A MONTE CARLO PROCEDURE FOR HAMILTONIANS WITH SMALL NONLOCAL CORRECTION TERMS

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Lattice field theories are considered whose hamiltonians contain small nonlocal correction terms. It is proposed to do simulations for an auxiliary polymer system with field-dependent activities. If a nonlocal correction term to the hamiltonian is small, it need be evaluated only rarely.

In this note we would like to describe a Monte Carlo procedure that can cope with complicated nonlocal [+1] bosonic hamiltonians for lattice field theories as are expected to result from exact analytical or accurate numerical renormalization group calculations. It can be used to advantage when most of the nonlocal correction terms are small. Let us initially suppose that the hamiltonian $\mathcal{H}(\varphi)$ is given, as a function of some fields $\varphi = \{\varphi_x\}$ (spin or gauge fields, for instance) on a finite set Λ of sites x (e.g. points or links of a lattice). Let us assume that $\mathcal{H}$ can be split as

$$\mathcal{H}(\varphi) = \mathcal{H}_0(\varphi) + \mathcal{H}_1(\varphi) , \tag{1}$$

where $\mathcal{H}_0$ has good locality properties so that it is suitable for treatment by standard Monte Carlo simulation techniques, and $\mathcal{H}_1$ is small in a suitable sense (cp. inequality (3) below). Expanding $\exp(-\mathcal{H}_1)$ in a Mayer series (high-temperature series) one may obtain a polymer representation of the Boltzmann factor of the form [1,2]

$$\exp[-\mathcal{H}(\varphi)] = \exp[-\mathcal{H}_0(\varphi)]$$

$$\times \left(1 + \sum_{\mathcal{X} \neq \emptyset} \prod_{P \in \mathcal{X}} A(P, \varphi) \right) . \tag{2}$$

Here $\mathcal{X}$ are collections of mutually compatible non-

empty subsets P of Λ, called polymers. For the moment, two polymers P_1 and P_2 are to be regarded as compatible if they do not overlap. We write $P_1 \sim P_2$ in this case. Later on we shall consider a generalization. The activities $A(P, \varphi)$ will only depend on φ_x for $x \in P$. If the fields take their values in a compact space, inessential φ-independent terms can be added to the hamiltonian so that the activities are nonnegative (see below)

$$A(P, \varphi) \geqslant 0 .$$

We will assume that this is true. Generalization to situations where the activities are negative with very small probability is possible. [One considers an auxiliary polymer system with activities $|A(P, \varphi)|$ and takes care of the signs when computing averages.] It is required that there exists $\xi_\varphi < \infty$ for every φ such that for all x

$$1 + \sum_{P:x \in P} A(P, \varphi) \leqslant \xi_\varphi . \tag{3}$$

This is a basic stability condition for polymer systems [2].

We propose to do simulations for an auxiliary statistical system whose states are pairs $(\mathcal{X}, \varphi)$. The Monte Carlo procedure will generate a sequence of pairs $(\mathcal{X}, \varphi)$. One sweeps through all sites x of Λ. For each x, updating "at x" may change $\varphi(x)$ and $\mathcal{X}$. A change in $\mathcal{X}$ may consist in adding or removing (or altering) a polymer P that contains x. Given x and $\mathcal{X}$, the new φ_x

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is computed with probability distribution

$$d \, \text{prob}(\varphi_x) = \mathcal{N}_{\mathcal{X}}^{-1} \, \exp[-\mathcal{H}_0(\varphi)]$$

$$\times \prod_{P \in \mathcal{X}: x \in P} A(P, \varphi) \, d\varphi_x \,. \tag{4}$$

$\mathcal{N}_{\mathcal{X}}$ is a normalization factor, and the right-hand side is to be considered as a function of φ_x, for fixed $\{\varphi_y\}_{y \neq x}$. Given φ, the collections $\mathcal{X}$ are to be generated with probability

$$\text{prob}(\mathcal{X}) = \mathcal{N}_{\varphi}^{-1} \prod_{P \in \mathcal{X}} A(P, \varphi) \,. \tag{5}$$

The first 1 in the large brackets in eq. (2) is to be understood as the contribution from the empty collection $\mathcal{X} = \emptyset$, and eq. (5) must also hold for $\mathcal{X} = \emptyset$. (Empty products are read as 1). To achieve this one performs updating "at x" with transition probabilities $W_x(\mathcal{X} \to \mathcal{X}')$ that satisfy the condition of detailed balance [3].

$$\text{prob}(\mathcal{X}) W_x(\mathcal{X} \to \mathcal{X}') = \text{prob}(\mathcal{X}') W_x(\mathcal{X}' \to \mathcal{X}) \,. \tag{6}$$

A possible choice of transition probabilities $W_x(\mathcal{X} \to \mathcal{X}')$ for $\mathcal{X} \neq \mathcal{X}'$ is as follows

$$W_x(\mathcal{X} \to \mathcal{X}')$$

$$= \xi_{\varphi}^{-1} \quad \text{if } \mathcal{X}' = \mathcal{X} - \{P\} \text{ for some } P \ni x \,,$$

$$= \xi_{\varphi}^{-1} A(P, \varphi) \quad \text{if } \mathcal{X}' = \mathcal{X} + \{P\} \text{ and } x \in P \,,$$

$$= 0 \quad \text{otherwise} \,. \tag{7}$$

The condition $\mathcal{X}' = \mathcal{X} + \{P\}$ is to be understood as: $\mathcal{X}' = \mathcal{X} \cup \{P\}$ and P is compatible with all polymers in $\mathcal{X}$. ξ_{φ} is to be chosen so that inequality (3) holds (i.e. the total transition probability is ≤ 1). The computer remembers the state by storing for each x both φ_x and the polymers $P \in \mathcal{X}$ with $x \in P$.

The general procedure outlined so far starts from a polymer representation (2) of the Boltzmann factor. Given that, one does not actually need an expression for $\mathcal{H}$ itself (i.e. one avoids taking logarithms). This could be significant for the following reason. Rigorous analytical work on renormalization group transformations [4] suggests that series representations (like eq. (8) below) for effective hamiltonians may be inappropriate (badly nonlocal and divergent) when φ is in the large field region where $\exp[-\mathcal{H}(\varphi)]$ becomes very small, but that a well-behaved polymer expan-

sion (2) for the Boltzmann factor continues to hold there.

In the following we will suppose, however, that $\mathcal{H}_1(\varphi)$ is given as a series such as

$$\mathcal{H}_1(\varphi) = \sum_Q V_Q(\varphi) \,. \tag{8}$$

The label Q will specify a subset supp Q of Λ such that $V_Q(\varphi)$ depends on φ_x only for $x \in$ supp Q. Consider for instance a lattice gauge theory with gauge group G and lattice gauge field U that specifies parallel transporters $U(C) \in$ G. Q might have the form

$$Q = (C_1, \tau_1; C_2, \tau_2; \dots C_n, \tau_n) \,, \tag{9}$$

where C_i are closed paths and τ_i are characters of irreducible representations of G, and

$$V_Q(U) = \rho(Q) \prod_{i=1}^{n} \tau_i(U(C_i)) + \text{c.c.} \tag{10}$$

with complex coefficients $\rho(Q)$.

We will derive a special polymer representation of the Boltzmann factor which appears be particularly convenient for computation. It involves the Q in eq. (8) as polymers. This amounts to a slight generalization of the notion of polymers introduced after eq. (2), because different polymers Q may now occupy the same subset P = supp Q of Λ. We will write $x \in$ Q in place of $x \in$ supp Q. Two polymers Q will now be regarded as compatible if they are not identical.

If necessary we add field-independent constants c_Q to $V_Q(\varphi)$ so that $V_Q(\varphi) \leq 0$. In the example (10), $c_Q = 2|\rho(Q)||\Pi \tau_i(1)|$ will do. We define activities $A(Q, \varphi) \geq 0$ by

$$\exp[-V_Q(\varphi)] = 1 + A(Q, \varphi) \,.$$

It follows that

$$\exp[-\mathcal{H}_1(\varphi) + \text{const.}]$$

$$= \prod_Q \exp[-V_Q(\varphi)] = \prod_Q [1 + A(Q, \varphi)]$$

$$= \sum_{\mathcal{X}} \prod_{Q \in \mathcal{X}} A(Q, \varphi) \,,$$

and polymer representation (2) holds except for an inessential overall constant factor. This polymer system can be simulated as described before.

If V_Q is small, then also $A(Q, \cdot)$ is small, and the probability of finding $Q \ni x$ in the state $\mathcal{X}$ while at x is also small. Therefore $V_Q(\varphi)$ for any particular such Q needs to be computed only rarely. In contrast it would need to be computed at every updating step at $x \in Q$ in the standard Monte Carlo procedure.

References

[1] E. Seiler, Gauge theories as a problem in constructive quantum field theory and statistical mechanics, Lecture Notes in Physics, Vol. 159 (Springer, Berlin, 1982).
[2] C. Gruber and H. Kunz, Commun. Math. Phys. 22 (1971) 133.
[3] K. Binder, in: Monte Carlo methods in statistical physics, ed. K. Binder (Springer, Berlin, 1979);
M. Creutz, L. Jacobs and C. Rebbi, Phys. Rep. 95 (1983) 201.
[4] K. Gawedzki and A. Kupiainen, Commun. Math. Phys. 99 (1985) 197.