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STRUCTURES IN QUANTUM CELLULAR AUTOMATA

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For cellular automaton machines getting increasingly smaller in size, a regime will be entered where effects due to matter waves may become dominant. Studying the evolution of one-dimensional and locally interacting cellular automata governed by generalized quantum mechanical rules, we discuss irreversibility as it appears in the evolution of structures in quantum cellular automata.

1. Introduction

Cellular Automata (CA's) are n-dimensional arrays whose evolution is given by rules connecting the values of the individual sites of the arrays at various times with each other [1]. For cellular automata getting increasingly smaller in size, a regime will be entered where quantum effects cannot be neglected. Ultimately, such effects may very well be dominant [2]. Quantum mechanically this fact is described by introducing probability amplitudes implying that one will not be able to know for certainty whether the value at a given site is 0 or 1 at a given instant of time.

This implies that questions on the foundations of quantum theory, such as the quantum mechanical measurement process or the transition from microscopic to macroscopic, or from reversible to irreversible physical processes, respectively, will enter the domain of cellular automata research.

Such a procedure, besides being of a fundamental interest, should also be of significance for the problem of understanding the impact of quantum physics on computer operation. Notwithstanding the fact that today no accepted view of computing in the quantum domain exists, this may be implied by the equivalence of certain classes of cellular automata to Turing machines [3].

One way to arrive at a quantum cellular automaton (QCA) is to attribute some complex number c_{IJ} to each site of the cellular automaton and to construct transition rules in such a way that superposition of probability amplitudes is permitted. For simplicity, we study the evolution of one-dimensional cellular automata and we focus on strictly local (i.e. nearest neighbor) interaction.

Approximating the unitary evolution operator U by the first order term of its expansion,

$$U = \mathrm{e}^{-\mathrm{i}Ht/\hbar} \simeq 1 - \mathrm{i}Ht/\hbar\,,$$

and introducing periodical boundary conditions, the Hamiltonian becomes essentially

$$H = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ \ddots & 0 & \delta & & & & 0 \\ & \delta^* & 0 & \delta & & & \\ & & \delta^* & 0 & \delta & & \\ & & & \delta^* & 0 & \delta & \\ & & & & \delta^* & 0 & \ddots \\ & 0 & & & & \ddots & \ddots \end{pmatrix}. \qquad (1)$$

Also, we decided to normalize the one-dimensional QCA at any given time. This procedure, though seemingly reasonable from the quantum mechanical viewpoint, would have also to be relaxed eventually in the transition between quantum and classical CA's, because the latter

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are not normalized (see [1]). It is important to note that eq. (1) represents a unitary evolution for small values of δ only. For larger values of δ, other matrix elements farther off the diagonal would have to be nonzero in a very specific way to preserve unitarity.

2. Some results

The results are presented in the form of probability maps, i.e. we plot the "temporal" evolution of one-dimensional quantum cellular automata in terms of the normalized probability values $P_{IJ} = c^*_{IJ}c_{IJ}$ for each site J at each time step I. Different shades of grey represent different probabilities.

We have studied the evolution of quantum cellular automata as a function of the size of the off-diagonal elements δ in the Hamiltonian. That is, we have investigated the dependence of the resulting patterns on the relative weighing of the nearest neighbor's contributions [4].

In the plots of the probability maps the number of pixels is 120×532 for one image. Generally, we vary the size of the off-diagonal contributions $\delta = \delta_c(1 + i)$ by varying δ_c and we vary the initial point configurations.

To show a characteristic result, fig. 1 presents an example with one initial site of non-zero amplitude. We plot a quantum cellular automaton with $\delta_c = 20$ and one initial point. The ellipses typical for this range of δ_c gradually flatten and eventually form "plane-wave surfaces." Other observed features of the probability maps are striped wave-like patterns, interference patterns, ripples, and the like. Generally, probability maps with $n \geq 2$ initial points exhibit the following properties:

i) high sensitivity to the number (odd versus even) of zero-value sites between non-zero initial points,
ii) high sensitivity to slight variations of the values of individual initial points,
iii) rapid stabilization of the pattern structure for symmetric initial point configurations.

Now we shortly discuss global pattern formation as caused by the local evolution rules applied. For $\delta_c \gtrsim 1$, three "phases" of global evolution can be clearly distinguished:

1) a mostly complex development from the initial states to the first appearance of recognizable large-scale periodical structures,
2) strictly periodical "ellipse-like" structures,
3a) an "infinite-time state" which represents the stable final state resembling a plane-wave pattern, or
3b) a stable large-scale periodic structure.

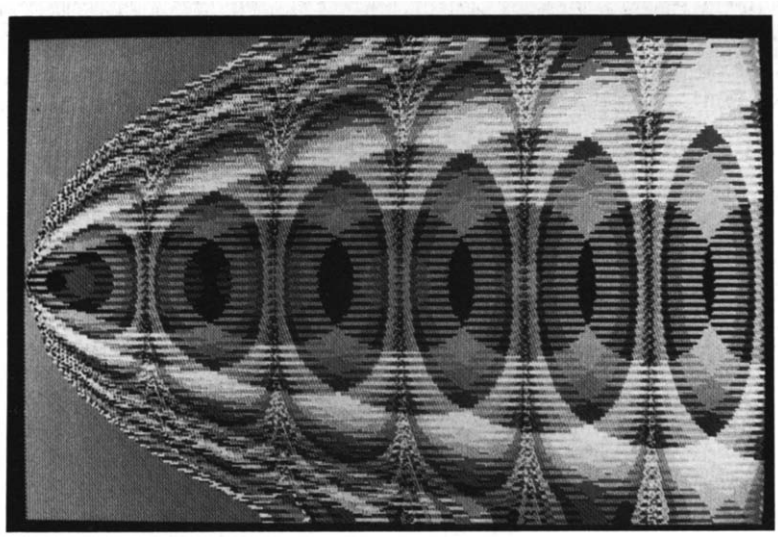

Fig. 1. Quantum cellular automaton with $\delta_c = 20$ and one initial point. The ellipses typical for this range of δ_c gradually flatten with time and eventually form "plane wave surfaces". The time axis runs from left to right.

3. Irreversibility

Suppose one begins QCA evolution at time I using the evolution rule

$$c_{I+1,J} = \frac{1}{\sqrt{N}} (c_{I,J} + \mathrm{i}\delta_{c_{I,J-1}} + \mathrm{i}\delta^*_{c_{I,J+1}}) , \tag{2}$$

i.e. using the corresponding evolution operator

$$U = \frac{1}{\sqrt{N}} \begin{pmatrix} \ddots & \ddots & \ddots & & & \\ \ddots & 1 & \mathrm{i}\delta^* & & & 0 \\ & \mathrm{i}\delta & 1 & \mathrm{i}\delta^* & & \\ & & \mathrm{i}\delta & 1 & \mathrm{i}\delta^* & \\ & & & \mathrm{i}\delta & 1 & \mathrm{i}\delta^* \ddots \\ & 0 & & & \mathrm{i}\delta \ddots & 1 \ddots \\ & & & & \ddots & \ddots \end{pmatrix} . \tag{3}$$

If at time $I+1$ one applies the Hermitian conjugate rule of [2], one obtains

$$U^{\dagger}U = \frac{1}{N} \begin{pmatrix} \ddots & \ddots & \ddots & \ddots \\ \ddots & 1+2\delta\delta^* & 0 & \delta^{*2} \ddots \\ \ddots & 0 & 1+2\delta\delta^* & 0 \ddots \\ \ddots & \delta^2 \ddots & 0 \ddots & 1+2\delta\delta^* \ddots \end{pmatrix}$$

$$\neq \begin{pmatrix} \ddots & & & \\ & 1 & & 0 \\ & & 1 & \\ & & & 1 \\ & 0 & & \ddots \end{pmatrix} \tag{4}$$

such that only for small values of δ the "inverted value" $\bar{c}_{I,J}$ becomes

$$\bar{c}_{I,J} = c_{I-2,J} . \tag{5}$$

Thus, for non-negligible values of δ, the evolution becomes non-unitary. That is, the off-diagonal terms in (4) begin to dominate the QCA evolution which has thereby become irreversible. We therefore conclude that the quantization of state space (under maintainance of continuous phase relations) implies that for large enough values of the "mixing parameter" δ strictly local unitary evolution becomes impossible. To arrive at unitary, reversible quantum mechanics one has to relax the locality condition. In contrast, relaxing unitarity as done here provides a possible mechanism for a transition to macroscopic irreversibility.

How does this finding relate to other notions of irreversibility in the context of the relation between quantum mechanics and macroscopic physics? In answering this question, we restrict ourselves to a comparison of our non-unitary QCA's with work done by George, Prigogine, and Rosenfeld (GPR) on "The Macroscopic Level of Quantum Mechanics" [5]. The latter discusses another possible model for the transition from quantum mechanical to macroscopic irreversible descriptions of a physical system.

GPR describe the temporal evolution of quantum systems via a Liouville equation

$$\mathrm{i}\dot{\rho}(t) = \frac{1}{\hbar}[H, \rho(t)] , \tag{6}$$

where the density operator

$$\rho(t) = \sum |\psi(t)\rangle\langle\psi(t)|$$

is as usual composed of states $|\psi(t)\rangle$ in Hilbert space $\mathcal{H}$. Since the density operator describes both density distributions within pure states and correlations between pairs of states, GPR view $\rho(t)$ as being a function which describes system evolution in the product space $\mathcal{H} \times \mathcal{H}$ which they call "superspace". Then the solution of (6) becomes

$$\rho(t) = \mathrm{e}^{-\mathrm{i}Lt}\rho(0)$$

$$\text{with} \quad L \equiv \frac{1}{\hbar}\{H \times \mathbb{1} - \mathbb{1} \times H\} , \tag{7}$$

where the time evolution superoperator $T(t) = \exp(-\mathrm{i}Lt)$ can be factorized into

$$T(t) = \mathrm{e}^{-\mathrm{i}Lt} = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\,\mathrm{e}^{+\mathrm{i}Ht/\hbar} . \tag{8}$$

Thus the Liouville superoperator is self-adjoint, and the time evolution superoperator is unitary.

The important ansatz to combine quantum mechanical and macroscopic description is the proposal by GPR to decompose the density superoperator into

$$\rho(t) = \rho_0(t) + \rho_c(t) ,$$

with

$$\rho_0(t) = P_0\rho(t) , \quad \rho_c(t) = P_c\rho(t) . \tag{9}$$

The density $\rho_0(t)$ represents the average distribution of states of the system, while the supervector $\rho_c(t)$ describes the effects of fluctuating correlations among these states. One thus arrives at an equivalent description both at the quantum mechanical and at the macroscopic level, where in both cases a corresponding Liouville equation is in operation.

In the context of our considerations it is important to note that the GPR model introduces an additional assumption (i.e. not inherent in the usual quantum mechanical formalism) which the authors call the "condition of dissipativity". In doing so, the possible appearance of (thermodynamic) irreversibility on the macroscopic level is traced back to a mixing of correlations on the microscopic level as described by $\rho_c(t)$. In such a case, initial phase relations between the state vectors may eventually be "smeared out" as an effect of the assumed fluctuations on the microscopic level.

Comparing this model of GPR with our irreversible quantum mechanical CA's, one finds that our evolution operator (3), if interpreted as a projection operator, does fulfil the condition of adjoint symmetry, but not the condition of idempotency; two conditions however, which would have to be fulfilled simultaneously if our description were a description based on projection operators in superspace.

One can clearly see a certain complementarity between the ansatz using quantum mechanical CA's and that of ref. [5]. The GPR approach introduces as additional assumption the "condition of dissipativity", i.e. the "smearing out" of phase correlations for long times (i.e. for the macroscopic domain), while the states themselves always obey a Liouville equation implying, among other features, also nonlocality. Our ansatz in turn is characterized by the additional assumption of a discretization of state space under operation of local rules, while the phase correlations are maintained for all times. The mixing of states in our case is a consequence of the applied evolution rule for the QCA.

Therefore, despite some similarities, the two approaches to irreversibility as discussed here are fundamentally different. However, these differences are easily explained since they follow from the different additional assumptions introduced. The common point of departure for both models is irreversibility considered as the result of the mixing of correlations. How this mixing comes into being is a question of the additional assumptions introduced into the quantum mechanical description. Which of the two approaches is more relevant for the question of quantum computation is certainly open. From the point of view of a practical realization of a quantum apparatus, we point out that our model has the distinct advantage of its time evolution being described within the system itself as opposed to the practically unrealizable superspace system.

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