The Role of Correlation in the Operation of Quantum-dot Cellular Automata

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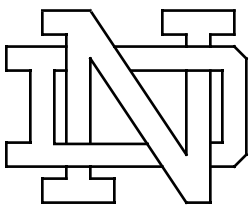

Nano Devices Group

Max Planck Institute, Dresden, May 2001

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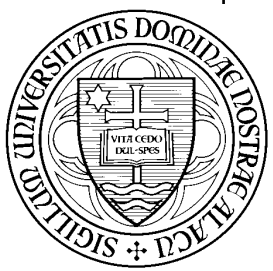


Outline

- Introduction
  - Motivations for QCA
  - QCA Review
  - Implementations
- Modeling QCA circuits
  - Quantum dynamics of QCA cell line (Scrödinger equation, dynamical equation for the density matrix)
  - An alternative: the coherence vector formalism
  - Reducing the number of variables by approximating the higher order correlations with lower order ones
  - Examples to compare the exact and the approximate method
- Conclusions

What is the Quantum-dot Cellular Automata paradigm?

The QCA concept is a transistorless alternative of nowadays circuit technology for digital computing at nanoscale. Why do we need alternatives? Because scaling down traditional transitor based circuits has its own limits.

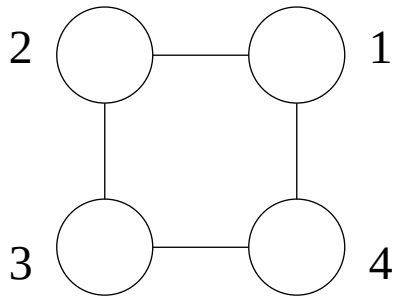
Problems at nanoscale:

- **Few carriers in the nanocurrent**
- **Barriers that modulate current can leak**
- **Difficult to cascade devices: Need to transform small current into substantial voltage (V) to switch next device.**

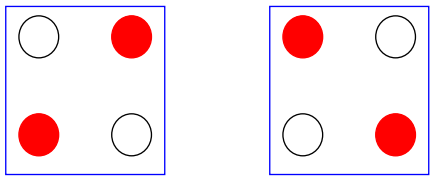
Solution: do not code information with charged current, do not switch current on and off.

The QCA cell

Structure: four quantum dots, two extra electrons, tunneling is possible between adjacent dots

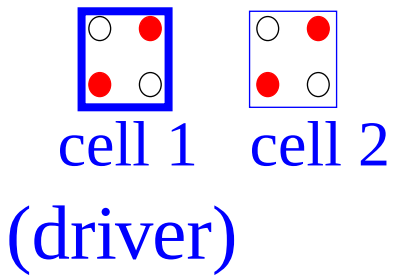


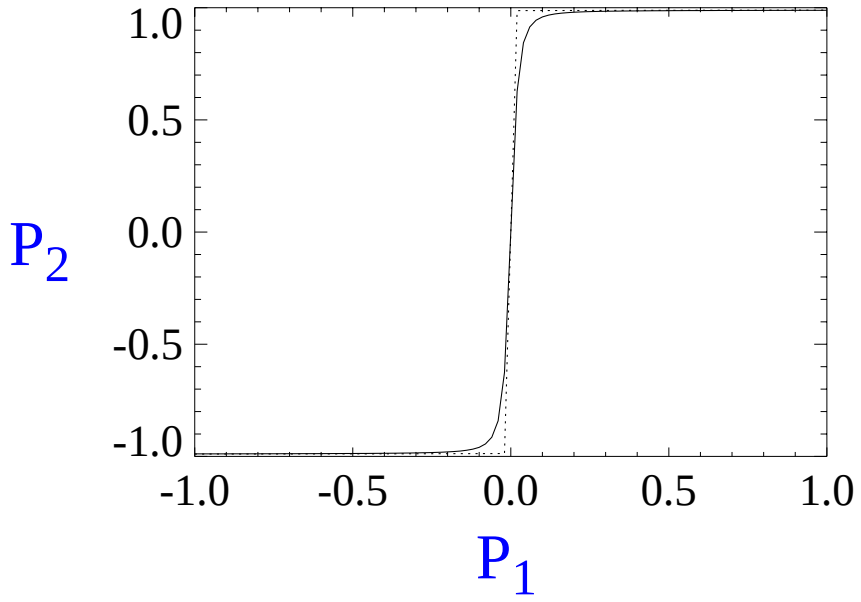
Two bistable states belonging to polarization P=+1 and P=-1, respectively



The QCA intercell coupling

Nonlinear cell-to-cell response function

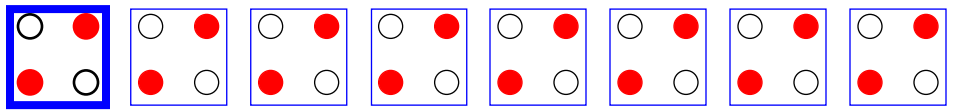




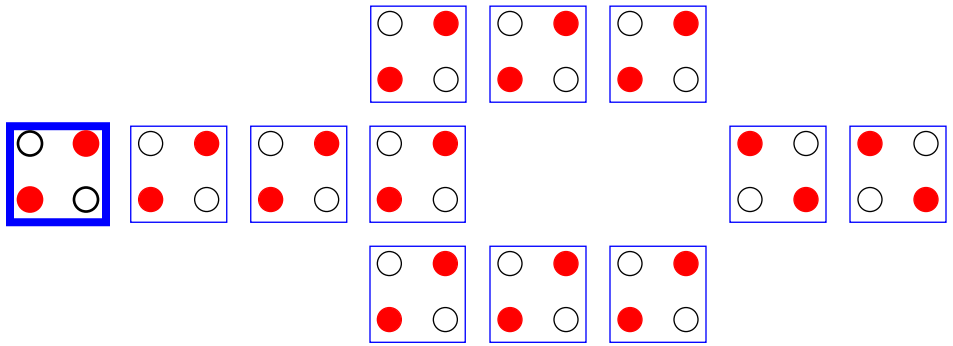
Coulombic coupling between cells.

Complex QCA structures

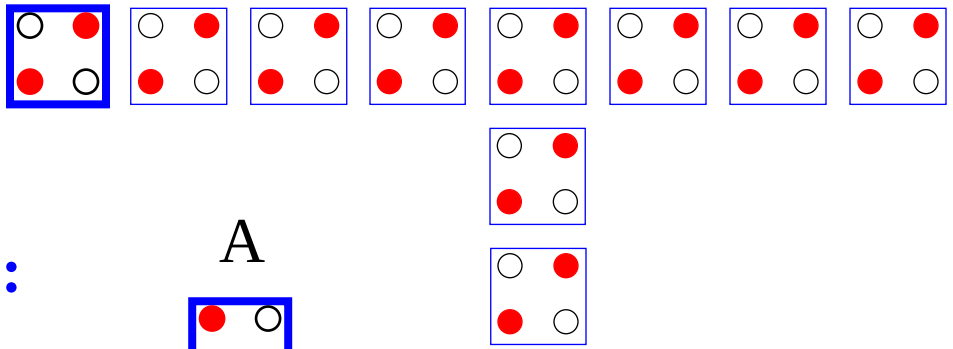
Cell line:



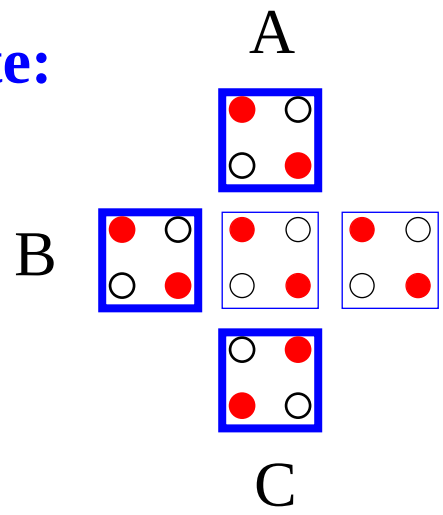
NOT:

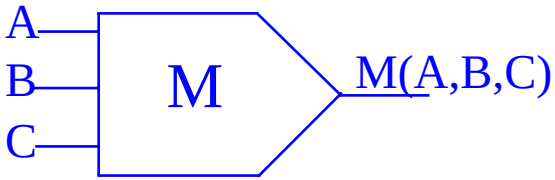


Fan-out:



Majority gate:
(AND/OR)



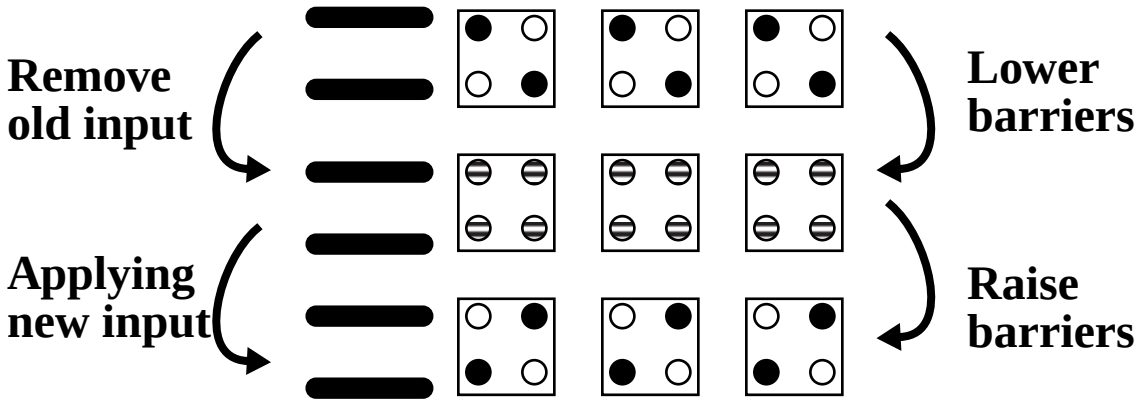


Adiabatic switching

The solution of a logical problem is mapped to the ground state of a physical system: ground state computing.

Problem: the trajectory is not controlled, we may end up in a metastable state.

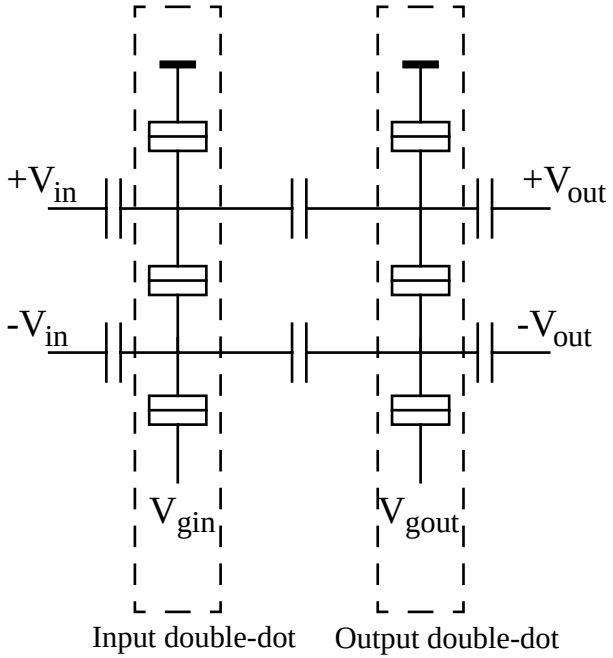
Solution: during an adiabatic process we stay near ground state, thus the trajectory can be controlled.



Lowering the barriers between applying the old and the new inputs increases the energy difference between the ground state and the first excited state.

Possible QCA implementations

(1. Metal island implementation with single electron tunneling circuits)



Successful experiments at 70mK
Modeled as quasi classical circuit. (Capacitance, charging energy instead of Hamiltonian, wave function ...)

2. Semiconductor quantum-dot implementation

3. Molecular implementation

Quantum dynamics

Quantum dynamics of QCA I.

A cell is approximated as a two-state system. The Hamiltonian for a cell line of N cells is

$$\hat{H} = -\gamma \sum_{i=1}^{N} \hat{\sigma}_x(i) - \frac{E_k}{2} \sum_{i=1}^{N-1} \hat{\sigma}_z(i)\hat{\sigma}_z(i+1),$$

where γ is the tunneling energy. It is zero if the interdot barriers are high, and there is no tunneling. It is large, if the barriers are low and tunneling is easy. E_k is the "kink energy". This is the energy of two cells being oppositely polarized.

The polarization is defined as

$$P(i) = -\langle \hat{\sigma}_z(i) \rangle$$

Quantum dynamics of QCA II.

1. Dynamics based on the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle.$$

The state vector is a 2^N element vector. The size of the Hamiltonian is $2^N * 2^N$.

2. Dynamics based on density matrices (Liouville equation):

$$i\hbar\frac{\partial}{\partial t}\hat{\rho} = [\hat{H}, \hat{\rho}].$$

The size of the density matrix is 2^Nx2^N. Advantage: density matrices can describe mixed state/decoherence.

Redundancies in the density matrix

The elements of an MxM density matrix are not independent from each other.

M^2 complex = $2M^2$ real elements

Hermiticity --> M^2 real constraints

Trace is unity --> 1 real constraints

Real degrees of freedom=$2M^2$-M^2-1=M^2-1.

How can we extract the "informative" part of the density matrix?

Dynamics with the coherence vector

If the real degrees of freedom for an *M*x*M* density matrix are M^2-1 then the *M*x*M* density matrix can be written as a linear combination of M^2-1 basis operators.

$$\hat{\rho} = \frac{1}{M}\hat{1} + \frac{1}{M}\sum_i \lambda_i \hat{\lambda}_i \quad .$$

Question: what $\hat{\lambda}_i$ basis operators should we choose?

For a two state system (a single QCA cell), the density matrix is 2x2. The three basis operators are the three Pauli spin matrices.

$$\hat{\rho} = \frac{1}{2}\hat{1} + \frac{1}{2}\sum_{a=x,y,z} \lambda_a \hat{\sigma}_a; \qquad \lambda_a = \langle \hat{\sigma}_a \rangle; \qquad a=x,y,z.$$

The three element vector containing λ_a's is called the coherence vector.

(Mahler, Weberruss: *Quantum Networks*, Springer)

Basis operators for a cell line

For N coupled two level systems (coupled QCA cells) the basis operators are the form of:

$$\left\{\begin{array}{c}\hat{1}\\ \hat{\sigma}_x(1)\\ \hat{\sigma}_y(1)\\ \hat{\sigma}_z(1)\end{array}\right\}\left\{\begin{array}{c}\hat{1}\\ \hat{\sigma}_x(2)\\ \hat{\sigma}_y(2)\\ \hat{\sigma}_z(2)\end{array}\right\}\left\{\begin{array}{c}\hat{1}\\ \hat{\sigma}_x(3)\\ \hat{\sigma}_y(3)\\ \hat{\sigma}_z(3)\end{array}\right\}\times\ldots\times\left\{\begin{array}{c}\hat{1}\\ \hat{\sigma}_x(N)\\ \hat{\sigma}_y(N)\\ \hat{\sigma}_z(N)\end{array}\right\}.$$

Some of the basis operators for N=3:

$\hat{\sigma}_x(1)\hat{\sigma}_y(2)\hat{\sigma}_x(3)$, $\hat{\sigma}_y(1)\hat{\sigma}_z(3)$, $\hat{\sigma}_z(1)$.

Now the coherence vector has 2^{2N}-1=4^N-1 elements. (The density matrix has 2x2^{2N} real elements.*)*

Coherence vector description of a single cell

The Hamiltonian of a cell with a driver $\hat{H} = -\gamma\hat{\sigma}_x + \frac{E_k}{2}P_{driver}\hat{\sigma}_z$

Time dependence of the Pauli spin matrices in the Heisenberg picture:

$$\frac{d\hat{\sigma}_x}{dt} = -\frac{i}{\hbar}[\hat{\sigma}_x, \hat{H}] = E_k P_{driver}\hat{\sigma}_y \qquad \frac{d\hat{\sigma}_y}{dt} = -\frac{i}{\hbar}[\hat{\sigma}_y, \hat{H}] = -E_k P_{driver}\hat{\sigma}_x + 2\gamma\hat{\sigma}_z$$

$$\frac{d\hat{\sigma}_z}{dt} = -\frac{i}{\hbar}[\hat{\sigma}_z, \hat{H}] = -2\gamma\hat{\sigma}_y.$$

Dynamical equation for the coherence vector:

$$\hbar\frac{d}{dt}\begin{bmatrix}\hat{\sigma}_x\\ \hat{\sigma}_y\\ \hat{\sigma}_z\end{bmatrix} = \begin{bmatrix}0 & E_k P_{driver} & 0\\ -E_k P_{driver} & 0 & 2\gamma\\ 0 & -2\gamma & 0\end{bmatrix}\begin{bmatrix}\hat{\sigma}_x\\ \hat{\sigma}_y\\ \hat{\sigma}_z\end{bmatrix} \qquad \hbar\frac{d}{dt}\vec{\lambda} = \begin{bmatrix}0 & E_k P_{driver} & 0\\ -E_k P_{driver} & 0 & 2\gamma\\ 0 & -2\gamma & 0\end{bmatrix}\vec{\lambda}$$

Coherence vector description of two cells

For two cells the basis operators are:

$\hat{\sigma}_x(1), \hat{\sigma}_y(1), \hat{\sigma}_z(1)$; --> $\vec{\lambda}(1)$

$\hat{\sigma}_x(2), \hat{\sigma}_y(2), \hat{\sigma}_z(2)$; --> $\vec{\lambda}(2)$

$\hat{\sigma}_x(1)\hat{\sigma}_x(2), \hat{\sigma}_x(1)\hat{\sigma}_y(2), \hat{\sigma}_x(1)\hat{\sigma}_z(2)$;

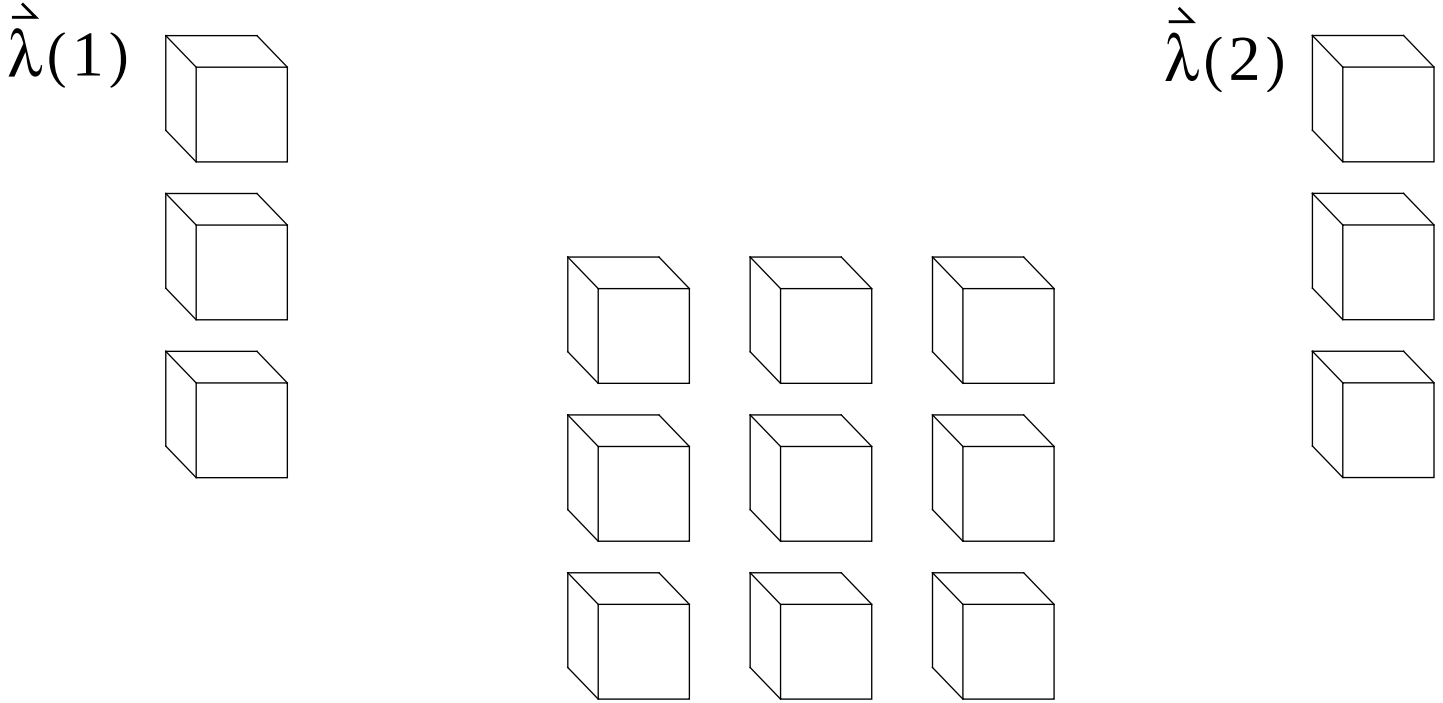
$\hat{\sigma}_y(1)\hat{\sigma}_x(2), \hat{\sigma}_y(1)\hat{\sigma}_y(2), \hat{\sigma}_y(1)\hat{\sigma}_z(2)$; --> $\vec{K}(1,2)$ **(correlation)**

$\hat{\sigma}_z(1)\hat{\sigma}_x(2), \hat{\sigma}_z(1)\hat{\sigma}_y(2), \hat{\sigma}_z(1)\hat{\sigma}_z(2)$.

The 15 element coherence vector is constructed as

$\vec{\lambda} = \begin{bmatrix} \vec{\lambda}(1) \\ \vec{\lambda}(2) \\ \vec{K}(1,2) \end{bmatrix}$. **The dynamics are given as** $\frac{d}{dt}\vec{\lambda} = \hat{\Omega}(t)\vec{\lambda}$.

Coherence vector description of two cells



Notice: the state variables of a multi-cell state can be divided into variables corresponding to the first cell, to the second cell and to the two-cell correlations. The state vector description do not have this feature.

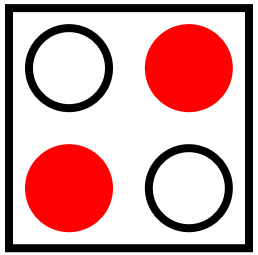
Coherence vector description of a cell line

In the general case, the basis operators are:

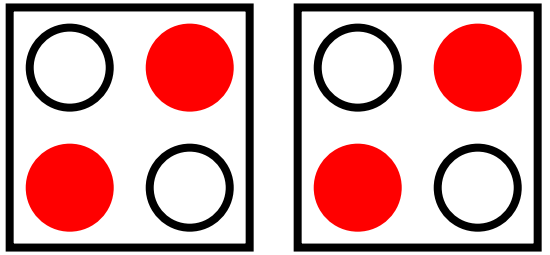
- **Single cell operators, like** $\hat{\sigma}_x(1)$, $\hat{\sigma}_z(3)$, $\hat{\sigma}_y(4)$.
- **Two-cell operators, like** $\hat{\sigma}_z(1)\hat{\sigma}_x(3)$, $\hat{\sigma}_z(2)\hat{\sigma}_y(7)$.
- **Three-cell operators, like** $\hat{\sigma}_z(1)\hat{\sigma}_y(\hat{2})\sigma_x(3)$.
- **N-cell operators ...**

The coherence vector contains the expectation values of all these operators. The expectation values of the two cell operators are the two-point correlations, the expectation values of the three cell operators are the three-point correlations.

The number of state variables increases exponentially with the number of cells

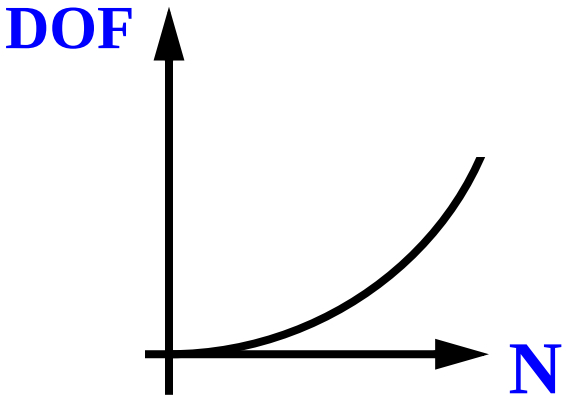


$\overline{\lambda}=(\lambda_x,\lambda_y,\lambda_z)$ **coherence vector**



$\overline{\lambda}(1)$ $\overline{\lambda}(2)$

N QCA cells together have more degrees of freedom than N-times the degrees of freedom one cell has.

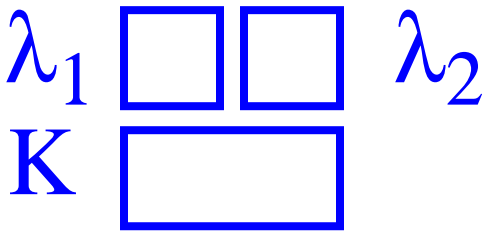


$$\vec{K} = \begin{bmatrix} K_{xx} \\ K_{xy} \\ K_{xz} \\ \cdots \\ K_{zz} \end{bmatrix}$$

correlation vector

Dynamical equations

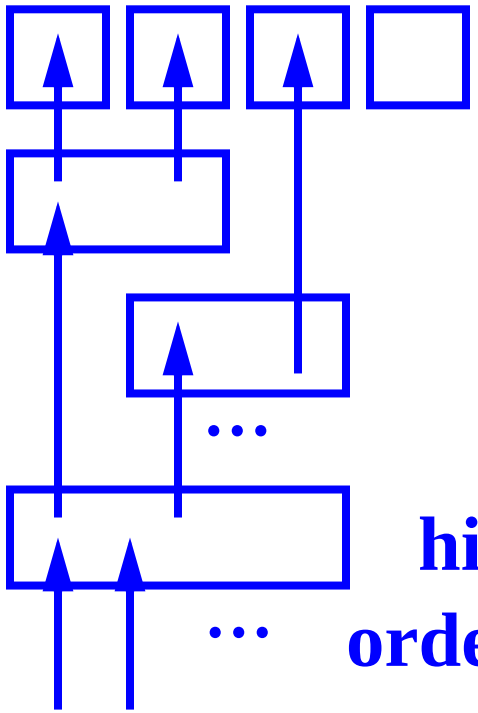
Two cells



$$\frac{d\lambda_1}{dt} = f(\lambda_1, K) \qquad \frac{d\lambda_2}{dt} = f(\lambda_2, K)$$

$$\frac{dK}{dt} = f(K, \lambda_1, \lambda_2)$$

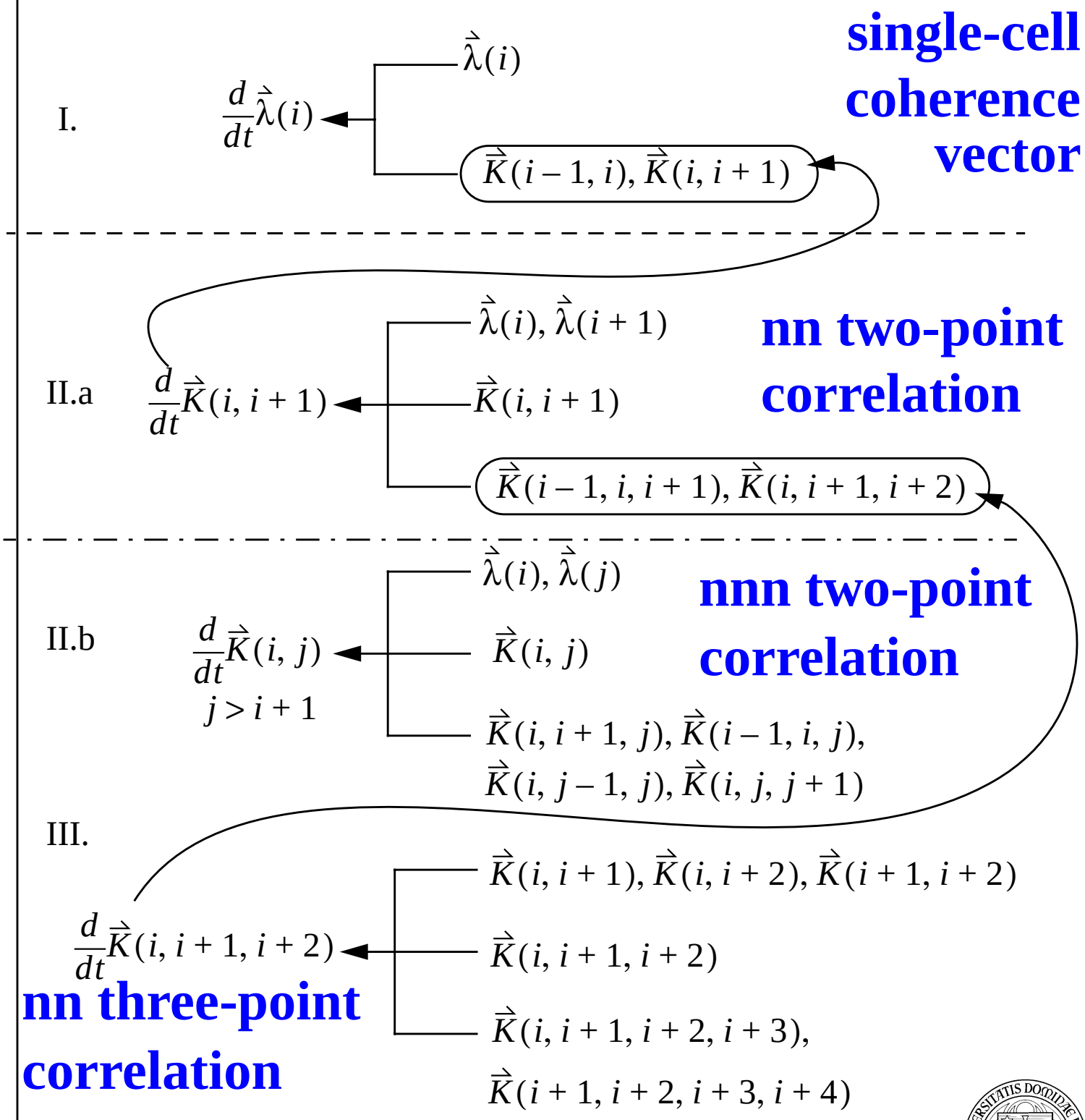
Many cells



higher order correlations

The hierarchy of dynamical equations must be truncated in order to get a computationally feasible model.

Truncation of the hierarchy of equations



Two-point correlations

- **The elements of $\vec{\lambda}(k)$ are defined as**

$$\lambda_a(k) = \langle \hat{\sigma}_a(k) \rangle; \quad a = x, y, z.$$

- **The elements of the *two-point* correlation vector $\vec{K}(k, l)$ are**

$$K_{ab}(k, l) = \langle \hat{\sigma}_a(k) \hat{\sigma}_b(l) \rangle; \quad a, b = x, y, z.$$

- **The elements of the *two-point* correlation vector proper $\vec{M}(k, l)$ are defined as**

$$M_{ab}(k, l) = \langle (\hat{\sigma}_a(k) - \langle \hat{\sigma}_a(k) \rangle) \times (\hat{\sigma}_b(l) - \langle \hat{\sigma}_b(l) \rangle) \rangle$$

$$M_{ab}(k, l) = K_{ab}(k, l) - \lambda_a(k) \lambda_b(k).$$

If the two cells are uncorrelated then the $\vec{M}(k, l)$ is zero.

The intercellular Hartree approximation

Reducing the number of state variables assuming

$$M_{ab}(k,l) = K_{ab}(k,l) - \lambda_a(k)\lambda_b(k) = 0 \ .$$

Thus all the two point correlations can be approximated as

$$K_{ab}(k,l) = \lambda_a(k)\lambda_b(l)$$ **. (Similar to <AB>=<A><B>.)**

This model does not keep correlations at all.

Three-point correlations

Similarly the three-point correlation is defined as

$$K_{abc}(k,l,m) = \langle \hat{\sigma}_a(k)\hat{\sigma}_b(l)\hat{\sigma}_c(m)\rangle; \quad a,b,c = x,y,z.$$

The three-point correlation proper is given as

$$M_{abc}(k,l,m) =$$
$$\langle(\hat{\sigma}_a(k) - \langle\hat{\sigma}_a(k)\rangle)\times(\hat{\sigma}_b(l) - \langle\hat{\sigma}_b(l)\rangle)\times(\hat{\sigma}_c(k) - \langle\hat{\sigma}_c(k)\rangle)\rangle$$

or

$$M_{abc}(k,l,m) = K_{abc}(k,l,m) - K_{ab}(k,l)\lambda_c(m) -$$
$$K_{ac}(k,m)\lambda_b(l) - K_{bc}(l,m)\lambda_a(k) + 2\lambda_a(k)\lambda_b(l)\lambda_c(m).$$

Keeping only the two-point correlations

Taking all three-point correlation propers to be zero, the three-point correlations can be obtained from lower order correlations:

$$M_{abc}(k,l,m) = K_{abc}(k,l,m) - K_{ab}(k,l)\lambda_c(m) - K_{ac}(k,m)\lambda_b(l) - K_{bc}(l,m)\lambda_a(k) + 2\lambda_a(k)\lambda_b(l)\lambda_c(m) = 0.$$

Hence

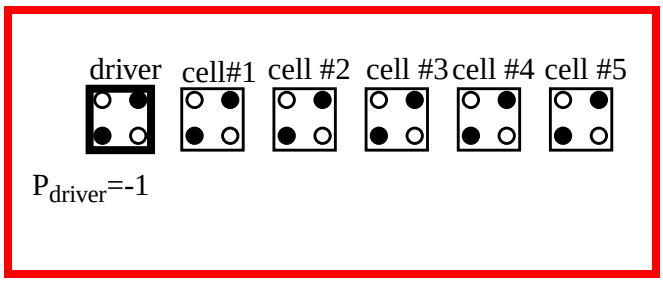
$$K_{abc}(k,l,m) = K_{ab}(k,l)\lambda_c(m) + K_{ac}(k,m)\lambda_b(l) + K_{bc}(l,m)\lambda_a(k) - 2\lambda_a(k)\lambda_b(l)\lambda_c(m).$$

Justification: the three-point correlation proper is small.

Reducing the number of state variables

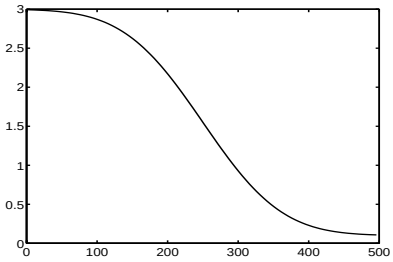
# of cells	Hartree method (no correla-tions)	Nearest-neighbor pair-correla-tions only	Pair-correla-tions only	Size of state vector for the exact model	Size of density matrix
1	3	3	3	2	4
2	6	15	15	4	16
3	9	27	36	8	64
5	15	51	105	32	1024
10	30	111	435	1024	$4x10^6$
15	45	172	990	32768	10^9
...	...	...	...	...	...
N	3N	12N-9	$4.5N^2$-1.5N	2^N	2^{2N}

Line of five QCA cells



The interdot tunneling barriers are raised for each cell.

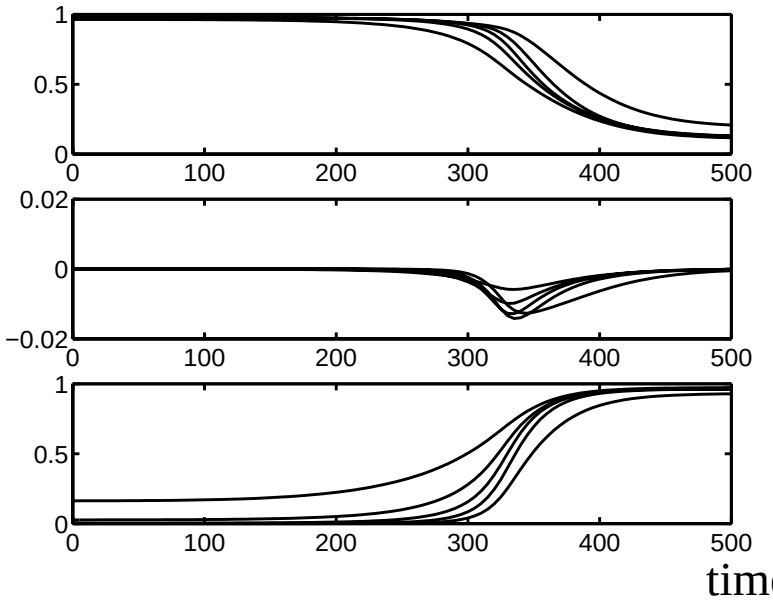
$\gamma(t)$



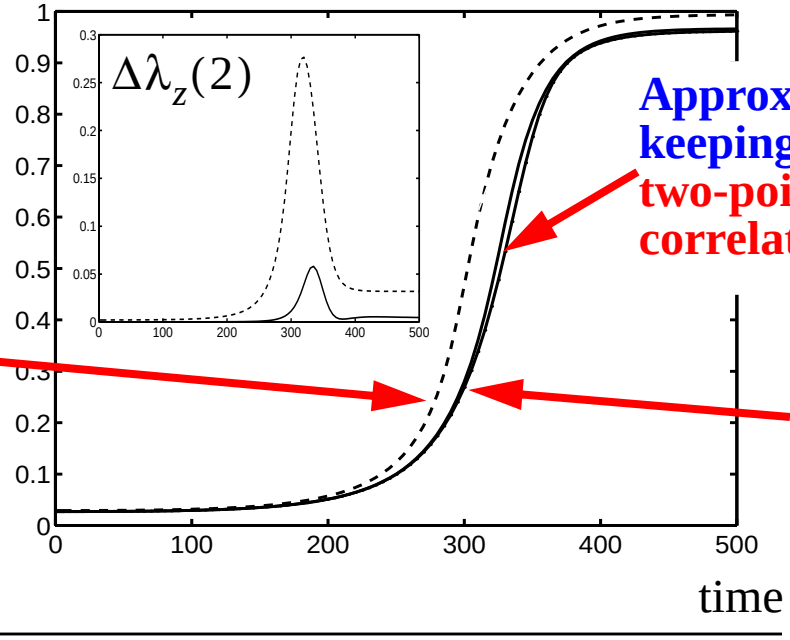
λ_x

λ_y

λ_z



$\lambda_z(2)$



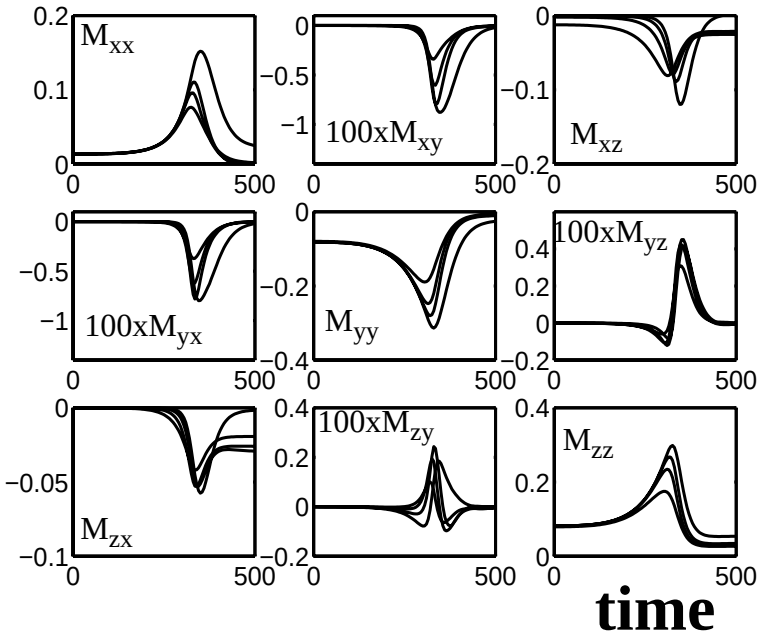
Approximation keeping the nn two-point correlations

Hartree approximation

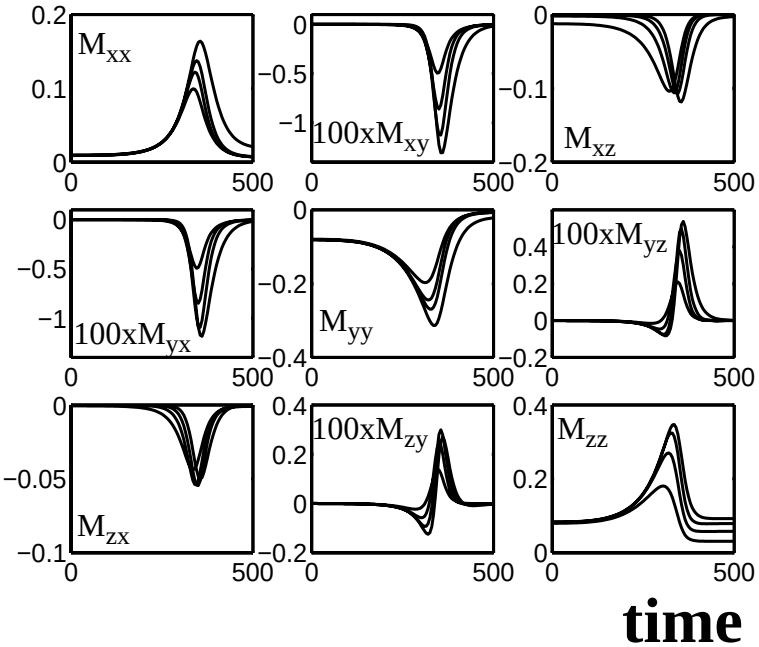
Exact

Line of five QCA cells - Dynamics of pair correlations proper

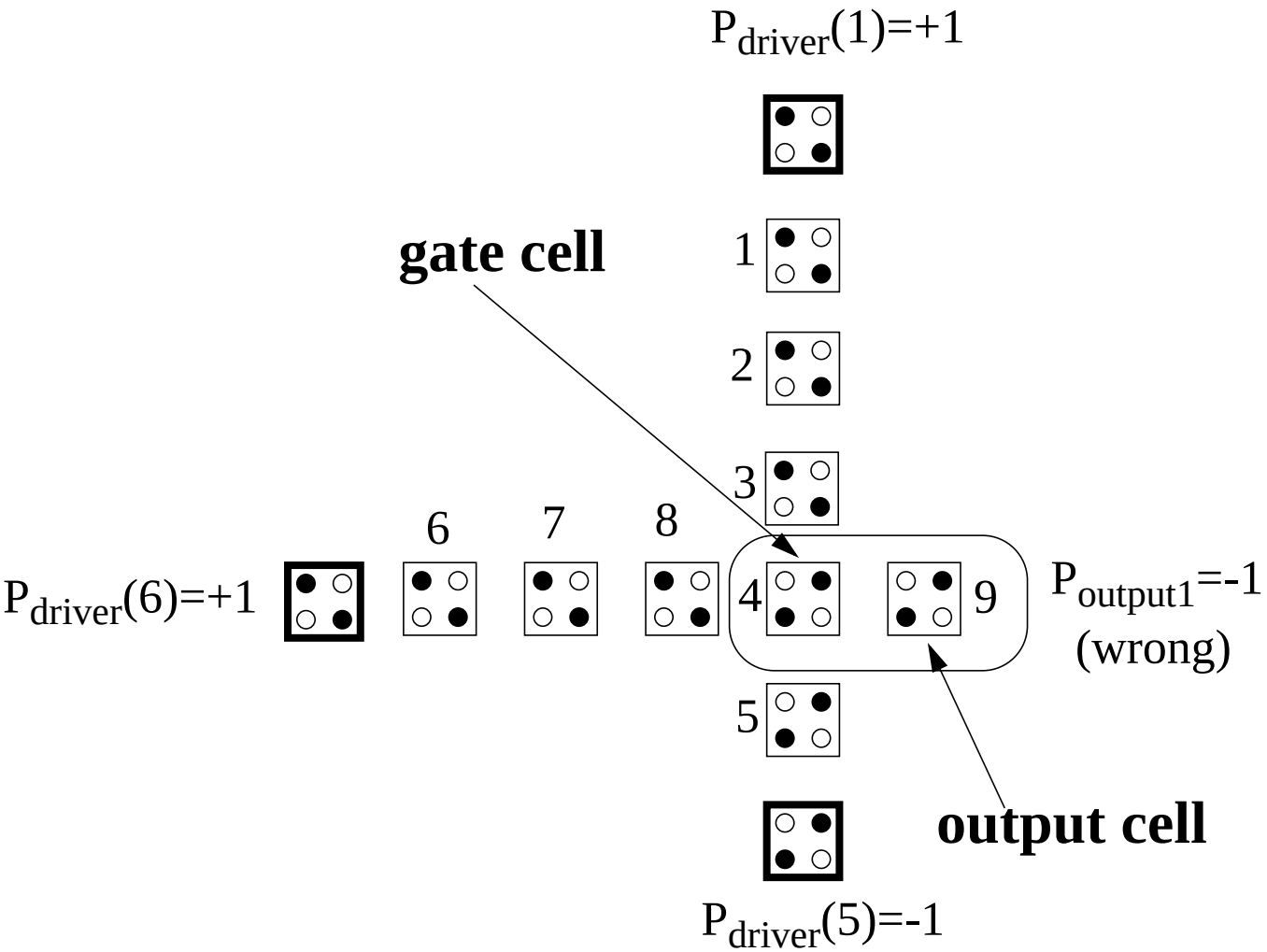
Exact model



Model keeping the nearest neighbor two-point correlations

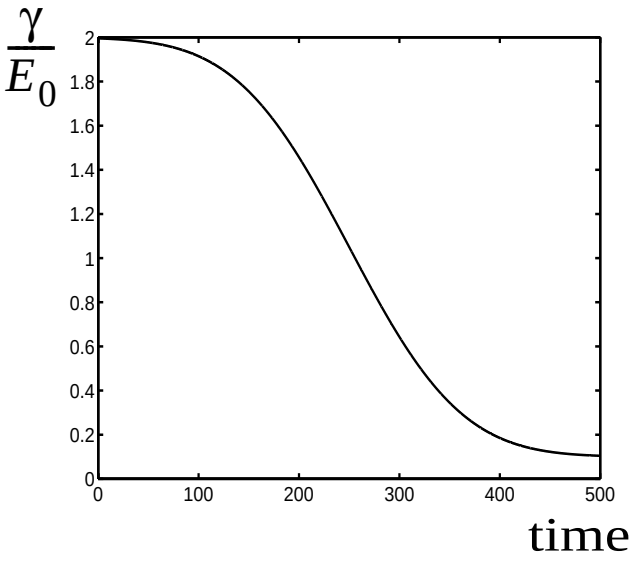


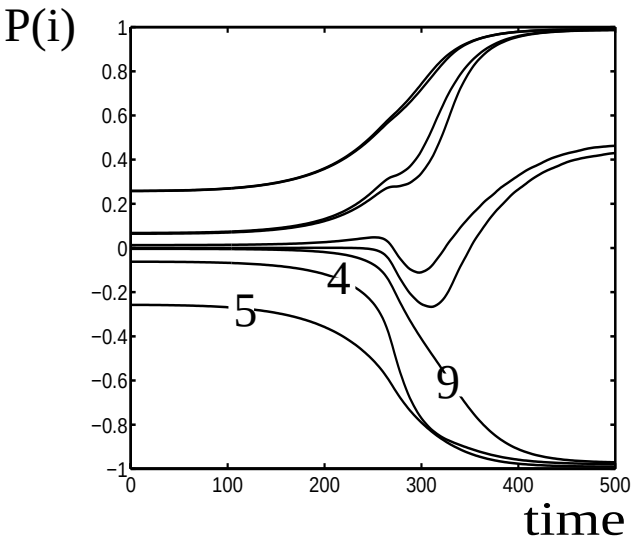
Majority gate with unequal input legs - the output is wrong with the Hartree approximation



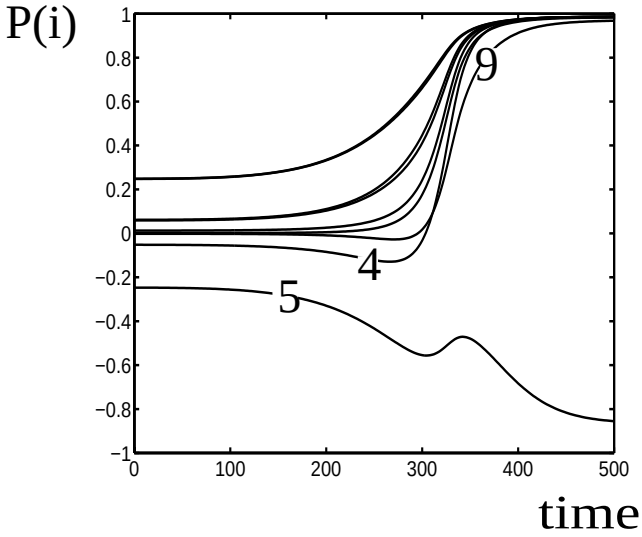
Majority gate with unequal input legs - by including the correlations in the cross region we are able to model the gate correctly

Time dependence of the tunneling





Incorrect results of the Hartree approximation



Correct results with the model including correlations only in the cross region

Conclusions

- The Quantum-dot cellular automata (QCA), as a transistorless alternative of traditional circuit technology was introduced.
- The coherence vector formalism was presented.
- The formalism was used to interpret correlations.
- The formalism was used to decrease the number of variables used for state description.
- The model makes it possible to include as much correlation as necessary to get the correct dynamics.

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