Canonical Sampling of a Lattice Gas

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It is shown that a novel sampling algorithm, recently proposed in conjunction with a lattice gas model of nuclear fragmentation, samples the canonical ensemble only in an approximate fashion. A residual weight factor has to be taken into account to calculate correct thermodynamic averages. Then, however, the algorithm is numerically inefficient.

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In a series of recent publications [1–3], Pan and Das Gupta introduced a lattice gas model for the schematic description of fragmentation in heavy-ion collisions. The basis of their treatment is a lattice with N sites where each site can be either empty or occupied by one of n particles. In the simplest case, the interaction is an attractive nearest neighbor coupling given by the Hamiltonian

$$\mathcal{H} = -\epsilon \sum_{<i,j>} \pi_i \pi_j \quad \text{with} \quad \pi_i = \begin{cases} 1 & \text{occupied} \\ 0 & \text{empty} \end{cases} \tag{1}$$

where $< i,j >$ indicates a sum over all nearest neighbor site pairs. This is nothing but an Ising model interpreted as a lattice gas [4]. Control parameters are temperature T and particle number n, or, in other words, the canonical ensemble is used in contrast to an earlier approach by Samaddar and Richert [5] that employed the grand-canonical ensemble.

The focus of this brief report is, however, not the model as such or a comparison with fragmentation data (see e.g. [6,7]) but the new sampling algorithm which was introduced in conjunction with the model. The algorithm for generating a configuration with n particles consists of the following steps: (i) Start with an empty lattice. (ii) The site for the placement of a particle is chosen with a *probability proportional to* $\exp(-\beta\Delta E)$ among the empty sites. ΔE is the energy change due to the chosen placement in each step and $\beta = 1/kT$. (iii) The previous step is repeated until n particles are placed. It is worth noting that, in absence of external potentials, the first particle is placed on a random site.

The claim of Refs. [1–3] is that this algorithm samples the canonical ensemble, or more specifically, generates a configuration c with a probability of

$$P^{(c)} = \frac{\exp(-\beta E^{(c)})}{\mathcal{Z}} \quad \text{with} \quad \mathcal{Z} = \sum_c \exp(-\beta E^{(c)}), \tag{2}$$

such that thermodynamic averages can be calculated by summing over the generated configurations with *equal* weight.

The probability to occupy site i_k in a configuration with $k-1$ already occupied sites $i_1, \ldots, i_{k-1}$, denoted as $(i_1, \ldots, i_{k-1})$, is therefore

$$p_{i_k}^{(i_1,\ldots,i_{k-1})} = \frac{\exp(-\beta\Delta E_{i_k}^{(i_1,\ldots,i_{k-1})})}{A^{(i_1,\ldots,i_{k-1})}} \tag{3}$$

where $\Delta E_{i_k}^{(i_1,\ldots,i_{k-1})}$ is the energy change if site i_k is filled and the step normalization

$$A^{(i_1,\ldots,i_{k-1})} = \sum_{i_j} \exp\left(-\beta\Delta E_{i_j}^{(i_1,\ldots,i_{k-1})}\right) \tag{4}$$

is given by a sum over all empty sites. The straightforward implementation of Eq. (3) leads to a computing time per configuration which grows quadratically with lattice size N at constant density $\rho = n/N$ even for short range interactions. However, using a rejection technique rather than the explicit evaluation of a distribution function leads to an implementation with a computing time proportional to the lattice size N. By construction, the new algorithm produces statistically independent configurations. Therefore, the new algorithm is free of 'critical slowing down' [8] and would be of considerable general interest, if it were valid.

Before we turn to a detailed analysis of the new algorithm it is important to distinguish between a *configuration* which is determined by a *set* of occupied sites and denoted as $(i_1, \ldots, i_n)$ and a particular *sequence* that is used to occupy the sites by the algorithm, denoted as $[i_1, \ldots, i_n]$. From Eq. (3) it follows that the probability to generate a n particle sequence $[i_1, \ldots, i_n]$ is

$$\begin{aligned} P^{[i_1,\ldots,i_n]} &= \prod_{k=1}^{n} p_{i_k}^{(i_1,\ldots,i_{k-1})} \\ &= \prod_{k=1}^{n} \frac{\exp(-\beta\Delta E_{i_k}^{(i_1,\ldots,i_{k-1})})}{A^{(i_1,\ldots,i_{k-1})}} \\ &= \frac{\exp(-\beta E^{(i_1,\ldots,i_n)})}{W^{[i_1,\ldots,i_n]}} \end{aligned} \tag{5}$$

where the total energy and the normalization are given by

$$\begin{aligned} E^{(i_1,\ldots,i_n)} &= \sum_{k=1}^{n} \Delta E_{i_k}^{(i_1,\ldots,i_{k-1})} \\ W^{[i_1,\ldots,i_n]} &= \prod_{k=1}^{n} A^{(i_1,\ldots,i_{k-1})}\ , \end{aligned} \tag{6}$$

respectively. It should be noted that in general the normalization explicitly depends on the sequence and not only on the configuration. The probability to generate the n particle configuration c is given by the sum over $n!$ possible sequences s leading to the same configuration:

$$P^{(c)} = \sum_{s \text{ of } c} P^{[s]} = \frac{\exp(-\beta E^{(c)})}{B^{(c)}} \tag{7}$$

with

$$B^{(c)} = \left(\sum_{s \text{ of } c} \frac{1}{W^{[s]}} \right)^{-1} \tag{8}$$

From comparing Eqs. (2) and (7) it follows immediately that the normalization $B^{(c)}$ should be independent of the configuration c and equal to the partition function $\mathcal{Z}$. On the other hand, for the Hamiltonian given in Eq.(1) one quickly sees that this is *not* true. The partition function can be written as a polynomial

$$\mathcal{Z} = \sum_m \Omega_{(m)} x^m \quad \text{with} \quad x = \exp(\beta\epsilon),$$

where $\Omega_{(m)}$ is the number of configurations with energy $-m\epsilon$. The step and sequence normalizations (4) and (6) are indeed polynomials in x. However, the configuration normalization $B^{(c)}$ given by Eq. (8) is a rational function in x and will, in general, not reduce to a polynomial, and thus differ from $\mathcal{Z}$.

From Eq. (5) it follows that the correct way to calculate a thermodynamic average of a quantity Q is

$$< Q > = \frac{\sum Q_i W_i}{\sum W_i} \tag{9}$$

where W plays the role of a *residual weight.* In this form, the algorithm is conceptually somewhere between a direct Monte Carlo, where configurations are chosen randomly and weighted with $\exp(-\beta E)$, and a Metropolis sampling, where configurations are chosen with probability $\exp(-\beta E)$ and weighted evenly [9]. The distribution of sequence weights W is approximately lognormal. Therefore, the weighted averages are dominated by only a very small fraction of the generated configurations, which makes this form of the algorithm numerically inefficient.

The original algorithm gives in many cases results close to the correct solution. For example, the total energy and specific heat for a 3d lattice gas with 4^3 sites and 16 particles at the critical temperature $T/\epsilon = 1.1277$ deviates only a few percent from the values obtained with Metropolis sampling. However, it is easy to construct examples where the algorithm fails drastically or to check that the particle-hole symmetry of the Hamiltonian Eq.(1) is broken by the algorithm.

In summary, it has been shown that the algorithm proposed recently by Pan and Das Gupta samples the canonical ensemble only approximately. Correct thermodynamic averages can be obtained by taking a residual weight factor into account. Then, however, the algorithm is numerically inefficient.

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