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# KNOT INVARIANTS AND THE THERMODYNAMICS OF LATTICE GAS AUTOMATA

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**David A. Meyer**

*Project in Geometry and Physics*
*Department of Mathematics*
*University of California/San Diego*
*La Jolla, CA 92093-0112*
dmeyer@euclid.ucsd.edu

## 1. Progress to date

### *1.0. Goals*

The goal of this project has been to build on the understanding of the connections between knot invariants, exactly solvable statistical mechanics models and discrete dynamical systems gained in earlier work [1,2], toward an answer to the question of how early and robust thermodynamic behavior appears in lattice gas automata. These investigations have recently become relevant, unanticipatedly, to crucial issues in quantum computation.

### *1.1. A cellular automaton model*

In [3] we showed that a specific reversible cellular automaton model with a conserved quantity is equivalent, in the sense that the ensemble of $1+1$ dimensional spacetime evolutions is the same as the equilibrium ensemble of 2 dimensional configurations, to a solvable statistical mechanics model. This model, the asymmetric six vertex model, is obtainable as a critical limit of the eight vertex model, which is also solvable. The dominant characteristic of criticality is scale or conformal invariance, which means that probability distributions of states are invariant and correlation functions transform covariantly under conformal transformations. Thus, if our cellular automaton were really at a critical point, *i.e.*, $N \to \infty$ as well as $T = T_{\text{critical}}$, the local distribution of states would be that of the thermodynamic limit, a result consistent with the canonical distribution observed in simulations. For finite $N$ this will be moderated by finite-size effects which round off the critical singularity.

### *1.2. A lattice gas model*

Having applied these ideas successfully to the simple case of a reversible cellular automaton, we moved on to the more interesting case of lattice gases. In [4,5] we detail the

construction of a family of $1+1$ dimensional lattice gas automata. In an effort to clarify which features of the lattice gas automata are the consequences of which constraints, we proceed systematically: first setting the kinematics of the model, then exploring the effect of requiring that the dynamics be local, and finally constructing the possible dynamics consistent with the imposed constraints.

In [3] we used the conserved quantity of the cellular automaton to define the weights of the equivalent statistical mechanics model. In this lattice gas model there is also a conserved quantity; we use it to effect a radical transformation of the model to one which is again equivalent to a 2 dimensional statistical mechanics model. The partition function of the resulting statistical mechanics model is exactly the transition probability in the lattice gas, given specific initial and final boundary conditions.

In fact, the model lies on a first order critical line between disordered and totally ordered regimes of the six vertex model. We observe that this result applies to ensembles of systems, in the thermodynamic limit. That the correlation length vanishes, for example, does not mean that there is no correlation between states of the probabilistic lattice gas automaton at successive time steps. Nor would a nonvanishing correlation length mean that there were necessarily spacelike correlations in a given initial state. Instead, the interpretation is that deep in the interior of a system, far from the boundary conditions and thus/or subject to essentially random boundary conditions, a domain of sufficiently large size is in thermodynamic equilibrium. Thus our results provide evidence for the first step in the derivation of the macroscopic equations of motion—the assumption of local thermodynamic equilibrium, as well as demonstrating the efficacy of constructing and analyzing lattice gas automata according to (spacetime) symmetry principles.

*1.3. Irreversible models*

The models described in Sections 1.1 and 1.2 are reversible—there is no preferred time direction. While it is very likely that at the smallest scales physical processes are reversible (quantum mechanical processes are unitary, as we will describe in Section 2), certainly at macroscopic scales those of most interest are not. This means that an effective or phenomenological theory above some mesoscopic scale will not be reversible. Lattice gas automata exemplify this situation particularly clearly. The microdynamics in most lattice gas models conserves mass, energy and momentum—and is at least probabilistically reversible. Nevertheless, at macroscopic scales lattice gas automata appear to model the Navier-Stokes equations *with viscosity* extremely well, at least in some parameter ranges.

Our results for the lattice gas model described in Section 1.2 apply to the existence of local thermodynamic equilibria in the lattice gas. They do not explain the approach to this state from non-equilibrium configurations, nor do they apply to the macroscopic irreversibility of the fluid equations being modelled. To begin to understand such systems one approach is to generalize the dynamics of these models to allow for irreversible interactions.

Perhaps the simplest model to generalize is the standard square lattice Ising model. Just as in the six vertex model equivalent to the lattice gas described in Section 1.2, the edges of the lattice are interpreted to be particle trajectories in $1+1$ dimensions and interactions to occur at the vertices of the lattice shown in Figure 1. Rather than consider a dynamics based on isooriented triangles in the lattice as is sometimes done to model anisotropy, we simply consider each edge to be oriented upward (*i.e.*, to the upper left or upper right), in the direction of increasing time, and allow the dynamics to depend on this orientation. Specifically, we investigate a spacetime Ising model [6]: *states* $\sigma$ are assignments of $\pm 1$ to each vertex and the energy of a state is a sum of contributions from edges $(p,q)$ with $p$ preceeding $q$:

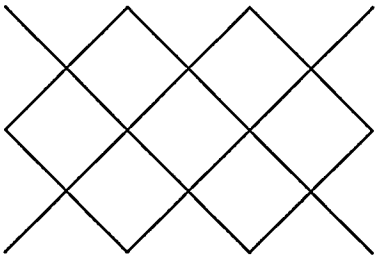

**Figure 1.** Part of the trajectory lattice for the spacetime Ising model.

$$E(\sigma) := -\sum_{(p,q)} E_1\delta(\sigma_q - \sigma_p) + E_2\mathrm{sgn}(\sigma_q - \sigma_p), \tag{1}$$

where $\delta(x)$ vanishes unless $x = 0$, in which case it equals one, and $\mathrm{sgn}(x) := x/|x|$ unless $x = 0$ in which case it vanishes. The Boltzmann weights are $W(\sigma) := e^{-\beta E(\sigma)}$, so the partition function is

$$Z(E_1, E_2; \beta) = \sum_{\sigma} W(\sigma). \tag{2}$$

In [6] we show that the spacetime Ising model defined by (2) and (3) is exactly solvable as a consequence of the exact solvability of the standard Ising model, and that all thermodynamic quantities derivable from the free energy are identical in the two models. There are other interesting quantities in the spacetime model, however. Specifically, analogously to the magnetism, we may define the *temporalization* $\tau$ to be the expectation value of $\sum \mathrm{sgn}(\sigma_q - \sigma_p)$. This measures the extent to which the direction of time is reflected in the conversion of $-1$s to $+1$s; in various lattice gas models it should be related to change in particle number or dissipation. The temporalization is nonnegative if the function $\mathrm{sgn}(\sigma_q - \sigma_p)$ in the second term of (1) is replaced by $\theta(\sigma_q - \sigma_p)$, where $\theta(x)$ vanishes unless $x > 0$, in which case it equals one, since this eliminates all configurations with any edge having a $+1$ preceeding a $-1$. This model is closely related to crystal growth problems as well as to the directed animal models for polymers in a flow field. In [7] we show that for this case there is a phase transition at positive temperature between phases with $\tau = 0$ and $\tau > 0$.

### *1.4. Random spacetime lattices*

The identification between lattice gas automata and statistical mechanics models on a square lattice is special to $1+1$ dimensions and a single particle speed. To investigate higher dimensional lattice gases or those with multiple speed particles, one must work in a more general setting. There has been considerable recent success in the analysis of statistical mechanics models on random 2 dimensional lattices; this, together with the considerations of Section 1.3, provides motivation for considering random lattices with a given time direction. Most specific lattice gas automata will have more kinematical constraints than this, of course, but this is the most general kinematical setting.

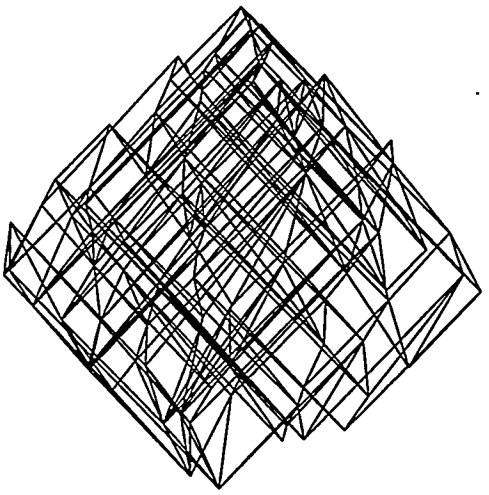

**Figure 2.** A random spacetime lattice with 100 vertices.

In [6] we study the spacetime Ising model of Section 1.3 on a lattice obtained by placing $N$ vertices randomly in the region $\mathcal{A} := \{(t,x) \mid 0 < t+x < \sqrt{2N},\ 0 < t-x < \sqrt{2N}\}$ and connecting each vertex to its nearest future neighbors that can be reached by particles with speeds less than 1. Figure 2 shows such a lattice with 100 vertices. The model is defined by its partition function

$$Z_N(\beta) := \int_{\mathcal{A}} dx_1 \ldots \int_{\mathcal{A}} dx_N Z_{P(x_1,\ldots,x_N)}(E_1, E_2; \beta) e^{-\beta L E_1}. \tag{3}$$

Here the subscript $P(x_1,\ldots,x_N)$ on $Z$ indicates that the spacetime Ising model partition function of (2) is to be evaluated on the random lattice defined by these points, and $L$ denotes the total number of edges (links) in this lattice. In [6] we show that at $T = 0$ and $E_1 = E_2$ this partition function can be evaluated exactly for all $N$, not just in the thermodynamic limit, giving:

$$Z_N(\infty) = I_0(2\sqrt{N}), \tag{4}$$

where $I_0$ is the modified Bessel function of the first kind of order zero. The elegance of this remarkable formula leads us to hope that, at least in the thermodynamic limit, the model might be solvable at positive temperatures as well.

The techniques which lead to (4) will not apply in exactly the same way to a nonrandom lattice such as would arise in the case of a lattice gas with a finite number of speeds. If this number is greater than one, however, the lattice will not be the tightly constrained square lattice of Figure 1, so these more general techniques will apply in some form.

Solvability in a random lattice or multiple speed model seems unlikely to result directly from the same type of knot invariant/Yang-Baxter equation analysis that applies in the

case of a square lattice. On the other hand, there is a direct connection between the skein relations satisfied by knot invariants and the linear recurrence relations satisfied by some partition functions. With this observation as motivation, in [8] we study the family of partition functions on random lattices with a time direction (equivalently, invariants of partially ordered sets) which satisfy a linear recurrence relation of the form

$$Z_P = \alpha Z_{P/(p,q)} + \alpha Z_{P/(q,p)} + \beta Z_{P/(p=q)}, \tag{5}$$

(where there is no edge connecting $p$ and $q$ in $P$, $P/(x,y)$ denotes $P$ with the edge from $x$ to $y$ added, and $P/(p=q)$ denotes $P$ with $p$ and $q$ identified; in each case, any resultingly non-nearest neighbor edges are removed.) We find that for $\alpha = 1$, any values of $\beta$ and $Z_{[N]}$ (where $[N]$ denotes the $0+1$ dimensional chain of $N$ points) define a consistent, and at least recursively solvable, model.

Any partition function which might arise in even an irreversible, multiple speed lattice gas model should satisfy a locality condition and a conservation of probability (unitarity) condition since it would derive from a particle scattering rule. In [9] we consider, although from a somewhat different perspective, the most general models of this form. We find that various forms of locality, together with unitarity and homogeneity, are actually very restrictive conditions.

## 2. Current developments

### *2.0. Quantum computation*

The fact that incentives to develop smaller and faster computers will eventually drive the devices from which they are constructed into the quantum regime motivated research into quantum mechanical limitations on deterministic computation as early as the 1970s. The subsequent conceptions of universal quantum simulator by Feynman and quantum Turing machine by Deutsch initiated a series of investigations into how aspects of quantum mechanics, specifically superposition and interference, might be exploited for computational purposes. Shor's remarkable discovery last year of a polynomial time quantum algorithm for factorization (and the centrality of the factoring problem to modern cryptography) has led to redoubled interest in the design and construction of quantum computational nanodevices. It should be emphasized that the goal here is a computational device which will run *quantum* algorithms, not a quantum device which will run deterministic or probabilistic algorithms.

For a variety of reasons—the wire and gain problems, and the pragmatic observation that an array of simple devices is often easier to design and build than a single, more complicated device—it seems likely that massive parallelism will optimize nanoscale computer architecture. In this paradigm, a quantum computer is a quantum cellular automaton: the state of each simple device (cell) in the array depends on the states of the cells in some local neighborhood at the previous timestep. Unlike the original cellular automaton models for parallel computation of von Neumann and Ulam, where this dependence

is deterministic or probabilistic, here the dependence is quantum mechanical: There is a (complex) probability amplitude for the transition to each possible state, subject to the condition that the evolution be unitary, so that the total probability—the sum of the norm squared of the amplitude of each configuration—is always one.

*2.1. Quantum lattice gases*

Quantum cellular automata, therefore, provide a laboratory for analyzing both potential quantum computer architectures and algorithms; this is our motivation for initiating the study of them using some of the ideas and techniques we developed in the work described in Section 1. In [10] we begin by proving:

NO-GO LEMMA. *In* $1+1$ *dimensions there exists no nontrivial, homogeneous, local, scalar quantum cellular automaton. More explicitly, every band* $r$*-diagonal unitary matrix which commutes with the 1-step translation matrix is also a translation matrix, times a phase.*

and then continue by showing that even a slight weakening of the homogeneity/translation invariance condition allows nontrivial unitary evolution. We find a one parameter family of evolution rules which are best interpreted as those for a one particle quantum automaton (one particle of a quantum lattice gas). This model is naturally reformulated as a two component cellular automaton which we demonstrate to limit to the Dirac equation. There are two generalizations of this automaton, the second of which, to multiple interacting particles, is the correct definition of a quantum lattice gas.

*2.2. Quantum cellular automaton mechanics*

The power of quantum algorithms derives from two aspects of quantum mechanics: superposition and interference. Superposition of computational basis states in the wave function provides effective parallelism, while quantum interference can be exploited to make amplitudes of undesirable computational paths cancel, leaving only correct outcomes with positive probabilities. In order for quantum interference to occur, phase coherence must be maintained throughout the computation. A simplest-assumptions calculation by Unruh of the decoherent influence on a quantum computer memory by a quantum field predicts that this will be difficult: while there is a vacuum dominated regime in which decoherence can be effectively delayed by reducing the coupling to the environment, this only lasts for computational time comparable to the thermal time scale ($\sim 10^{-9}$sec. at 1°K); beyond this time scale decoherence increases exponentially faster and reducing the coupling has little effect. Since standard error correction techniques (*e.g.*, multiple runs in series or parallel) are ineffective against this loss of coherence, the consequence is a severe limit on the number of time steps over which a quantum algorithm can run, *unless the physical representations of computational tokens can somehow be protected against decoherence.*

Quantum cellular automata/lattice gases not only model potential architectures for quantum computers but are also systems in which the *dynamical* effects of decoherence (rather than just its effect on static memory) can be investigated. The first steps in such an investigation are to understand planewaves, wave packets, boundary conditions,

and potentials in these models. Work on these aspects of quantum cellular automaton mechanics is in progress as is some preliminary work on decoherence itself. These problems are not as far from those we began this project studying as they may appear at first sight: decoherence is one aspect of the relaxation to thermodynamic equilibrium in quantum systems.

## 3. Publications

[1] D. A. Meyer, "State models for link invariants from the classical Lie groups", in Kawauchi A., ed., *Knots 90*, Proceedings of the International Conference on Knot Theory and Related Topics, Osaka, Japan, 15–19 August 1990 (Berlin: W. de Gruyter 1992) 559–592.

[2] B. Hasslacher and D. A. Meyer, "Knot invariants and cellular automata", *Physica D* **45** (1990) 328–344.

[3] B. Hasslacher and D. A. Meyer, "Knots, criticality and thermodynamics in discrete dynamical systems", UCSD/LANL preprint.

[4] B. Hasslacher and D. A. Meyer, "Lattice gases and exactly solvable models", *J. Stat. Phys.* **68** (1992) 595–610.

[5] B. Hasslacher and D. A. Meyer, "Lattice gases and exactly solvable models", in D. Frederick, ed., *Synergism of Analysis, Modeling, and Experiment*, Proceedings of the Tenth Symposium on Energy Engineering Sciences, Argonne National Laboratory, 11–13 May 1992 (Argonne, IL: Argonne National Laboratory 1992) 112–119.

[6] D. A. Meyer, "Spacetime Ising models", to appear in *Int. J. Mod. Phys. B.*

[7] D. A. Meyer, "Why do clocks tick?", Honorable Mention, Gravity Research Foundation essay contest (1992), *Gen. Relativ. Grav.* **25** (1993) 893–900.

[8] D. A. Meyer, "Recursive generalization of the order polynomial", UCSD preprint.

[9] D. A. Meyer, "Induced actions for causal sets", UCSD preprint.

*[10] D. A. Meyer, "From quantum cellular automata to quantum lattice gases", UCSD preprint.

* indicates that a copy of the (p)reprint is enclosed.