Extensions of Q2R: Potts model and other lattices

1988 J. Phys. A: Math. Gen. 21 3297

(http://iopscience.iop.org/0305-4470/21/15/018)

J. Phys. A: Math. Gen. **21** (1988) 3297-3299. Printed in the UK

COMMENT

Extensions of Q2R: Potts model and other lattices

Y Pomeau† and G Y Vichniac‡

† Département de Physique de l'Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

‡ Plasma Fusion Center, Massachusetts Institute of Technology, Cambridge, MA 02139, USA and BBN Communications Corporation, Cambridge, MA 02140, USA

Received 21 April 1988, in final form 10 May 1988

Abstract. We extend the Q2R rule from the Ising to the Potts model, and also to random lattices. Remedies against the lack of unique ergodicity of Q2R are also presented.

Q2R is a two-states-per-site cellular automaton which is both deterministic and reversible [1, 2]. Therein one flips a spin if this flip does not change the energy of the corresponding nearest-neighbour spin-$\frac{1}{2}$ Ising model on the square lattice. In order to avoid the simultaneous update of two adjacent sites, the square lattice is split into two sublattices, and the spins in each sublattice are alternatively updated in parallel and kept fixed. The model has been extended to the cubic lattice [2]. This comment discusses further extensions to the following systems:

(i) the q-states Potts model (q positive integer, Ising is $q = 2$);

(ii) other lattices and disordered systems.

This comment also suggests ways that could help the spin system escape the observed non-uniquely ergodic behaviour of Q2R [3].

(i) The energy of a configuration of the Potts model is $E = -\Sigma_{(nn)}\, \delta_{\sigma i \sigma j}$ where δ is the Kronecker symbol, σ belongs to a set of q different objects (called later a, b and c for $q = 3$), and where the sum is carried over all the neighbouring pairs of lattice sites i, j.

For $q = 3$ this energy E is conserved with the following discrete dynamics. The state at the vertex is s at one time step and s' at the next one; then, for the configurations

$$\begin{array}{ccc} & a & \\ & | & \\ a-s-a & & \\ & | & \\ & a & \end{array} \qquad \begin{array}{ccc} & b & \\ & | & \\ b-s-c & & \\ & | & \\ & c & \end{array} \qquad \begin{array}{ccc} & a & \\ & | & \\ a-s-c & & \\ & | & \\ & b & \end{array}$$

if $s = a$, then $s' = s = a$, if $s = b$ (or c) then $s' = c$ (or b). If

$$\begin{array}{ccc} & a & \\ & | & \\ a-s-b & & \\ & | & \\ & c & \end{array}$$

0305-4470/88/153297+03$02.50

then $s' = s$. From these rules all possible cases are covered by permutation of the four neighbours or by the required symmetry under permutation in (a, b, c). For $q > 3$ the generalisation of Q2R is no longer unique, When a fourth state d is available, then

$$\begin{array}{ccccc} & & a & & \\ & & | & & \\ a & - & s & = & b - a \\ & & | & & \\ & & a & & \end{array}$$

could yield either $s' = c$ or d. This ambiguity is removed by imposing a circular lexicographic order; $b < c < d$. Note that the time-reversal symmetry implies then a reversal in this lexicographic order.

(ii) In the triangular lattice, where each site has six neighbours, a splitting into at least three sublattices, rather than two, is required. In technical (and here somewhat pedantic) terms, the triangular lattice is not a bipartite graph. In a random 2D lattice with nearest neighbour interaction, the higher parallelism is implemented with exactly four passes per glocal sweeping without simultaneous updating of adjacent cells. This results from the four-colour theorem (or conjecture) [4] as applied to the map where the 'countries' are the Wigner-Seitz (or Voronoi-Dirichlet) cells of the random lattice. On such a random lattice, as pointed out by a referee, there is possible blocking of spins (if $q = 2$, i.e. for Ising) with an odd number of neighbours, because the local magnetic field is never zero. This blocking does not seem to remain at higher q.

Let us turn to amendments aiming to alleviate the so-called lack of ergodicity of Q2R and lengthen the period of cycles. The observed lack of unique ergodicity (=the phase space available at a given energy is not spanned by a single trajectory; see [5] for more details) is perhaps not in contradiction with the fact that most trajectories in the large-N limit yield the same average properties as a Gibbs-Boltzmann ensemble for an infinite system, at least for the thermodynamically relevant quantities. A connection between Q2R and spin-glass behaviour has been suggested early on (see 5.1 of Vichniac in [1]). Recent numerical work has furthermore shown the existence of exponentially (in N) many different trajectories on an energy surface [3] or long transients in damage spreading [6]. However, the ergodic/non-ergodic nature of Q2R is not yet fully understood as far as this thermodynamic limit is concerned. As already suggested [7], this limit—to be reached at sufficiently low temperature—could require values of N such that $\ln N$ is very large. This would agree with the observation (see Pomeau in [1]) that the Gibbs-Boltzmann ensemble is stationary under the Q2R dynamics for an infinite system.

Let us notice that, viewing the Q2R dynamics as a determinisitc pseudorandom number generator, the period should be of order of the square root to the number of states, that is $2^{N/2}$ instead of 2^N, according to a result of Euler for random drawings in a finite sample. Hence unique ergodicity is not expected in such systems. The question is more concerned with how a random trajectory samples the surface energy.

The changes we propose in Q2R are as follows: Q2R splits the 2D square lattice into two sublattices (red and black); let us instead make another independent splitting into five sublattices, each containing an equal amount of red and black sites of the initial two sublattices (see below for a heuristic justification of this). The five sublattices, labelled from 1 to 5, are shown on an 8×8 square lattice in the following diagram.

Notice that these spins are related by chess-knight moves.

1	2	3	4	5	1	2	3
4	5	1	2	3	4	5	1
2	3	4	5	1	2	3	4
5	1	2	3	4	5	1	2
3	4	5	1	2	3	4	5
1	2	3	4	5	1	2	3
4	5	1	2	3	4	5	1
2	3	4	5	1	2	3	4

The idea behind this is the following: flipping at random an arbitrary number of spins (adjacent or not), computing the total energy E' of the resulting configuration, and accepting only those configurations with $E' = E$ is a prohibitively slow but exact way to obtain all correct microcanonical averages in the limit of an infinite sampling. The suggested method of five sublattices is (in computer allocation) a poor man's way of doing this in the spirit of Q2R. The hope is that the jump in configuration at each time step is bigger with this five-sublattice method and so would allow a faster sampling of the configuration space. In particular this would avoid short periods of oscillation of small clusters, known to exist in Q2R, a phenomenon certainly related to its lack of ergodicity at low temperature. Finally, one could also forgo the advantages of parallelism and update each site sequentially [8]. This would be an 'N-sublattice' method.

Acknowledgments

This work was initiated at the Institute for Scientific Interchange (Turin, October 1987) and completed at a conference held at Valparaiso in December 1987. One of us (GYV) wishes to thank D Stauffer for his encouragement and his interest in that work, and both authors thank E Tirapegui for the stimulating meeting in Chile.

References

[1] Vichniac G V 1984 *Physica* **10D** 96
Pomeau Y 1984 *J. Phys. A: Math. Gen.* **17** L415
Creutz M 1986 *Ann. Phys., NY* **167** 62
Hermann H J 1986 *J. Stat. Phys.* **45** 145
Toffoli T and Margolus N 1987 *Cellular Automaton Machines* (Cambridge, MA: MIT Press)
Takesue S 1987 *Phys. Rev. Lett.* **59** 2499
[2] Lang W M and Stauffer D 1987 *J. Phys. A: Math. Gen.* **20** 5413
Desai R C and Stauffer D 1988 *J. Phys. A: Math. Gen.* **21** L59
[3] Hermann H J, Carmesin H D and Stauffer D 1987 *J. Phys. A: Math. Gen.* **20** 4939
Schulte M, Stieefelhagen W and Demme E S 1987 *Period in the chaotic phase of Q2R automaton. Preprint* Institute for Theoretical Physics, University of Cologne
[4] Saaty T L and Kainen P C 1986 *The Four Colour Problem* (New York: Dover)
[5] Halmos P R 1986 *Lectures in Ergodic Theory* (New York: Chelsea)
[6] Stanley H E, Stauffer D, Kertesz J and Herrmann H 1987 *Phys. Rev. Lett.* **59** 2326
[7] Aizenman M, Griffeath D and Lebowitz J 1988 to be published
[8] Stauffer D 1988 private communication