Characterizing Quantum-Dot Cellular Automata

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May 2014

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Chapter 1

Characterization

1.1 The three-cell wire

We choose a simple QCA system, the three-cell wire that we had already introduced in Fig. **??**(b) in the first chapter, to investigate general time-independent characteristics of QCA circuits. Specifically, we are interested in how the polarization of one cell *responds* to the polarization of a second cell, and how cell polarizations depend on cell-cell distance and inter-cell angle. For the three-cell wire we use a nearest-neighbour Coulomb repulsion $V_1 = 40$ and the cell-cell distance is $d/a = 2.2$, where a is the edge length of the cell. Most of our calculations will be at finite temperature, $T = 1$, and we will concentrate on horizontal wires for now (meaning the inter-cell angle is $\theta = 0°$). Both the Coulomb energy scale V_1 and the temperature T are in units of the hopping t, with $t = 1$. For these parameters the bond approximation is valid, which we deploy unless otherwise noted. We investigate systems both without compensation charges $q = 0$, here the net cell charge is $-2e$, and with a compensation charge of $q = \frac{1}{2}$, yielding charge-neutral cells.

The driver cell sets the input for the three-cell wire with its polarization P_D taking values in the range -1 to $+1$. The three active cells respond to the driver polarization. For our discussion, we define the linear polarization response of cell k with respect to cell l as

$$\chi_{kl} = \frac{\partial P_k}{\partial P_l}\Big|_{P_l=0}. \tag{1.1}$$

Fig. 1.1(a) and (b) show the polarization of the first cell with respect to the driver cell, the polarization of the second cell with respect to the first cell, and so on. For the first cell, the response is non-linear and shows gain, therefore $\chi_{1D} > 1$. In contrast, the polarization response between cells interior to the wire is linear and does not exhibit gain, i.e. $\chi_{21} \leq 1$ and $\chi_{32} \leq 1$. Generally, the polarization decreases monotonically from cell to cell, $|P_D| \geq |P_1| \geq |P_2| \geq |P_3|$. In fact, for the $q = 0$ system the polarization rapidly drops to zero for the chosen parameters. The transmission is much improved for charge neutral cells. In that case, the response is almost perfect, $\chi_{21} \sim \chi_{32} \sim 1$.

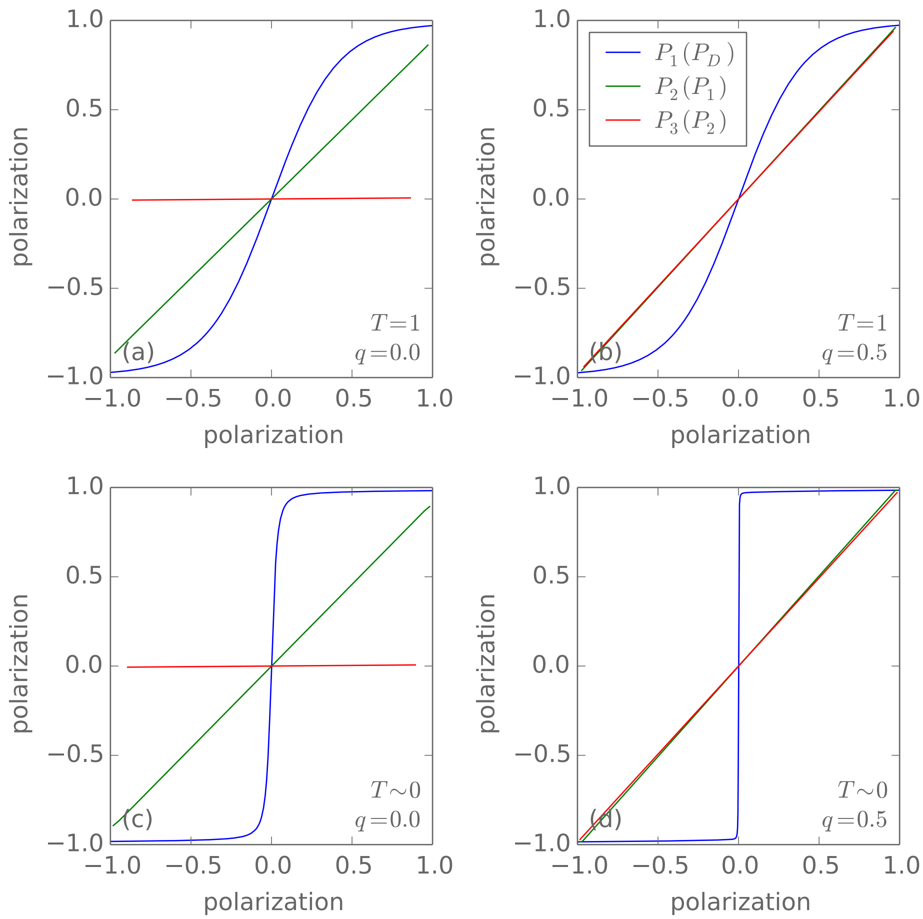


Figure 1.1: The cell-cell polarization response. The response of the first cell with respect to the driver cell is non-linear and exhibits gain. In contrast, the response of the second cell with respect to the first cell, and similarly for the third with respect to the second, is linear and without gain. At zero temperature, the responses are generally improved, but the qualitative behaviour remains the same.

It is worth pointing out that at zero temperature, where we have to use the fixed charge model rather than the inapplicable bond approximation, we observe the same polarization response characteristics, as demonstrated in Fig. 1.1(c) and (d). Quantitatively, for the same system parameters the response is improved at zero temperature compared to $T = 1$. For example, the first cell's polarization response becomes a near-perfect step function for the chosen parameters. But, importantly, it remains true that the response inside the wire (χ_{21}, χ_{32}) is always linear and without gain. Without compensation charges, the polarization of the third cell remains zero even in the ground state, indicating that the cells are so closely spaced that charge buildup pushes the electrons of the rightmost cell to the rightmost edge.

In the literature, the non-linear nature of $P_1(P_D)$ has been noted [1] [2], and the apparent gain $\chi_{1D} > 1$ has been invoked to argue for the robustness and fault-tolerance of the QCA scheme. However, as our graph shows, this is only strictly true for the response with respect to the driver cell. We believe that the picture where each cell switches with gain with respect to its neighbours is an artifact of the intercellular Hartree approximation (ICHA), which we had introduced in more detail in chapter **??**. ICHA treats each cell individually in the static charge mean field of the other cells in the system. In other words, in the ICHA scheme, for each cell the rest of the system is approximated by an effective driver cell.

We now fix the driver polarization at $P_D = 1$ and look at how the polarizations of the active cells depend on the cell-cell distance d/a, see Fig. 1.2(a) and (b). At $d/a = 2$ all quantum dots in the system are equally spaced, cells are placed a distance a apart. At this separation and smaller, our basic assumption of no inter-cell hopping breaks down, as some dots in adjacent cells are now placed closer together than the dots inside each cell. Thus $d/a \leq 2$ is an unphysical limit. Conversely, at very large cell-cell distances we expect the cells to become decoupled and therefore all polarizations to be zero. Obviously, neither extreme limit is of interest if our aim is to build functional QCA devices.

As already observed above, and in line with our intuition, polarizations generally decrease from cell to cell as we go further away from the driver cell. Without compensation charges ($q = 0$) the polarization quickly falls off to very small values, whereas for charge neutral cells ($q = \frac{1}{2}$) the situation is much improved. The graph shows that there is a cell-cell distance that yields maximal polarization for each cell. For the $q = 0$ system—non-charge-neutral cells—the optimal distance increases from cell to cell, due to charge buildup. In contrast, with charge-neutral cells ($q = \frac{1}{2}$) the cell-cell distance yielding optimal polarization does not change notably from cell to cell. In fact, here a range of distances gives very good polarizations, as the polarization saturates at values close to $P = 1$. Of course, for a wire what really matters is the output polarization. For the chosen parameters, this calculation demonstrates that for a $q = 0$ system we should choose $d/a \sim 2.9$. For $q = \frac{1}{2}$ the range $d/a \sim 1.3 \ldots 2.3$ gives the best output polarization. Worryingly, this range is very close to the lower, unphysical limit!

Especially for the non-charge-neutral system it is beneficial to allow for different dis-

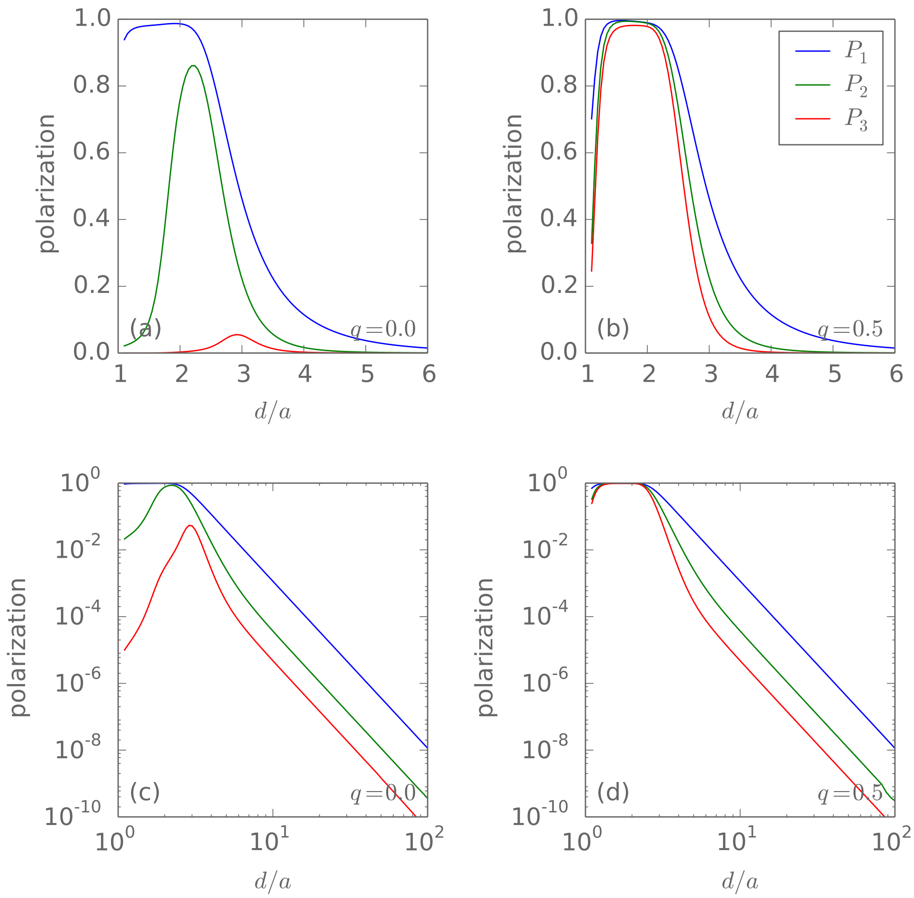


Figure 1.2: (a)(b) Cell polarization over cell-cell distance. In the non-charge-neutral system ($q = 0$), due to charge buildup the maximum polarization for consecutive cells is at increasingly large cell-cell distances. Even at optimal distance the output polarization P_3 is very small. The output polarization is drastically improved for the charge-neutral system. Each cell attains its optimal polarization in the same range of cell-cell distances. (c)(d) Cell polarization over very large cell-cell distances. For large distances $d/a > 10$ the polarizations settle into an universal long distance tail d^{-5}, independent of q and as predicted by the Ising interaction J.

tances between different adjacent cells along the wire. Thus a single d/a parameter is replaced by d_k/a with $k = 1, 2, 3$ for the three-cell wire. Using a stochastic optimization scheme introduced by Sandvik *et al.* [3], we can optimize the d_k/a for optimal output polarization. We find that the output polarization is significantly improved from $P_3 = 0.06$ for uniformly spaced cells to $P_3 = 0.15$ for cells with individual cell-cell distances. Not surprisingly, cells are farther spaced to the right (the output) and closer spaced to the left (the input). This is a manifestation of charge buildup in the system. The situation is very similar for longer wires and different parameters for non-charge-neutral wires. Of course, non-uniformely spaced cells have implications for the directionality of transport in a wire, which would have to be considered when designing QCA circuitry. More generally, we should be able to optimize the functionality of any given non-charge-neutral QCA layout by allowing for slightly adjustable cell placement. We can do the same stochastic optimization for charge-neutral wires ($q = 1/2$), but find that little is gained by allowing non-uniform cell-cell distances. Looking at Fig. 1.2 this is really not surprising at all, and simply a consequence of having no charge buildup in the system. It should be emphasized how much better the output polarization is for charge-neutral wires. At least for the chosen parameters, even very short wires seem unrealistic for a non-charge-neutral system.

It is instructive to plot the polarizations over cell-cell distance up to very large distances in a log-log graph as shown in Fig. 1.2(c) and (d). Even though large distances come with extremely small polarizations that are not of practical interest, this graph yields valuable insights into the nature of the interaction that mediates the polarization. At distances $d/a > 10$ we see that the polarization settles into an universal long range tail with $P(d) \sim d^{-5}$. This is consistent with our understanding that the polarization is mediated by a quadrupole-quadrupole interaction. For these large distances the polarization is exactly the same for both the $q = 0$ and the $q = \frac{1}{2}$ systems. Hence, having non-charge-neutral cells does not actually alter the characteristics of the cell-cell interaction. Instead, it suppresses the cell-cell interaction at small distances. That is, charge repulsion competes with the quadrupole interaction. The graph exactly confirms our analysis from chapter **??**. There, we had derived an approximate expression for the mediating cell-cell interaction in the Ising picture, $J \sim d^{-5}$, to leading order, and the derived J was independent of q. At the time we had seen that, in general, we can only map QCA to a modified Ising model with an additional cell-cell interaction J', which does depend on q. However, for the horizontal wire J' vanishes and we are left with the pure Ising model, and at large enough distances the behaviour of the polarization is just as predicted. Of course, we are mostly interested in small distances, where the polarization is relatively large. Here, the polarization falls off faster than d^{-5} and, remembering the derivation of J, we would need to include higher order corrections in the multipole expansion to accurately describe this behaviour. Even with higher order terms the Ising model and its J cannot, however, correctly reproduce the suppression of the quadrupole interaction at short distances in the case of $q = 0$.

From the discussion of the Ising model in chapter **??**, we already know that cell polarizations should change with the inter-cell angle. The polarizations are mediated by

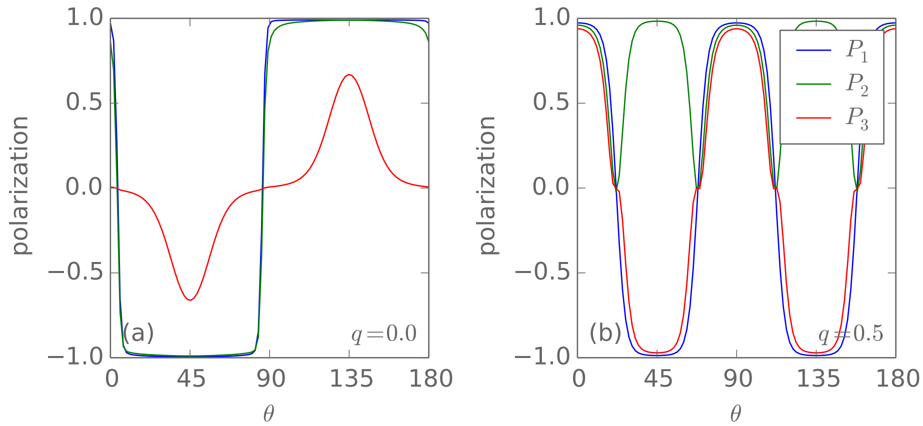


Figure 1.3: Cell polarization over the inter-cell angle. The charge-neutral system is invariant under rotations by 90° and closely matches the behaviour predicted by the Ising J. At 45° cell polarizations are alternating. For the non-charge-neutral system, the polarizations are predominantly set by the angle, and not by the driver polarization. The system is invariant under rotations by 180°, as predicted by the modified Ising J'. In the non-charge-neutral case QCA does not work at all, except for horizontal or vertical wires.

the cell-cell interactions J and J', and specifically we had found $J \sim \cos 4\theta$, whereas $J' \sim \sin 2\theta$. We rotate the three-cell wire from a horizontal configuration ($\theta = 0°$) over diagonal ($\theta = 45°$) to vertical ($\theta = 90°$), and back to horizontal ($\theta = 180°$), and look at the cell polarizations in the process. Fig. 1.3(b) shows the polarization as a function of the angle for the charge-neutral system, where $J' = 0$. Indeed, the cell polarizations follow the behaviour predicted by J: they are rotationally invariant under rotations by 90° and peak at the angles $0°, 90°$, and so on, where $J > 0$. At 45°, where $J < 0$, cell polarizations are alternating, e.g. $P_D \sim 1$, $P_1 \sim -1, P_2 \sim 1$, and $P_3 \sim -1$. In between, for example at $\theta = 22.5°$, $J = 0$ and the polarization is zero accordingly. The wire can be used to transmit signals in a range of about 20° around $\theta = n \cdot 45°$, where n is an integer and the usable angle range depends on the chosen system parameters. Of course, at 45° we have to make sure to use an even number of cells for transmission, as the signal will be inverted otherwise. Conceivably, the nodes at $22.5°, 67.5°$, and so on could be used to decouple closely spaced cells.

The situation is very different for non-charge-neutral systems, as shown in Fig. 1.3(a). In this case, $J' \neq 0$ and we see that the polarization is actually predominantly set by J', which is rotationally invariant under rotations by 180°. This is in line with our derivation where we had found, to leading order, $J' \sim d^{-3}$, whereas $J \sim d^{-5}$, and thus, J' was expected to dominate. The graph shows that the cell polarizations are much larger in

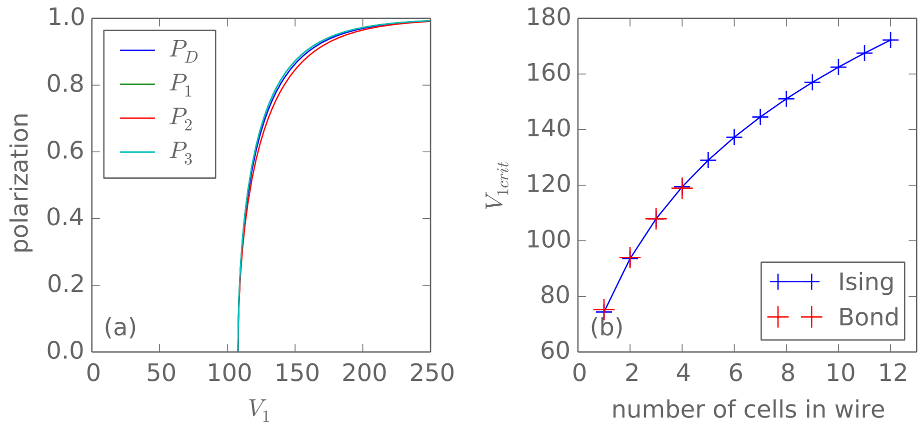
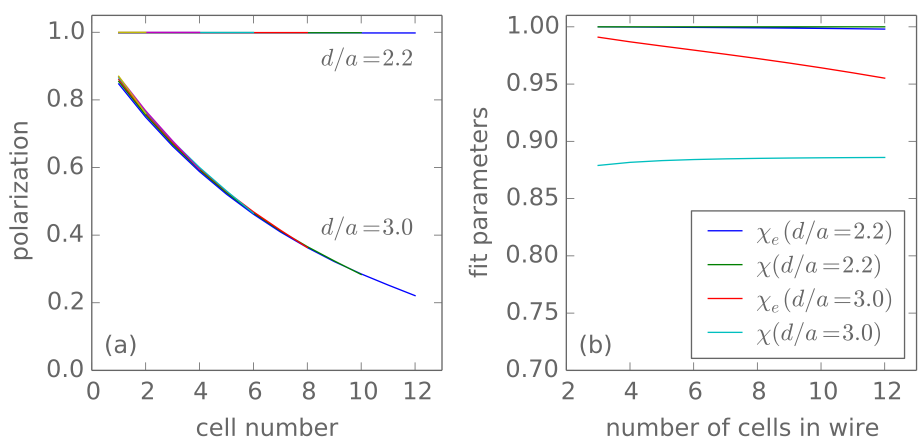


Figure 1.4

magnitude away from $0°, 90°$, and so on, where we know that the system behaves as expected. In fact, the presented graph looks exactly the same for $P_D = 1$ and $P_D = -1$, except for a small range of angles of about $5°$ around $\theta = n \cdot 90°$, where the angle range again depends on the chosen system parameters. In short, the cells' polarizations are set by the inter-cell angle, and not by the driver polarization. The importance of charge neutrality had first emerged in our discussion of the Ising model. Here we see this finding most impressively confirmed. The non-charge-neutral system will never work as a QCA circuit unless all we want to do is build linear chains of cells. Even in this case the system becomes very fragile with respect to angular displacement. Thus, for QCA charge-neutral cells, $q = \frac{1}{2}$, are absolutely essential. In the literature charge neutrality has usually been assumed, either explicitly or implicitly, but as far as we know, no one else has previously identified its crucial role.

1.2 Workable parameters for QCA



1.0
0.8
0.6
0.4
0.2
0.0
polarization
0
2
4
6
8
10
12
cell number
$d/a = 2.2$
$d/a = 3.0$
(a)
1.00
0.95
0.90
0.85
0.80
0.75
0.70
fit parameters
2
4
6
8
10
12
number of cells in wire
$\chi_e(d/a = 2.2)$
$\chi(d/a = 2.2)$
$\chi_e(d/a = 3.0)$
$\chi(d/a = 3.0)$
(b)

Figure 1.5

Bibliography

[1] C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, "Quantum cellular automata," *Nanotechnology* **4** (1993) 49.

[2] C. S. Lent and P. D. Tougaw, "Lines of interacting quantum-dot cells: A binary wire," *Journal of Applied Physics* **74** (1993) 6227–6233.

[3] J. Lou and A. W. Sandvik, "Variational ground states of two-dimensional antiferromagnets in the valence bond basis," *Phys. Rev. B* **76** (Sep, 2007) 104432. `http://link.aps.org/doi/10.1103/PhysRevB.76.104432`.