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LETTER TO THE EDITOR

Invariant in cellular automata

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Abstract. For a subclass of the set of reversible cellular automata, we give the form of an exact time invariant quantity, which can be seen as a kind of energy. With the ergodic assumption, this is a model of two interacting Ising spin systems.

There is at present a growing interest in cellular automata (Vichniac 1984, Wolfram 1984, Hayes 1984), owing in particular to their physical realisation by inexpensive electronic hardware (Toffoli 1984, see also Margolus 1984). Some of these systems are even able to model dynamical systems such as the flow equations (Hardy *et al* 1976). In this letter we explain the computation of a non-trivial invariant for a class of reversible models invented by Fredkin (see Vichniac 1984). This invariant may be seen as a kind of energy, although its derivation does not use the methods of Hamiltonian mechanics.

Let us consider a lattice of points, regular or not. Indeed finite periodic lattices can be considered as imbedded in infinite periodic lattices. We shall not, therefore, worry about the problem of the thermodynamic limit that does not appear explicitly in our formal computations.

Let us define at each site of this lattice two Boolean variables σ_i and $\hat{\sigma}_i$, where i is the site index. At a given (discrete) time each of these quantities takes either the value 0 or 1. Let ν_i be a neighbourhood of i such that if $j \in \nu_i$ then $i \in \nu_j$. We shall refer to this as the property of symmetry of the neighbourhoods. Now one introduces a deterministic rule for computing the σ's and $\hat{\sigma}$'s at time $(t+1)$ from the σ's and $\hat{\sigma}$'s at time t. Actually, the reversible rules that we want to consider were given originally as two time step rules with a single Boolean variable at each lattice site. However, this may be readily transformed into single time step rules with two Boolean variables at each site. The class of rules that we shall consider has the general form

$$\hat{\sigma}_i^{t+1} = \sigma_i^t \tag{1a}$$

$$\sigma_i^{t+1} = \hat{\sigma}_i^t + A_i^t - 2\hat{\sigma}_i^t A_i^t \tag{1b}$$

or

$$\sigma_i^{t+1} = \hat{\sigma}_i^t + A_i^t(1 - 2\hat{\sigma}_i^t) \tag{1c}$$

where t is the discrete time index and A_i is a function with Boolean values of the σ_j's in the neighbourhood ν_i of site i. The algebra will now be simplified by using the concept of truth value of a statement S, denoted as $(S)_T$. If S is true, then $(S)_T = 1$, otherwise $(S)_T = 0$. Now consider the cases where $A_i = (\Sigma_{j\in\nu_i} \sigma_j = q_i)_T$ where q_i is a natural integer less than or equal to the cardinality of ν_i. Thus the right-hand side of

(1*b*) or (1*c*) is equal to $(A_i^t \neq \hat{\sigma}_i^t)_T$. For an explicit rule, such as the Q2R rule of Vichniac (1984) ($q_i = 2$ in this rule, which explains the 2 in Q2R, the meaning of Q and R will be given below) A_i can be written as a symmetric polynomial with integer coefficients on the σ's in ν_i.

We now want to prove that the quantity

$$\Phi^t = \sum_{i,j \in \nu_i} \sigma_i^t \hat{\sigma}_j^t - \sum_i (\sigma_i^t + \hat{\sigma}_i^t) q_i \tag{2}$$

does not depend on time. In equation (2) the products and sums are to be understood in the usual sense of the operations on integers and not mod 2, although all variables are Boolean. Thus if the cardinality of ν_i is uniformly bounded, Φ^t is of the order of the number of sites for large lattices.

To show that Φ is t-independent, let us compute Φ^{t+1}. With rule (1) one has

$$\Phi^{t+1} = \sum_i (\hat{\sigma}_i^t + A_i^t(1 - 2\hat{\sigma}_i^t)) \left(\sum_{j \in \nu_i} \sigma_j^t - q_i \right) - q_i \sigma_i^t. \tag{3}$$

However, the product $A_i^t(\Sigma_{j \in \nu_i} \sigma_i^t - q_i)$ is equal to zero because A_i^t is the truth value of $(\Sigma_{j \in \nu_i} \sigma_i^t = q_i)$. Thus

$$\Phi^{t+1} = \sum_{i,j \in \nu_i} \hat{\sigma}_i^t \sigma_j^t - \sum_i q_i(\sigma_i^t + \hat{\sigma}_i^t). \tag{4}$$

From the symmetry of the neighbourhoods $j \in \nu_i \Leftrightarrow i \in \nu_j$, one may interchange $\hat{\sigma}$ and σ in the quadratic term on the right-hand side of (4) to obtain finally $\Phi^t = \Phi^{t+1}$. This derivation raises some questions that we shall now comment on.

(1) Are there other invariants? This is certainly so in a quite trivial sense. As shown by Vichniac (1984) the rule Q2R is consistent with a time dependent behaviour strictly confined in a fixed region of a two-dimensional lattice. Thus by an obvious argument of translational invariance the splitting of the phase space by the invariant is certainly less fine than the one defined by the dynamics. In this case, this points to the existence of local invariants.

(2) Vichniac's set of rules lead us to consider the following type of possible choice for A_i

$$A_i = \left(\sum_{j \in \nu_i} \sigma_j = p_i \right)_T + \left(\sum_{j \in \nu_i} \sigma_j = q_i \right)_T$$

with $p_i \neq q_i$, both p_i and q_i being natural integers less than or equal to the cardinality of ν_j. So the question is: is there an invariant as Φ for this class of rules?

(3) It is quite natural to look for possible connections between this class of automata and other models of statististical mechanics, such as the Ising spin system. Consider for instance the QR rules on a regular square lattice. In this case ν_i is the set of the four (quatre in French, this explains the Q in QR, R being for 'reversible') nearest neighbours of site i. Furthermore, let us put $s = \sigma - \frac{1}{2}$ and $\hat{s} = \hat{\sigma} - \frac{1}{2}$, so that s and $\hat{s}$ are the usual spin-half variables of an Ising model. The invariant becomes

$$\Phi = \sum_{(i,j)} s_i \hat{s}_j + \sum_i (2 - q_i)(s_i + \hat{s}_i) + \sum_i (1 - q_i)$$

where (i,j) means summation over all distinct pairs of nearest neighbours. This is the energy of two distinct Ising models, each model having spins s over a sublattice and spins $\hat{s}$ on the other sublattice. The quantity $(2 - q_i)$ plays the role of an external magnetic field. This could be used to model a deterministic dynamics of the Ising model. Note, however, that as previously mentioned in point (1), such a deterministic dynamics is not necessarily ergodic. It could be ergodic in some weak sense for large systems with 'random' initial conditions, this being enough to make statistical mechanics meaningful in those large systems.

(4) The extension of this to automata on lattices of an arbitrary dimensionality is straighforward. It is also of interest to notice that one may extend the definition of A_i as

$$A_i = \left(\sum_{j\in\nu_i} J_{ij}\sigma_j = q_i \right)_{\mathrm{T}}$$

where J_{ij} are integers such that $J_{ij} = J_{ji}$ (the previous condition of symmetry of the neighbourhoods is a particular formulation of this condition), and where the q_i's are now restricted by

$$|q_i| \leqslant \sum_{j\in\nu_i} |J_{ij}|.$$

Then the corresponding invariant is

$$\Phi = \sum_{i,j\in\nu_i} J_{ij}\sigma_i\hat{\sigma}_j - \sum_i q_i(\sigma_i + \hat{\sigma}_i).$$

(5) As there is an invariant quantity as time goes on and if the usual assumptions of thermohydrodynamics work, the long wavelength perturbations of the invariant relax according to the Fourier heat equation. The heat conductivity that appears in this equation is given by a Green–Kubo expression, that can be derived as in Hardy *et al* (1974) the shear viscosity of the lattice gas model. Let us give this form of the heat conductivity for the case $q = 2$ and $J_{ij} = 1$ and for a regular lattice. To do this we shall need some more notations. We shall assume that the Boltzmann–Gibbs statistical weight has the usual form: $Z^{-1}\exp(-\Phi/\Theta)$, Z being the partition function Φ the energy as given in equation (4) for $q_i = 2$ and Θ the temperature measured with the same (dimensionless) units as Φ. Furthermore, the formal expression of the α Cartesian component of the microscopic heat flux at time τ and site i is

$$J_{i,\alpha} = \tfrac{1}{2} \sum_{j\in\nu_i} r_{ij,\alpha}(\sigma_i^\tau \hat{\sigma}_j^\tau - \sigma_j^\tau \hat{\sigma}_i^\tau)$$

where $r_{ij,\alpha}$ is the α component of the vector $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$ whose ends are at neighbouring sites i and j of the lattice. With all these notations the formal expression of the heat conductivity reads

$$\kappa_{\alpha\beta} = \frac{1}{\Theta^2} \sum_{t=0}^{\infty} \left\langle J_{i,\alpha}(0) \sum_k J_{k,\beta}(t) \right\rangle$$

where the average is taken over a Boltzmann–Gibbs distribution of initial conditions for the dynamics in phase space. The heat conductivity tensor is defined in such a way that the heat transport equation reads

$$\frac{\partial\Phi(\boldsymbol{r}, t)}{\partial t} = \sum_{\alpha,\beta} \kappa_{\alpha\beta} \frac{\partial^2\Theta}{\partial r_\alpha\, \partial r_\beta}$$

where $\Phi(\boldsymbol{r}, t)$ is the local value of the energy per site. This is related to the local temperature through the equilibrium equation of state in the near equilibrium situations where the Fourier equation is valid. On the other hand it is well known (Pomeau and Resibois 1975) that transport coefficients often diverge in two dimensions. If one assumes that there is only one global conserved quantity, Φ, in this model it does not seem that those divergences affect the previous expression of the heat conductivity.

(6) A very fascinating result, among many others, was proved by Onsager for the 2D Ising model at the Curie temperature: pair correlation functions between spins on the same line are rational numbers. It has been conjectured since, but as far as we know never proved that any equilibrium correlation is a rational number in the same conditions. If this is true, an immediate consequence is that any time correlation function of the equilibrium fluctuations of our model are also given by rational numbers at the Curie temperature when the cellular automaton is equivalent to two Ising models on a square lattice.

This work was initiated at the 1984 conference on 'Physics and Computation' held at Drake's Anchorage, where I was introduced to the problem of the invariants of the reversible rules by Gerard Vichniac. I have greatly benefited from discussions with him and with Charles Bennett, and have been very much inspired by the work of Tom Toffoli and Norm Margolus with the CAM machine.

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