Statistical Mechanics of Probabilistic Cellular Automata

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The necessary and sufficient conditions under which fully probabilistic cellular-automata (PCA) rules possess an underlying Hamiltonian (i.e., are "reversible") are established. It is argued that, even for irreversible rules, continuous ferromagnetic transitions in PCA with "up-down" symmetry belong in the universality class of kinetic Ising models. The nonstationary (e.g., periodic) states achieved for asymptotically large times by certain PCA rules in the (mean field) limit of infinite dimension are argued to persist in two and three dimensions, where fluctuations are strong.

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Cellular automata (CA) are regular arrays of variables, each of which can assume two or more discrete values and evolves in discrete time steps according to a set of local rules which may be either deterministic or probabilistic.[1] They are used to model problems in physics, chemistry, biology, and computer science. The goal is to determine, for any given rule, the nature of the state of the system for asymptotically large time ($t \rightarrow \infty$), and to identify the universality classes of the phase transitions that occur as the rules are varied. In this paper we study probabilistic cellular automata (PCA) with two states per site. Our main results follow:

(1) We establish the necessary and sufficient condition under which a PCA rule is "microscopically reversible," i.e., the transition probabilities obey detailed balance for some underlying Hamiltonian; as $t \rightarrow \infty$ the system is therefore described by the stationary (equilibrium) Boltzmann distribution corresponding to that Hamiltonian. The condition depends on whether the rule is applied by updating the spins simultaneously or sequentially.[2]

(2) Continuous transitions into stationary ferromagnetic states of PCA which do not have associated Hamiltonians (i.e., are "irreversible") but which do have the "up-down" symmetry familiar from Ising models, are argued to fall, for both statics and dynamics, in the same universality classes as kinetic Ising models.[3] Thus, at ferromagnetic critical points, fully PCA coarse grained to sufficiently large length scales possess underlying Hamiltonians, even if they do not on microscopic scales.

(3) As in[4] equilibrium statistical mechanics, there exists a systematic expansion for PCA in inverse powers of d, the dimension. In the $d=\infty$ limit one obtains mean-field theory (MFT): The evolution of the CA is described by an iterative map[5] with one variable—the average magnetization—which, for appropriate rules, exhibits time-dependent asymptotic behavior, including limit cycles, chaos, etc.[6] We argue that such time dependence is not an artifact of MFT, but survives the strong fluctuations present in few dimensions. Guided by the analytic results available at $d=\infty$, we construct fully probabilistic, local rules in $d=2$ which produce, under numerical simulation, nonstationary states, viz., two-, three-, and four-cycles, as $t \rightarrow \infty$. We have also found rules which lead to what we believe are chaotic states.

We consider CA on d-dimensional hypercubic lattices with N sites, labeled i, each occupied by an Ising spin $S_i = \pm 1$. With $P(\{S_i\},t)$ the probability that the system is in the state $\{S_i\}$ at time t, the discrete master equation[7]

$$P(\{\tilde{S}_i\},t+1) = \sum_{\{S_i\}} P(\{S_i\},t) \prod_i Q(\tilde{S}_i | S_i, \{S_{i'}\}) \quad (1)$$

describes the PCA's time evolution. Here $Q(\tilde{S}_i | S_i, \{S_{i'}\})$ is the probability that the ith spin assumes the value $\tilde{S}_i$ at time $t+1$, given that this spin and its "neighborhood"—a set of z spins located on nearby sites $\{i'\}$—have the values S_i and $\{S_i'\}$, respectively, at time t. The rule is defined by specifying the neighborhood and the 2^{z+1} nonzero independent probabilities Q. We consider only "fully probabilistic" rules, i.e., *all* transition probabilities Q strictly greater than zero. Equation (1) clearly describes simultaneous (synchronous) updating of the spins; one can, alternatively, update single spins in a random sequence, i.e., sequentially. We reduce the number of independent Q's to $z+1$ by considering "totalistic" CA,[1] i.e., $Q = Q(\tilde{S}_i | S_i, \sum_{i'} S_{i'})$, and imposing up-down symmetry: $Q(\tilde{S}_i | S_i, \sum_{i'} S_{i'}) = Q(-\tilde{S}_i | -S_i, -\sum_{i'} S_{i'})$. The rule is then completely specified by the $z+1$ values of the function $f(M_i) = Q(-1|1, zM_i)$, where $M_i = (1/z)\sum_{i'} S_{i'}$ is the average magnetization of the neighborhood of i.

Kinetic Ising models [i.e., those (reversible) PCA which satisfy detailed balance for some associated Hamiltonian and so approach the Boltzmann distribution as $t \to \infty$] are well understood. Hence it is useful to derive conditions under which CA rules are reversible. First consider simultaneously applied rules. Detailed balance requires the existence of a Hamiltonian H such that for any two states $\{S_i\}$ and $\{\tilde{S}_i\}$,

$$\prod_i Q(\tilde{S}_i|S_i, \{S_{i'}\})/Q(S_i|\tilde{S}_i, \{\tilde{S}_{i'}\}) = \exp(H\{S_i\} - H\{\tilde{S}_i\}). \quad (2)$$

Consider for simplicity a one-dimensional, totalistic, up-down-symmetric PCA, the neighborhood of S_i consisting of the two near neighbors S_{i+1} and S_{i-1}, so that $z=2$. Q can then be written in the form

$$Q = A \exp[\tilde{S}_i(aS_i + bM_i + cS_iS_{i+1}S_{i-1})],$$

where A is an arbitrary even function of the S's but is independent of $\tilde{S}_i$, and a, b, and c are arbitrary constants. It follows from (2) that the associated H can consist of at most nearest- and next-nearest-neighbor two-spin interactions. It is then easy to check by considering two specific updatings of the system, viz., (1) only the ith spin flips (i.e., $\tilde{S}_i = -S_i$), and (2) only the ith and $(i+1)$st spins flip, that unless $c=0$ detailed balance cannot be satisfied for all pairs of states. Similarly, consideration of the updatings in which (1) only the ith spin flips, and (2) only the $(i+1)$st spin flips, shows that detailed balance can be satisfied for all pairs of states for *any* values of a and b. Invoking the fact that Q is a probability, i.e.,

$$\sum_{\tilde{S}_i = \pm 1} Q(\tilde{S}_i|S_i, 2M_i) = 1,$$

then immediately establishes the most general form of Q [or, equivalently, of $f(M)$] for reversible rules as

$$f(M) = [1 - \tanh(a + bM)]/2. \quad (3)$$

Extension of this reasoning to arbitrary dimension and z is straightforward but tedious; the result (3) continues to hold. Equation (3) implies that no simultaneously applied, up-down symmetric rule with more than two independent parameters can be reversible.

For *sequentially* applied rules the criterion for reversibility is simpler to derive since only single spin flips need be considered. The criterion depends on z. For nearest-neighbor rules ($z=2d$) the necessary and sufficient condition for the existence of an underlying Hamiltonian is $f(M) = f_e(M)[1 - \tanh(\lambda M)]$, where λ is an arbitrary parameter and f_e an arbitrary even function of M. As the range of the rule increases, the restriction on $f(M)$ required to ensure reversibility becomes progressively less stringent. For infinite-ranged CA ($z=N$) it can be shown that *every* f corresponds to an underlying Hamiltonian, H, which typically involves infinite-ranged, multispin interactions.

These results imply that there are, rather surprisingly, rules [viz., those of the form (3) with $a \neq 0$] which do not obey detailed balance under sequential updating, but which do when simultaneously applied. The converse is, of course, also true, and is not surprising. While we have considered only totalistic rules, our methods can be simply generalized to establish conditions for the existence of underlying Hamiltonians for arbitrary PCA.

We now discuss the universality classes of the continuous ferromagnetic transitions which can occur between stationary states of irreversible PCA with up-down symmetry when the probabilities f are varied. We first discuss MFT for PCA: From (1) one can readily construct an infinite hierarchy of coupled equations involving equal-time correlation functions of progressively higher order. For large z, this hierarchy can, just as in equilibrium statistical mechanics,[4] be systematically decoupled in an expansion in powers of $1/z$. The MF limit, $z=\infty$, is simple, even for *irreversible* CA: The time evolution is completely characterized by the average magnetization $M(t) = \langle S_i \rangle_t$. It is straightforward to verify from (1) that in this limit $M(t)$ obeys the one-variable recursion relation

$$M(t+1) = g(M(t)) = M(t) - 2[f_o(M(t)) + M(t)f_e(M(t))], \quad (4)$$

where f_o and f_e are the odd and even parts of f, respectively. This iterative map g has a fixed point at $M=0$ (corresponding to the "paramagnetic" state). Other fixed points with $M \neq 0$ ("ferromagnetic" states) may occur, depending on the details of $g(M)$. The stability criterion for a fixed point is[5] $|g'(M^*)| < 1$. Rules for which, at some critical value of the parameters, a stable ferromagnetic and an unstable paramagnetic fixed point coalesce, producing a stable paramagnetic fixed point, lead to continuous ferromagnetic phase transitions. From (4) one obtains the respective values $\frac{1}{2}$ and 1 for the associated critical exponents β and γ. These are the conventional MF results of equilibrium critical phenomena. Alternative formulations[8] of MFT for PCA in finite d yield the conventional values $\nu = \frac{1}{2}$, $\eta = 0$, and the mean-field dynamical exponent, $z=2$. In equilibrium critical phenomena, the upper critical dimension, d_c, can be identified as that d at which the hyperscaling relation $\beta = (\nu/2)(d-2+\eta)$ is satisfied by the MF exponents.[9] Postulating the validity of this identification for CA we find, as in the static equilibrium case, $d_c = 4$. For $d > 4$, then, all continuous transitions into ferromagnetic states in PCA are characterized by the standard MF exponents.

To study the effect of fluctuations for $d < d_c = 4$, consider the Langevin equation,[7]

$$\partial\psi_i/\partial t = Q_i(\{\psi_j\}) + \eta_i(t), \tag{5}$$

where ψ_i, a classical field at site i, assumes any value between $-\infty$ and $+\infty$, Q_i is an analytic function of the $\{\psi_j\}$, and η_i is a Gaussian random noise variable of zero mean. The critical behavior of kinetic Ising models is described[3] by (time-dependent Ginzburg-Landau) equations of the form (5) with $Q_i(\{\psi_j\}) = -\Gamma\,\partial H(\{\psi_j\})/\partial\psi_i$ and $\overline{\eta_i\eta_j} = 2\Gamma\,\delta_{ij}\,\delta(t-t')$. Here $H(\{\psi_j\})$ is the Ginzburg-Landau representation of the underlying Hamiltonian, Γ is the dissipation constant, and this specific choice for $\overline{\eta_i\eta_j}$ ensures[10] that in the $t\to\infty$ limit the system is described by the Boltzmann distribution, $e^{-H(\{\psi_j\})}$. Critical phenomena in kinetic Ising models have been intensively studied[3] through application of the ϵ expansion to this special case of (5).

It is natural to hypothesize that the critical behavior of PCA which do *not* admit underlying Hamiltonians can likewise be described[11] by Eq. (5), with Q analytic in $\{\psi_j\}$ but *not* expressible as $-\Gamma\,\partial H/\partial\psi_i$ for any H (i.e., with $\partial Q_i/\partial\psi_j \neq \partial Q_j/\partial\psi_i$). For short-ranged PCA with up-down symmetry, Q_i must then be an odd function of ψ_i and of some appropriate neighborhood, $\{\psi_{i'}\}$, of i. For example,

$$Q_i = A\sum_{\langle i'\rangle}\psi_{i'} + B\sum_{\langle i_1',i_2',i_3'\rangle}\psi_{i_1'}\psi_{i_2'}\psi_{i_3'} + O(\psi_{i'}^5) \tag{6}$$

(the various i' being summed over all nearest neighbors of i) represents, for arbitrary coefficients A and B, a nearest-neighbor rule. The absence of an underlying Hamiltonian for $B\neq 0$ eliminates the fluctuation-dissipation theorem[3]; $\overline{\eta_i\eta_j}$ can thus be taken to be an arbitary even function of the $\{\psi_j\}$, e.g.,[12] $\overline{\eta_i(t)\eta_j(t')} = \delta_{ij}\,\delta(t-t')[\Gamma_0 + \Gamma_1\psi_i^2 + \ldots]$, for constants Γ_0 and Γ_1.

Note that the difference between the $\{Q_i\}$ which result from CA with and without underlying Hamiltonians is quite subtle. For example, the standard nearest-neighbor ψ^4 Ginzburg-Landau Hamiltonian gives rise[3] to a Q_i which consists only of terms linear in ψ_i and $\psi_{i'}$ and a cubic term, ψ_i^3. It is therefore very similar to the Q_i of Eq. (6). The sole difference lies in the wave-vector dependence of the cubic terms in (6). Such wave-vector dependence is *irrelevant* under the renormalization group in $d = 4-\epsilon$.[3,13] Indeed, it is easily shown that in $d = 4-\epsilon$, the dynamical fixed point of the standard kinetic Ising model with no conserved variables is stable with respect to *all* additional analytic terms introduced by elimination of the underlying Hamiltonian without breaking of either the lattice or the up-down symmetry. One concludes (subject to the usual caveats concerning one's inability to establish more than *local* stability of fixed points and the dangers of extrapolating from $d = 4-\epsilon$ to physical dimensions) that fully PCA with up-down symmetry and a nonconserved order parameter fall, for both statics and dynamics, in the universality class of the ordinary Ising model with no conservation laws. Similar arguments show that rules which conserve the order parameter (and so are not fully probabilistic) give rise to ferromagnetic transitions in the universality class of the Ising model with conserved order parameter. Thus, near second-order phase transitions, irreversibility on microscopic length scales renormalizes away, producing, on large scales, reversible systems.

We now discuss nonstationary asymptotic behavior of PCA. It is known from the theory[5] of one-variable iterative maps that by suitable variation of $g(M)$ [viz., $g'(M^*) < -1$] the ferromagnetic fixed point of the (*simultaneously* updated) MF model (4) can be rendered unstable. At its stability limit, this fixed point can bifurcate to a two-cycle, wherein the average magnetization alternates in time between two distinct nonzero values. Indeed, for appropriate choices of g, it is possible to find all the diverse features of single-variable maps,[5] notably bifurcation sequences accumulating to states wherein M is a chaotic function of time. The occurrence of such nonstationary states in MF approximations of PCA has been previously pointed out,[6] but little is known about their stability with respect to fluctuations. [Note that the time-dependent asymptotic behavior in Refs. 6a and 6b occurs for *reversible* rules, either simultaneously (Ref. 6a) or sequentially (Ref. 6b) applied, treated in uncontrolled MF-like approximations. We believe that this is an artifact of the particular approximations employed, and that only *irreversible* PCA can exhibit time dependence. For simultaneously applied PCA it is easy to verify from (4) and the monotonicity of f in (3) that in the $d=\infty$ limit no reversible rule can produce time dependence.]

Since, for totalistic nearest-neighbor (i.e., $z = 2d$) rules, MFT is exact in the $d=\infty$ limit, fluctuation corrections to it are conveniently studied in the systematic $1/d$ (i.e., $1/z$) expansion mentioned earlier. As in statistical mechanics it is easy to show that[4] to $O(1/d)$ only $M(t)$ and the *nearest-neighbor* correlation function $G(t) = \langle S_iS_j\rangle_t - M^2(t)$ are required for a complete characterization of the time evolution; all other correlations are of $O(1/d^2)$. Similarly, to any finite order in $1/d$ the hierarchy of coupled equations reduces to an n-variable iterative map, for some finite n. Two-variable maps are known to exhibit the bifurcation route to chaos[5]; the qualitative features of MFT are thus preserved to $O(1/d)$ for appropriate rules. While the behavior of maps with more variables can be extraordinarily complex and few analytic results are known, one expects, as in statistical mechanics, that, for systems with discrete symmetry far from critical points (i.e., when spatial correlations are short) MFT should remain a good guide even for $d=2$ or 3; time-dependent states ought, therefore, to occur for appropriate rules.

To test this expectation we have performed Monte Carlo simulations on simultaneously updated PCA on square lattices in $d=2$. We computed $M(t)$ for $t=1,2,\ldots,t_{\max}$, and studied the power spectrum of M. Peaks in this spectrum which occur at rational frequency and which sharpen and grow as the sample size is increased, and do not broaden or shrink with increasing $t_{\max}$, were taken as the signature of periodic states. The parameter space of possible rules is, of course, vast; selecting simple rules in a relatively arbitrary way never led us to time-dependent states. We systematized the search by considering totalistic CA with neighborhoods consisting of $(2n+1)\times(2n+1)$ squares of sites for $n=1,2,\ldots,8$; thus $z=4(n^2+n)$. Using the known criterion [i.e., large $|g'(M^*)|$] for the occurrence of nonstationary states in MFT (which provides a progressively better description as z increases, becoming exact at $z=\infty$) as a guide, we succeeded in constructing rules which undergo limit cycles with periodicities 2, 3, and 4 on samples of size up to 150×150 and $t_{\max}$ of up to 100 000. The three- and four-cycles occurred, however, only for $n\geqslant 3$ (i.e., $z\geqslant 48$) and $n\geqslant 8$ ($z\geqslant 288$), respectively. We have also found rules (for $z=80$) which yield what we believe are chaotic states, as evidenced by a broad power spectrum which persists for the largest samples that we studied (200×200), but have yet to observe a periodic state with period >4, much less a complete bifurcation sequence, which MFT predicts. We therefore consider the evidence for the stability with respect to fluctuations of the chaotic state less compelling than for the two-, three-, and four-cycles. A noteworthy feature of the simulations is the strong stabilizing effect of fluctuations on stationary states: Rules which produce time-dependent states within MFT typically give stationary behavior, or at most two-cycles, until z gets rather large (~ 50). This does not preclude nonstationary states with large periods for smaller z, but indicates that they occupy progressively smaller regions of the huge available parameter space as z decreases.

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[1]See, e.g., S. Wolfram, Rev. Mod. Phys. **55**, 601 (1983); see also Physica (Amsterdam) **10D**, 1–247 (1984). (CA, as conventionally defined, are always updated simultaneously. We broaden the definition here to allow for sequential updating.)

[2]E. Domany and W. Kinzel, Phys. Rev. Lett. **53**, 311 (1984), have established the rather different result that *any* simultaneously updated PCA in d dimensions is equivalent to an equilibrium statistical mechanics problem in $d+1$ dimensions. See also E. Domany, Phys. Rev. Lett. **52**, 871 (1984); G. Y. Vichniac, Physica (Amsterdam) **10D**, 96 (1984).

[3]See, e.g., R. J. Glauber, J. Math. Phys. **4**, 294 (1963); P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[4]R. Brout, Phys. Rev. **118**, 1009 (1960).

[5]See, e.g., P. Collett and J.-P. Eckmann, *Iterated Maps on the Interval as Dynamical Systems* (Birkhaüser, Boston, 1980).

[6a]M. Y. Choi and B. A. Huberman, Phys. Rev. A **28**, 1204 (1983).

[6b]M. Y. Choi and B. A. Huberman, Phys. Rev. B **28**, 2547 (1983).

[6c]D. R. Smith and C. H. Davidson, J. Assoc. Comput. Mach. **9**, 268 (1962).

[7]See, e.g., N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[8]See, e.g., L. S. Schulman and P. E. Seiden, J. Stat. Phys. **19**, 293 (1978); G. Grinstein, C. Jayaprakash, and Y. He, unpublished.

[9]See, e.g., P. Pfeuty and G. Toulouse, *Introduction to the Renormalization Group and Critical Phenomena* (Wiley, New York, 1977).

[10]G. E. Uhlenbeck and L. S. Ornstein, Phys. Rev. **36**, 823 (1930).

[11]While the microscopic dynamics of the continuous-time Langevin equation (4) appear rather different from those of *simultaneously* applied irreversible rules, we hypothesize that irreversible PCA are like reversible ones (Ising models) in that *universality classes* for continuous ferromagnetic transitions are independent of how the rules are applied. This hypothesis certainly holds in MFT. Numerical results [C. H. Bennett and G. Grinstein, Phys. Rev. Lett. **55**, 657 (1985)] on a simultaneously applied irreversible rule in $d=2$ give a magnetization exponent β fully consistent with the Ising-model value of $\frac{1}{8}$.

[12]In the case of CA which are not fully probabilistic but have one absorbing state, $\Gamma_0=0$. This is what places such models in a different unversality class [see, e.g., W. Kinzel, Z. Phys. B **58**, 229 (1985); P. Grassberger, Z. Phys. B **47**, 365 (1982); H. K. Janssen, Z. Phys. B **42**, 151 (1981); and Ref. 2].

[13]K. G. Wilson and J. Kogut, Phys. Rep. **12C**, 75 (1974).