Lattice Field Theory as a Percolation Process

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For a given lattice spin or gauge theory an associated correlated band or plaquette percolation process is constructed. It is conjectured to reproduce the universal scaling behavior of the original model. Different field theories lead to different cluster weights generalizing a result by Fortuin and Kasteleyn for Potts models. The new representation lends itself to the design of Monte Carlo algorithms with reduced critical slowing down.

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It has been known for some time¹ that the q-state Potts model is equivalent to bond percolation² with a weight factor q for each cluster and a certain bond probability fixed by the classical temperature. More recently, Swendsen and Wang demonstrated³ that such a representation allows a Monte Carlo simulation of the Ising model at criticality with greatly reduced autocorrelation times on large lattices. Clearly the corresponding gain in computer-time efficiency would be highly welcome for simulations of other lattice field theories. In fact, several related efforts along different lines have been made.⁴ I am thus motivated to develop a percolation representa-

$$\overline{Z} = \sum_{\{k_{x\mu}=0,1\}} \int \prod_{x} d\mu(\sigma_x) \exp\left[\sum_{x\mu} k_{x\mu} [\kappa + s(\sigma_x \cdot \sigma_{x+\mu})]\right]$$

For a given $k_{x\mu}$ configuration the spin model is now bond diluted, and the free parameter κ plays the role of a bond chemical potential. The annealed summation over $k_{x\mu}$ is, of course, trivial, and \overline{Z} can again be written in form (1) with a new nearest-neighbor action

$$\overline{s}(\epsilon) = \ln[(1 + e^{\kappa + s(\epsilon)})/(1 + e^{\kappa})], \qquad (3)$$

where $\epsilon = \sigma_x \cdot \sigma_{x+\mu} \in [-1,1]$, and irrelevant constants are fixed by $s(1) = 0 = \overline{s}(1)$. The *q*-state Potts model distinguishes only between $\epsilon = 1$ and $\epsilon \neq 1$ by $s(\epsilon \neq 1)$ = -K, and (3) then simplifies to

$$-\bar{K} = \ln[(1 + e^{\kappa - K})/(1 + e^{\kappa})].$$
(4)

All spin correlations formed with (2) depend on this combination only, and Fortuin and Kasteleyn's representation corresponds to the choice $K = \infty$ with $\overline{K} = \ln(1 + e^{\kappa})$. For each bond configuration the lattice sites may be grouped into disconnected clusters,² and $K = \infty$ forces all spins in a cluster to be parallel. Then the spin summation can be carried out and results in a factor q^{N_c} (N_c = number of clusters).⁶ This innocent-looking factor is, however, a nonlocal function of $\{k_{x\mu}\}$ and thus

$$z_c(k_{x\mu}) = \int \prod_{x \in c} d\mu(\sigma_x) \exp\left[\beta \sum_{c \in x\mu} k_{x\mu}(\sigma_x \cdot \sigma_{x+\mu} - 1)\right].$$

tion for continuous spin and gauge fields. Detailed numerical tests in the two-dimensional O(3) σ model will be reported elsewhere.⁵

The partition function for a spin model on a hypercubic lattice,

$$Z = \int \prod_{x} d\mu(\sigma_{x}) \exp\left(\sum_{x\mu} s(\sigma_{x} \cdot \sigma_{x+\mu})\right), \qquad (1)$$

represents $O(n) \sigma$ models, Ising models (n=1), x-y models (n=2), or Potts models depending on the choice of the integration measure $d\mu$ and nearest-neighbor coupling s. System (1) is augmented by a two-valued variable $k_{x\mu}$ for each interaction bond:

in general cumbersome⁷ for Monte Carlo updating; Swendsen and Wang incorporate it in their simulation by keeping bond as well as spin variables and simulating their joint distribution.

If we now consider continuous spins σ_x (e.g., $n \ge 2$) with the standard action $s(\epsilon) = \beta(\epsilon - 1)$, then clearly $\overline{s}(\epsilon)$ will be a variant action different from the original one for $\kappa < \infty$. Universality, however, leads one to expect that wherever in the (β, κ) plane the model develops long-range spin correlations one is approaching the same continuum field theory. If the standard version of the model with parameters $(\beta_0, \kappa_0 = \infty)$ and a diluted form at $(\beta, \kappa < \infty)$ are to describe the same long-range physics, one will obviously have to choose $\beta > \beta_0$: Stronger ferromagnetism on the active bonds has to make up for the missing ones.

We may also analyze (2) from the percolation point of view; then the spin integrations are recognized to supply a weight factor for each cluster c:

$$\overline{Z} = \sum_{\{k_{x\mu}\}} \exp\left(\kappa \sum_{k_{x\mu}}\right) \prod_{c} z_{c}(k_{x\mu}), \qquad (5)$$

with

(6)

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(8)

For large β the fluctuations of the continuous spins now remain relevant for the bonds, because they typically arrange $1 - \sigma_x \cdot \sigma_{x+\mu} = o(1/\beta)$. Then (6) can be computed in perturbation theory after the introduction of collective coordinates to eliminate the zero modes corresponding to simultaneous SO(n) rotations of all spins in a cluster.⁸ The leading-order (Gaussian fluctuations) result of such a calculation⁵ for the O(n) σ model reads

$$z_c = (|c|\beta/2\pi)^{(n-1)/2} C_n (\det K_c)^{-(n-1)/2}.$$
(7)

Here |c| is the number of spins in cluster c, and $C_n = 2\pi^{n/2}/\Gamma(n/2)$ is the surface of the sphere in n dimensions. K_c is the (negative) diluted lattice Laplacian on c,

$$K_{c}(x,y) = \sum_{\mu} \{k_{x\mu}(\delta_{x,y} - \delta_{x+\mu,y}) + k_{y\mu}(\delta_{x,y} - \delta_{x,y+\mu})\},\$$

with $x, y \in c$, and det' K_c is the determinant of the $|c| \times |c|$ matrix K_c with the zero eigenvalue belonging to the constant mode omitted. We dropped a factor of the form $A^{|c|}$ which only contributes to the total normalization of \overline{Z} because $\sum_c |c| = \text{total number of spins.}$ Apart from the Gaussian determinant contribution, z_c represents the phase-space volume corresponding to the arbitrary orientation of the cluster's total spin normalized relative to the Gaussian modes. For $n \rightarrow 1$ (7) reduces to the Ising-model result of Fortuin and Kasteleyn, $z_c = 2$. If n > 1 there is an analogous factor $C_n(\beta/2\pi)^{(n-1)/2}$ for each cluster, but clearly the remaining part of the weight encodes further information on the geometric structure of the cluster.

Figure 1 shows some first numerical results for the O(3) σ model on a two-dimensional 20×20 lattice.



FIG. 1. Nearest-neighbor correlation E in the two-dimensional O(3) σ model vs β for various fixed fractions of active bonds. The percentages vary slightly along the curves (as indicated for the end points); this is a finite-size effect on the 20² lattice caused by the extra demon degree of freedom in the microcanonical algorithm (Ref. 9).

Rather than fixing κ , I employed the microcanonical demon algorithm⁹ to run at various fixed percentages of active links. The nearest-neighbor spin correlation E is plotted as a function of β with the line "100%" corresponding to the standard version of the model $(\kappa = \infty)$. Although E is a nonuniversal short-range quantity, I found it valuable for adjusting β , when the bond fraction is varied: For equal E also the magnetic susceptibility (indicative for the correlation length) turns out to be very similar.¹⁰ In Table I results of simulations on various $L \times L$ lattices are reported. Parameters were adjusted to approximately maintain $\chi \simeq 0.1L^2$ to mimic in a simple way the continuum limit at fixed physical volume. For each lattice this may be achieved with various degrees of dilution if β is tuned appropriately. The two choices found in the table represent the standard version and a value of 52.5% at which autocorrelation times turned out to be smaller than at neighboring values for which short test runs were conducted. The quoted values for the correlation time τ_{χ} were determined by analysis of connected correlations in computer time after reaching equilibrium. Ratios of correlations at successive time separations reached constant values at a separation $\sim \tau_{\chi}$ and could be followed to about $3\tau_{\chi}$ before getting overwhelmed by noise. Errors on autocorrelation times are notoriously hard to determine. Here they are somewhat subjectively based on oscillations of the ratios and experience with multiple independent runs.

The simulation of the O(3) model is accelerated by the performance of random, i.e., Haar-measure distributed, O(3) rotations of the independent clusters after each heat-bath sweep of the spin and bond variables. These collective modes leave the Boltzmann factor invariant and represent the natural generalization of the choice of random Potts spins for each cluster.³ The Hoshen-Kopelman¹¹ algorithm is used to divide spins into clusters after each bond sweep. This takes less computer time than the spin update itself. I make further use of the nonlocal information residing in the clusters to define improved (i.e., less noisy) estimators¹² for correlations. Since all correlations between spins in different clusters vanish because of their independent O(n) rotations, we may, for example, measure the two-point function as

$$G(x-y) = \langle \sigma_x \cdot \sigma_y \theta(x,y;k_{x\mu}) \rangle, \tag{9}$$

TABLE I. Results of various simulations on lattices of size $L \times L$. Autocorrelation times τ_x associated with the susceptibility χ are given in each case for bond fractions of 52.5% and 100% (standard formulation). The first column shows the number of sweeps in multiples of 1000.

(No. sweeps)/1000	L	P _b [%]	β	E	χ/L^2	τχ
30	20	100	1.3	0.520	0.095(2)	17(2)
20	20	52.5	5.5	0.532	0.105(2)	8(1)
30	28	100	1.4	0.563	0.094(3)	38(2)
20	28	52.5	7.5	0.563	0.094(2)	18(3)
50	40	100	1.5	0.602	0.102(3)	74(7)
50	40	52.5	11.5	0.587	0.107(1)	30(5)
30	56	100	1.6	0.636	0.109(7)	217(12)
20	56	52.5	15.5	0.593	0.123(2)	75(8)

with $\theta = 1$ if x and y belong to the same cluster as defined by the bonds $\{k_{x\mu}\}$, and $\theta = 0$ otherwise. In Table I reduced autocorrelation times are noticed for the new algorithm in all cases. Not unexpectedly the gain is not as dramatic as in the critical Potts model.³ Combined with the advantage of improved estimators it seems, however, profitable to use the percolation technique in simulations of the typical size that is manageable on present-day computers. Many more details on the numerical aspects will be published elsewhere.⁵

To conclude, a word on gauge theory: Obviously the bond variables in this case live on plaquettes which form clusters by connecting links. The links in each cluster may be gauge transformed independently. New moves different from just gauge transformations arise in this way if a site borders links belonging to different clusters; the gauge transformation at that site may be chosen independently for each cluster and applied to the respective links. As a consequence an improved estimator for fundamental Wilson loops may be taken to vanish exactly unless the loop is fully contained in one cluster. On the asymmetric torus appropriate for finite physical temperature, the deconfinement transition (nonvanishing Polyakov loop) can only take place when there is a finite probability for links to belong to an "infinite" cluster closing in the temporal direction, i.e., beyond a (generalized kind of) plaquette percolation threshold.

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²For a review on percolation theory, see D. Stauffer, Phys. Rep. **54**, 1 (1974); J. W. Essam, Rep. Prog. Phys. **43**, 833 (1980).

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⁶This result may be considered as the leading term in a low-temperature expansion that becomes exact for $K \rightarrow \infty$. Compare the continuous-variable case below.

⁷Problems similar to those encountered for dynamical lattice fermions would arise; see, however, M. Sweeny, Phys. Rev. B **27**, 4445 (1983), and the discussion at the end of Ref. 3.

⁸For finite lattice perturbation theory in the standard O(3) model, these modes have to be fixed, too: P. Hasenfratz, Phys. Lett. **141B**, 385 (1984); U. Wolff, Nucl. Phys. **B265** [FS15], 537 (1986).

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¹⁰This approximate "universality" is presumably due to the fact that I remain within the class of nearest-neighbor actions only.

¹¹J. Hoshen and R. Kopelman, Phys. Rev. B 14, 3438 (1976).
 ¹²Sweeny, Ref. 7.