interplay in the problems addressed here. To evaluate the efficiency of the schemes we made MC computations of

$$\langle H_N(\sigma) | \eta \rangle_{\varrho_\beta} = \int_{S_N} H_N(\sigma) \varrho_\beta(\sigma | \eta) \quad (4.1)$$

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 .

As β increases, in typical η 's most of the coarse-cells are covered: $\eta(k) = \pm Q$. In this case most of the information on the microscopic configuration is already given by η and first approximation schemes A and D are “perfect”. With deviant η 's almost all information on the microscopic configurations is lost in the transition micro-CG and the results of our experiments show that our higher order schemes are efficient in recovering this information. In particular the higher order schemes designed to deal with the $Q < L$ case show to be efficient *even at very low temperatures*.

In the Tables 4.1-4.6 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 [20] 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 $\int_{S_N} H_N(\sigma) \mathcal{G}_N^{(2)}(\sigma)$ with $\mathcal{G}_N^{(2)}$ given in Section 2.2.3.

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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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
 $N=512, L=16.$

| | $\beta=0.5$ | $\beta=1$ | $\beta=1.5$ | $\beta=2$ |
|----------------|-------------|-------------|-------------|-------------|
| Direct MC | -0.0124 | -0.0659 | -0.3579 | -0.4574 |
| Scheme F, Q=4 | -0.0124 0 % | -0.0659 0 % | -0.3579 0 % | -0.4574 0 % |
| Scheme F, Q=8 | -0.0124 0 % | -0.0659 0 % | -0.3579 0 % | -0.4574 0 % |
| Scheme F, Q=16 | -0.0124 0 % | -0.0659 0 % | -0.3579 0 % | -0.4574 0 % |