Physica D 31 (1988) 70–77
North-Holland, Amsterdam

A CONSERVATION LAW IN QUANTUM CELLULAR AUTOMATA

Gerhard GRÖSSING
Atominstitut der Österreichischen Universitäten, Schüttelstr.115, A-1020 Vienna, Austria

Anton ZEILINGER
Atominstitut der Österreichischen Universitäten, Schüttelstr.115, A-1020 Vienna, Austria and Hampshire College, Amherst, MA 01002, USA

Received 2 July 1987
Revised manuscript received 21 December 1987
Communicated by H. Flaschka

In the present study we identify various general features governing the evolution of quantum cellular automata which have been introduced as a means of extending general systems theory into the quantum domain. It is found that a conservation law connects the strength of the mixing of locally interacting states and the periodicity of the large-scale (global) structures which develop during the evolution of quantum cellular automata. Moreover, for a large class of quantum cellular automata, the global patterns exhibit irreversible behavior.

1. Introduction

One of the central topics of modern systems theory is the relationship between individual parts of a structure or of a process on the one hand and the overall evolution of that structure or process on the other hand. In other words, it is the relation between descriptions on a local and descriptions on a global level that has become a point of central interest. One example thereof is the possibility of generation of "order out of chaos" in complex systems. In this context, the question of an evolutionary "time arrow" has also been raised. This question arises if one considers how apparently local reversible rules could generate in a way to be understood irreversible processes on some other, more global, level (as, e.g., in morphogenetic models in biology).

Our main interest in this paper is to study such questions of systems theory in the context of quantum theory. This is part of a larger program, one of the goals of which is to work out on a general level similarities between general systems theoretical properties in classical and in quantum processes. Another goal is to understand the reason for the differences between the two domains. This should help us to understand both domains, and what distinguishes them, better. The tools with which we intend to obtain such understanding are cellular automata.

The reasons why we chose cellular automata for our study are twofold. Firstly, certain cellular automata are known, at least on the classical level, to be capable of universal computation [1] – a quite general systems modeling feature. And secondly, cellular automata are represented by N-dimensional arrays, the evolution being represented by rules connecting the values of the individual sites of the arrays at various times with each other [2]. We submit that this latter feature makes cellular automata particularly amenable to generalization into the quantum domain.

In order to achieve this generalization we have, in a previous paper [3], introduced cellular automata in a complex state space. That is, we have attributed some complex number c_{IJ} to each site of the cellular automaton. As is standard in quantum mechanics, these complex numbers are then

interpreted as probability amplitudes. Their evolution is governed by rules which are constructed such as to permit their superposition.

For such automata we have coined the term "quantum cellular automata" and we have begun to study the evolution of one-dimensional quantum cellular automata, focusing for the time being on strictly local (i.e. nearest neighbor) interaction. Approximation of the unitary evolution operator by

$$U = e^{-iHt/\hbar} \simeq 1 - iHt/\hbar$$

and introduction of periodical boundary conditions with a Hamiltonian of the form

$$H = \begin{pmatrix} \varnothing & \epsilon^* & & & & & & \cdots & \varnothing & \epsilon \\ \epsilon & \varnothing & \ddots & & & & & & \varnothing & \varnothing \\ & \ddots & \ddots & \epsilon^* & & & & & & \vdots \\ & & \epsilon & \varnothing & \epsilon^* & & & & & \\ & & & \epsilon & \varnothing & \epsilon^* & & & & \\ & & & & \epsilon & \varnothing & \epsilon^* & & & \\ & & & & & \epsilon & \varnothing & \epsilon^* & & \\ & & & & & & \epsilon & \ddots & \ddots & \\ \vdots & & & & & & & \ddots & \varnothing & \epsilon^* \\ \varnothing & \varnothing & & & & & & & \epsilon & \varnothing \\ \epsilon^* & \varnothing & \cdots & & & & & & & \end{pmatrix} \quad (1)$$

results with $\delta \equiv \epsilon t/\hbar$ in the following transition rule for our one-dimensional quantum cellular automaton:

$$c_{I+1,J} = \frac{1}{\sqrt{N}}\left(c_{I,J} + i\delta c_{I,J-1} + i\delta^* c_{I,J+1}\right). \quad (2)$$

For large δ, the evolution (2) becomes non-unitary but remains local. Here, I and J denote time-step and site location respectively, and N is a normalization factor such that

$$\sum_J |c_{IJ}|^2 = 1 \quad \text{for all } I.$$

In ref. [3] we have presented the results in the form of probability maps plotting the "temporal" evolution of one-dimensional cellular automata in terms of the normalized probability values $P_{IJ} = c_{IJ}^* c_{IJ}$ for each site J at each time step I, using different colors for different probabilities. Studying these maps, we have found typical quantum features like constructive and destructive interference, or beats. Moreover, certain large scale structures have appeared whose form changes upon variation of the coefficient δ_c of the off-diagonal element $\delta = \delta_c(1 + i)$ in the Hamiltonian [3]. (See, for example, plate I displaying a probability map for $\delta = 20(1 + i)$, i.e. $\delta_c = 20$, and one initial point.)

In this paper, we study the possibility of attributing a characteristic size of the periodically reappearing structures to a specific value δ or to other parameters, i.e. we explore the dependence of structures such as the "ellipse"-like ones in plate I upon variation of various parameters. More explicitly, since in all cases studied the size of such a structure is just twice its periodicity (i.e. the distance between neighboring centers of those overlapping patterns), we investigate the dependence of the periodicity of such "global" structures (as opposed to the "local" rules applied) on four kinds of variations:

i) variation of the periodical boundary conditions;

ii) variation of the number of initial points;

iii) variation of the size of the off-diagonal elements δ;

iv) variation of the quantum phase relations between the individual cellular automaton states by varying independently real and imaginary parts of δ.

2. General properties of the observed patterns

There are several results which hold generally for all quantum cellular automata with $\delta_c \gtrsim 1$ (note that, as has been shown in ref. [3], one generally obtains striped patterns for all quantum cellular automata with $\delta_c > \sqrt{2}$).

1) One can clearly distinguish three domains, or "phases", of the evolution on the global level: a) a mostly complex development from the initial states to the first appearance of recognizable large-scale periodical structures, b) strictly periodical, "ellipse"-like structures, and c) an "infinite-time state" which represents the stable final state that appears at the end of the total evolution and which resembles a plane wave pattern.

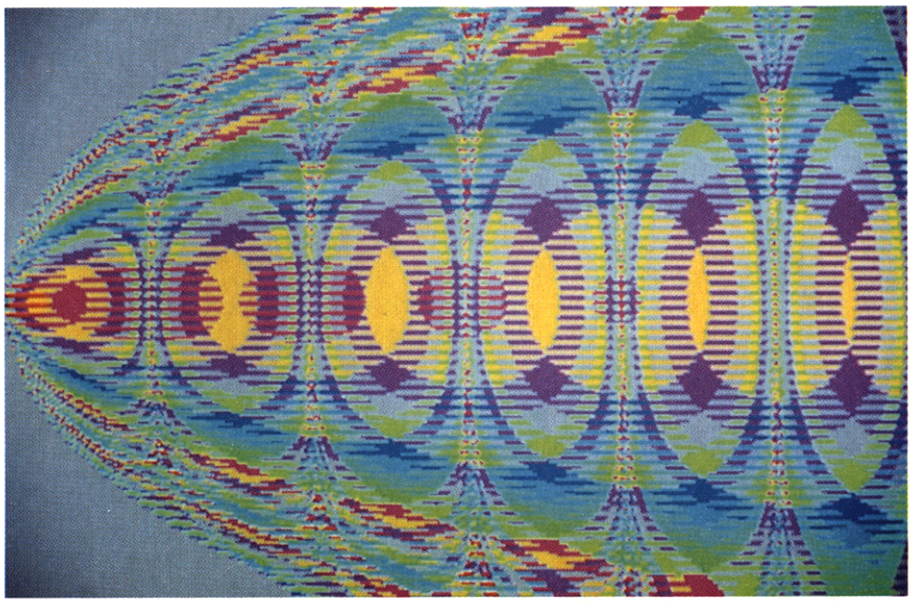
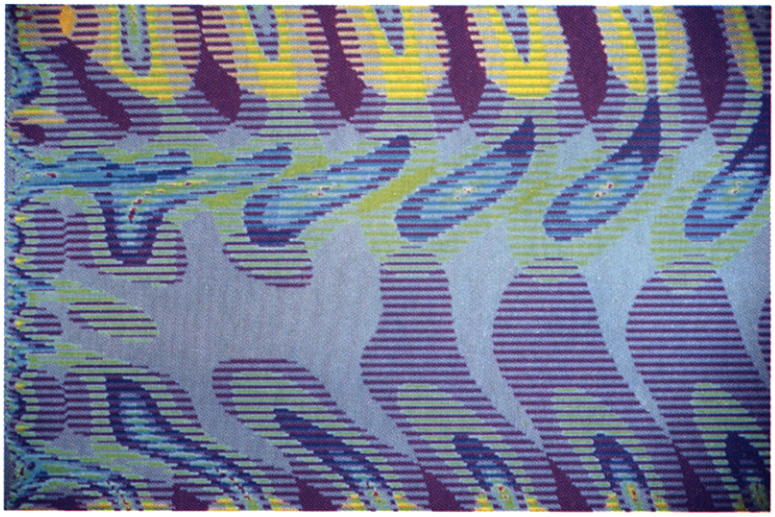


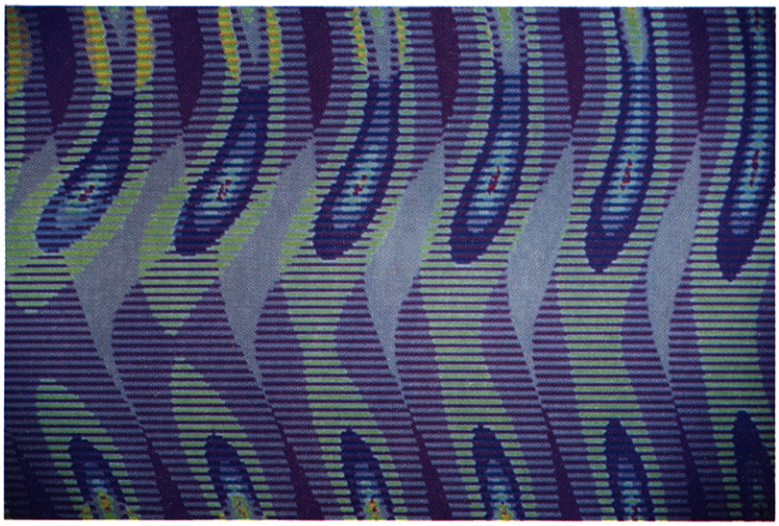
Plate I. Evolution of a quantum cellular automaton with one initial point ($\delta_c = 20$) and $J = 120$ sites (vertical). The time axis (index I) runs from left to right. Different colors represent different probabilities. The characteristic periodicity Δ is half the size of the nearly elliptical patterns.

Plate II. Same as plate I, but with only $J = 40$ sites. The periodicity Δ is the same as in plate I, but the evolution towards the infinite-time state is accelerated.

Plate III a–c. Same as plate I, but with 10 initial points at sites $J = 1$, 3, 9, 25, 30, 50, 60, 75, 90, 100. The time axis runs consecutively through plates a, b and c. Again, the same periodicity results as in plate I. The pattern gradually becomes more regular while information on the initial condition is slowly getting lost.



a



b

c

(An exception to c), however, is given under point 5).)

2) As noted above, calling the distance (measured in time steps) between two centers of neighboring patterns the "periodicity" of the quantum cellular automaton, it holds that the global patterns appearing are exactly twice as large as the corresponding periodicities (plate I). This is a consequence of the specific form of overlap between neighboring patterns which, we assume, is a result of the quantum nature of our cellular automata, i.e. quantum superposition.

3) The periodicity of the global structures is independent of the size of the quantum cellular automaton (i.e. the numbers of sites J used per time step before the periodical boundary condition becomes effective). The main effect of a narrowing down of the size of a quantum cellular automaton through reduction of the number of available states J is an acceleration of the global evolution towards the infinite time state. For illustration, we show in plate II the same quantum cellular automaton as for plate I (i.e. $\delta_c = 20$) except that the number of states used is 40 instead of 120. This implies that, because of the periodic boundary conditions, in plate II the site $J = 41$ corresponds to the site $J = 1$. However, the periodicity of the resulting pattern in plate II is exactly the same as the one in plate I. Note that the "plane wave" pattern, i.e. the infinite time state, appears already after a few time steps while with a cellular automaton of $J = 120$ sites they would appear much later (see plate IIIc).

4) The periodicity is also independent of the number of initial points. In plate III we display an initially irregular quantum cellular automaton with 10 initial points (again with $\delta_c = 20$) at sites $J = 1, 3, 9, 25, 30, 50, 60, 75, 90, 100$, which gradually becomes more regular. Measuring the distances between the centers of the overlapping global structures in plate IIIb or IIIc we obtain exactly the same result as for plate I where only one initial point had been used.

5) As we have reported in ref. [3], there is a specific condition called the "constancy in time criterion" that, if fulfilled, produces stable patterns periodically reappearing with the same size after a few hundred time steps: whenever the initial configuration is such that the location of the sets of initial points, with each set containing at least one initial point, is rotation symmetric with respect to the axis of the torus defined by the periodic boundary conditions, one obtains stable patterns which are then conserved for all later times.

It is important to note that only for the stable patterns mentioned in point 5) above one has a time-reversal symmetry on the global scale, while generally for all other quantum cellular automata with $\delta_c \gtrsim 1$ the patterns gradually become progressively flatter and eventually flatten out completely to create patterns that appear like plane waves (see, e.g. plate II or IIIc). In other words, in all the cases the state the evolution tends to with progressing time only depends on δ_c but is independent of the specific details of the initial condition. This implies that the longer the evolution lasts, the less information on the initial condition will be left in the cellular automaton.

Such a loss of information means that for the largest class of quantum cellular automata one obtains a definite time direction on the level of the global structures. As we have shown recently, this type of irreversibility results from the fact that the evolution (2) becomes non-unitary for large enough values of δ_c. For a more detailed discussion, see ref. [4].

3. Quantitative properties

In addition to studying the general features of patterns in quantum cellular automata, we have also investigated quantitatively the effects which arise upon variation of the off-diagonal elements δ of our Hamiltonian. The magnitude of these elements determines the relative admixture of the probability amplitudes at the neighboring sites $J - 1$ and $J + 1$ at time step $I - 1$ to the probability amplitude at site J at time step I. Therefore, δ

will henceforth be called "mixing parameter". Generally, the mixing parameter is a complex number

$$\delta = \delta_R e^{i\phi} = \delta_R(\cos\phi + i\sin\phi) =: \delta_c + i\delta_c'. \quad (3)$$

Thus, for the case $\delta = \delta_c(1+i)$, i.e. $\delta_c = \delta_c'$ (as always used in the previous examples) one attributes a quantum phase of $\phi = \pi/4$ to δ, and in general the phases are given by

$$\phi = \arctan\frac{\delta_c'}{\delta_c}. \quad (4)$$

In figs. 1 and 2 we present the dependence of the periodicity Δ of the global features of quantum cellular automata (measured in ΔI consisting of the units of time steps I) on the choice of the mixing parameters δ. It turns out that there exist two clearly distinguishable domains. In the first, depicted in fig. 1 where $\delta_R < 1$, no regularity could be found except for extremely small values of δ_R where Δ rapidly grows towards infinity. (The fact that for some values of δ_R, two values for Δ are given, is caused by the appearance of different superimposed structures which one can often clearly identify as beats.) The situation is completely different, however, for values $\delta_R \gtrsim 1$. As can be seen from fig. 2, for a constant value of ϕ the dependence of Δ on δ_R is strictly linear. Moreover, the whole domain of structures appearing upon variation of δ is confined by two linear equations, one holding for $\phi = 0, \pi/2, \pi, \ldots$, etc., and the other for $\phi = \pi/4, 3\pi/4, 5\pi/4, \ldots$, etc. For $\phi = n\pi/2$ $(n = 0, 1, 2, \ldots)$ it holds that

$$\Delta = \tfrac{7}{2}\delta_R, \quad (5)$$

and for $\phi = (2n+1)\cdot\pi/4$ $(n = 0, 1, 2, \ldots)$

$$\Delta = 5\delta_R. \quad (6)$$

For any other value of the quantum phase we also found a linear relationship with slope values

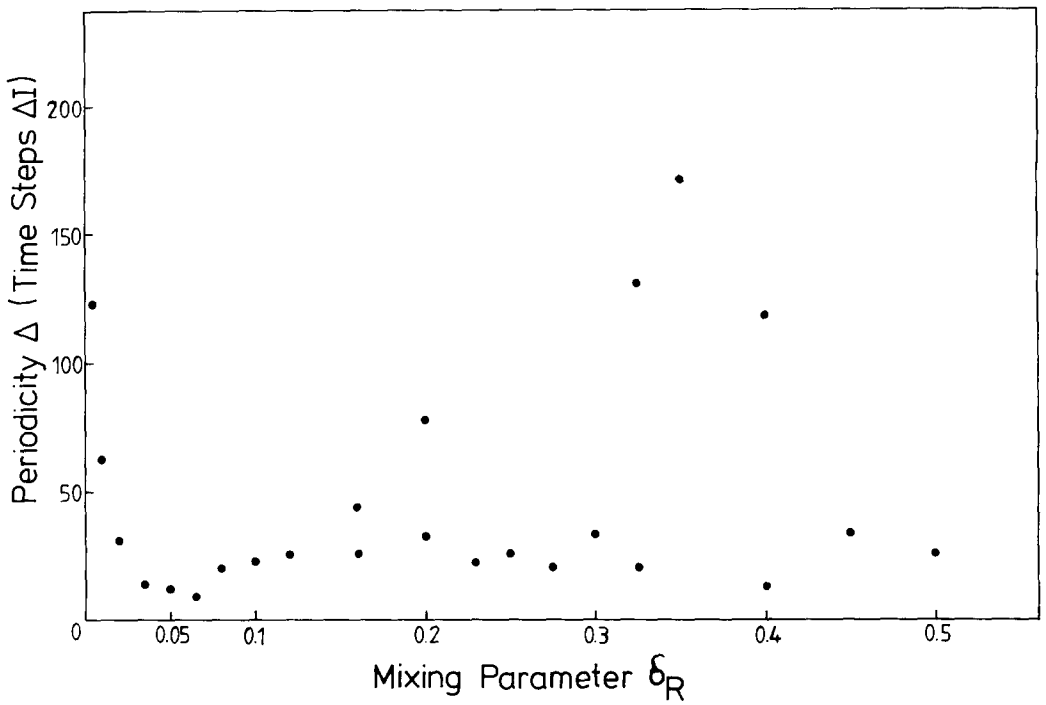


Fig. 1. Characteristic periodicity Δ measured in units of time steps ΔI versus small values of the mixing parameter δ_R, i.e. $\delta_R \lesssim 0.5$. No regularity can be observed except for extremely small values of δ_R where Δ rapidly grows towards infinity.

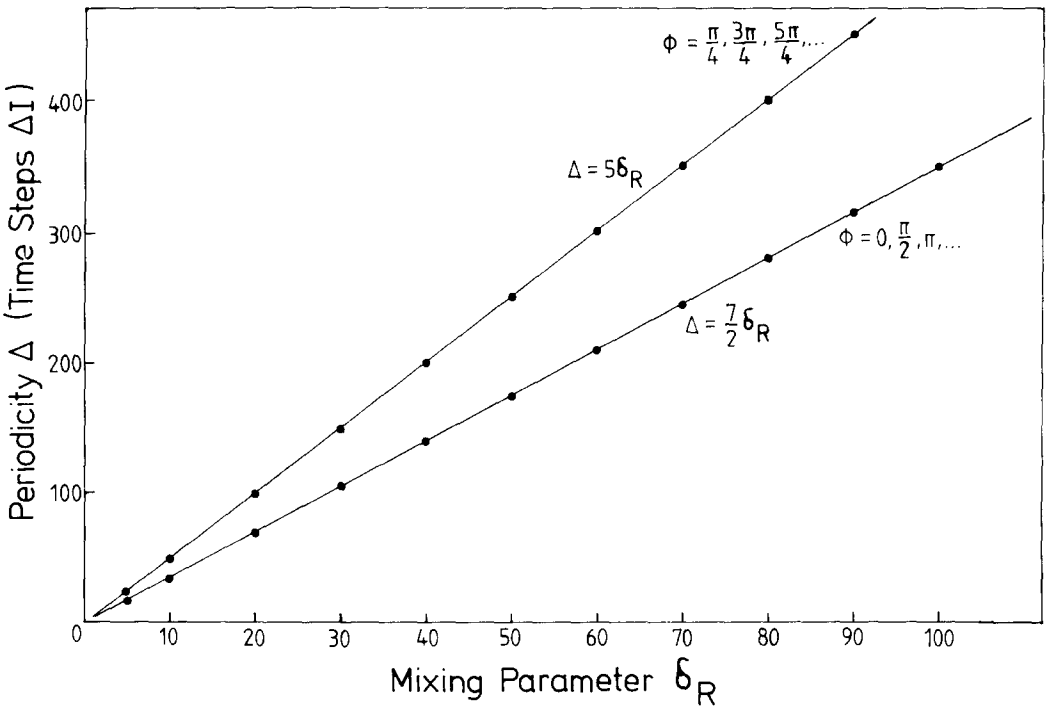


Fig. 2. Characteristic periodicity Δ measured in units of time steps ΔI versus large values of the mixing parameter δ_R, i.e., $1 \lesssim \delta_R \lesssim 100$. For a constant value of the quantum phase ϕ the dependence of Δ on δ_R is strictly linear with the slope being a function of the quantum phase ϕ. The cases of maximum and minimum slopes are shown.

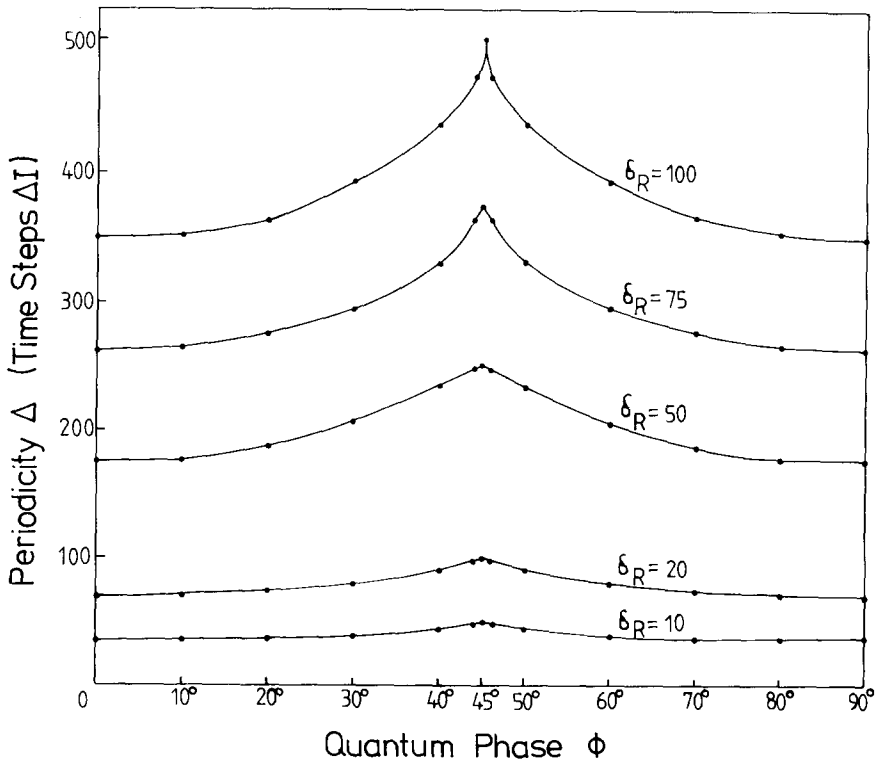


Fig. 3. Variation of periodicity Δ as a function of the quantum phase ϕ for various values of the mixing parameter δ_R.

in between these two cases. Thus, one can generally attribute to each given phase ϕ a slope k which is bounded as

$$\tfrac{7}{2} \leq k \leq 5. \tag{7}$$

This linear relationship permits us therefore to formulate a *conservation law for quantum cellular automata*. Since I describes the discrete time parameter, we may identify the inverse of the periodicity Δ of a pattern as the characteristic frequency ω of the quantum cellular automaton ($\omega = 1/\Delta$). It then generally holds for all automata with $\delta_R \gtrsim 1$ that

$$\delta_R \cdot \omega = \text{constant}. \tag{8}$$

The constant in eq. (8) is only a function of the quantum phase ϕ. The dependency of the constant on the phase ϕ is rather weak as can be seen from fig. 3 where we present "section cuts" through fig. 2 for constant δ_R. One can see that the resulting functions exhibit sharp maxima at $\Delta = 5\delta_R$ but stay mostly around the flat minima at $\Delta = 3.5\delta_R$.

6. Concluding comments

To summarize, it seems remarkable that one can observe an exact linear behavior for the largest domain of values δ_R ($\delta_R \gtrsim 1$): the periodicity and the size of the global structures are solely determined by the strength and (to a lesser degree, i.e. with less influence) by the phase relations of the local nearest neighbor couplings. This is a somewhat counterintuitive result, because one may have expected that the stronger the local couplings the faster the development and completion of a global pattern would be obtained. The opposite is true, however, and this fact can be put into the framework of the conservation law as formulated in eq. (8).

Moreover, one observes irreversibility of the global pattern evolution among the largest class of quantum cellular automata. This behavior is a consequence of the non-unitarity of the evolution operator (see ref. [4]). In the other cases, stable patterns occur. However, the common feature of all these quantum cellular automata is their strict periodicity in an exact linear dependence on the off-diagonal elements δ of their evolution operators. This may very well support the assumption that "chaos" is much less likely to appear on the level of quantum systems than on the classical level, the latter being represented by deterministic or stochastic cellular automata.

Acknowledgement

This work was supported by the Bundesministerium für Wissenschaft und Forschung under contract number Zl.19.153/3-26/85.

References

[1] J. von Neumann, Theory of Self-Reproducing Automata, A.W. Burks, ed. (Univ. of Illinois press, 1966).
[2] S. Wolfram, Statistical mechanics of cellular automata, Rev. Mod. Phys. 55 (1983) 642.
[3] G. Grössing and A. Zeilinger, Quantum cellular automata, paper presented at Int. Conf. on "Cellular Automata", M.I.T., Cambridge, USA (1986); proceedings in Complex Systems 2 (1988).
[4] G. Grössing and A. Zeilinger, Structures in quantum cellular automata, Physica B (1988), in press.