

Characterizing Quantum-Dot Cellular Automata

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Chapter 1

Approximations

1.1 Fixed charge model

Exact diagonalization scales exponentially with system size. For the full *grand canonical* QCA Hamiltonian, Eq. ??, only QCA devices of up to two cells are computationally feasible. Therefore, to access larger systems we need to introduce approximations. Approximating means to simplify. However, by carefully establishing successive approximations and their limits, we also reduce the problem to its essential ingredients and thus, hopefully, we gain a better understanding of the system. As a first step, we reduce the Hilbert space to a *fixed* number of particles per cell. We disallow any charge fluctuations, both for the system as a whole and for each individual cell. With that, we omit the chemical potential term in the Hamiltonian, $\mu = 0$, and prohibit inter-cell hopping. This is a major simplification. However, it is in line with the QCA idea: The approach requires a fixed number of charges per cell, typically two electrons, and cells are thought to interact only via Coulomb forces. In a sense we are shifting the starting point of our investigation. If the *fixed* charge approximation is not valid for a given system, then there is no hope of implementing QCA on it. On the other hand, for experimental systems like the atomic silicon quantum dots and for a given cell layout, it should always be possible, at least in principle, to tune the system parameters, especially the chemical potential, to get the system into the right particle number sector. The system has to be set up in a way that the two-electrons-per-cell sector is lowest in energy and other particle number sectors are sufficiently gapped out, that is, at an energy, compared to the ground state energy, much larger than temperature. Of course, in practice there are very clear limits as to how much the system parameters can be tuned and any QCA cell layout considered within the *fixed* charge approximation cannot necessarily be readily implemented on a given real-world material system.

For the *fixed* charge system, the state space scales as $N_s = \binom{8}{2}^{N_c} = 28^{N_c}$ (N_c is the number of cells). Using symmetries, the largest block of the Hamiltonian matrix is the spin zero sector, of size $N'_s = 16^{N_c}$. On conventional computer hardware, systems of

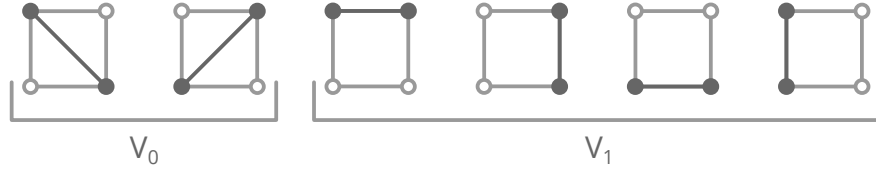


Figure 1.1: ...

up to four cells are possible, with memory requirements of 32GB. In practice, however, calculations for four-cell systems take too long and thus three cells is the practical limit for the *fixed*-number-of-particles-per-cell model.

1.2 Bond model

At its heart, QCA is a semi-classical idea. It relies solely on charge-charge interactions and ignores the particle spins. Therefore, as a next step in our quest to access larger system sizes, we neglect the spin degree of freedom in our model. The 28 states per cell of the *fixed* charge model can be reorganized into four doubly occupied dots and six bonds. The six bonds are illustrated in Fig. 1.1. Each bond corresponds to one spin singlet and three spin triplet states. The *bond* approximation only keeps one state for each bond and discards the doubly occupied states as well. With the *bond* model we thus assume that singlet and triplet states are qualitatively equivalent and energetically degenerate, and that doubly occupied dots are sufficiently gapped out, that is, $U \gg T$. As QCA ignores the spin, singlets and triplets should be qualitatively equivalent, but they are not quite degenerate. We expect that virtual double-occupancy lowers the energies of the singlet states and therefore introduces a small singlet-triplet splitting. Still, degeneracy is presumably not a bad assumption to start with and we will look at the singlet-triplet splitting in detail in due course. For the *bond* model the QCA Hamiltonian reduces to

$$H = - \sum_{\langle ij \rangle} t c_i^\dagger c_j + \sum_{i < j} V_{ij} (n_i - q) (n_j - q) . \quad (1.1)$$

With six bond states per cell, the Hilbert space of the *bond* model is $N_s = 6^{N_c}$ (N_c the number of cells). Five and six cells are doable, with memory requirements of 460MB and 16GB, respectively, but for practical calculations five cells really is the limit. For the *bond* model there are no symmetries that can be exploited.

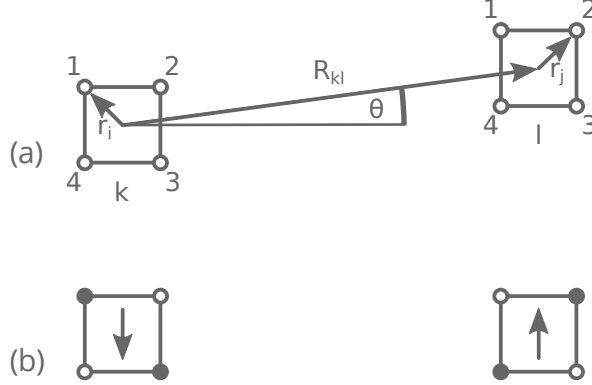


Figure 1.2: a) QCA cells k and l . b) The two-states-per-cell approximation identifies each cell with a spin \uparrow or \downarrow .

1.3 Ising model

A linear array of QCA cells where each cell has a state of logic 0 or 1 is reminiscent of a 1D spin $\frac{1}{2}$ chain. Indeed, if we reduce the basis to only two states per cell, down from six states in the *bond* picture, we can map the QCA system to a transverse-field Ising model with long-ranging interactions. This is an attractive proposition: The smaller Hilbert space allows for larger system sizes with our exact diagonalization method; more importantly, the transverse-field Ising model is amenable to sign-problem-free Stochastic series expansion (SSE) quantum Monte Carlo schemes [1]. These methods do not scale exponentially¹ and consequently allow access to much larger systems. Last, but not least, such a mapping connects the QCA approach to the established and well studied Ising model. The prospect hinges on the assumption that the two-states-per-cell basis actually is a good approximation for QCA systems. And while bistable two-state cells are certainly the picture we have in mind when we talk about QCA, it is not *a priori* clear whether this is a correct physical picture.

We use the *bond* Hamiltonian (1.1) as the starting point. We had already discussed in the last chapter that such a Hamiltonian can be decomposed into single-cell terms and cell-cell interaction terms,

$$H = \sum_k H_k^c + \sum_{k < l} H_{kl}^{cc}. \quad (1.2)$$

In comparison, the transverse field Ising model is described by

$$\tilde{H} = - \sum_k \gamma S_k^x + \sum_{k < l} J_{kl} S_k^z S_l^z. \quad (1.3)$$

¹SSE quantum Monte Carlo methods roughly scale as $N \ln N$ where N is the system size.

Thus, we would like to map the single cell term H_k^c to the transverse field term $-\gamma S_k^x$ and the Coulombic cell-cell interaction H_{kl}^{cc} to the Ising term $J_{kl} S_k^z S_l^z$. Each cell k is identified with a pseudo spin S_k^z , specifically the logic 0 with a spin down state and the logic 1 with a spin up state, as illustrated in Fig. 1.2(b). We will first look at how the QCA cell can be represented by only two states and derive an approximate expression for the transverse field γ . Then we will use a multipole expansion to derive J_{kl} from the cell-cell Coulomb interaction.

To arrive at a single-cell-basis with only two states we can, in principle, follow a similar prescription as for the fixed charge and bond approximations: We neglect high energy states which are assumed to be gapped out. In this case these are the four edge states with Coulomb energy V_1 , $|\psi_Q\rangle = \{|3\rangle, |4\rangle, |5\rangle, |6\rangle\}$ in Fig. 1.1, where we have introduced $|\psi_Q\rangle$ to denote the high-energy subspace of the single-cell Hilbert space. We only keep the low-energy, diagonal states $|\psi_P\rangle = \{|1\rangle, |2\rangle\}$ with Coulomb energy V_0 . Of course, these two are exactly our logic 0 and logic 1 state, or $|1\rangle \doteq |\downarrow\rangle$ and $|2\rangle \doteq |\uparrow\rangle$, respectively. Here, $|\psi_P\rangle$ denotes the low-energy subspace. For the high-energy states to be sufficiently gapped out we require $\Delta V = V_1 - V_0 \gg T$. In contrast to the fixed charge and bond models, merely truncating the Hilbert space is not sufficient for the Ising model. For our previous two approximations the Hamiltonian had remained essentially unchanged, apart from dropping no longer relevant terms, such as the chemical potential term or the Hubbard U term. The retained states were exactly the same states as in the full, untruncated model. But with only two states per cell the existing Hamiltonian (1.1) does not “work”: There is no process that takes the system from state $|1\rangle$ to $|2\rangle$. Therefore, for the Ising approximation we need to derive an effective, low-energy Hamiltonian from the bond model. In the bond picture, for the system to transition from state $|1\rangle$ to $|2\rangle$ it can take different paths, for example $|1\rangle \rightarrow |3\rangle \rightarrow 2$, consisting of two hopping processes with an interim high-energy edge state. We will treat those processes perturbatively, as *virtual* excitations, and derive an effective hopping term between the two states $|1\rangle$ and $|2\rangle$. This effective hopping term is precisely the transverse field γ which flips the spin in the Ising picture, $-\gamma S_k^x = -\gamma \frac{1}{2} (S_k^+ + S_k^-)$.

A single QCA cell is described by the time-independent Schrödinger equation $H_k^c |\psi\rangle = E_k |\psi\rangle$, with $|\psi\rangle = [|\psi_P\rangle, |\psi_Q\rangle]$. Our aim is to truncate the basis to $|\psi_P\rangle$ and derive an effective Hamiltonian \tilde{H}_k^c with the subspace Schrödinger equation $\tilde{H}_k^c |\psi_P\rangle = E_k |\psi_P\rangle$. The high-energy states $|\psi_Q\rangle$ have to be incorporated as virtual excitations. Using the basis depicted in Fig. 1.1 the single-cell bond Hamiltonian is very simple and can be written down explicitly. As the single-cell Hamiltonian is the same for all cells, we can drop the

index k .

$$\begin{aligned}
 H^c &= \left(\begin{array}{cc|cccc} V_0 & 0 & -t & -t & -t & -t \\ 0 & V_0 & -t & -t & -t & -t \\ \hline -t & -t & V_1 & 0 & 0 & 0 \\ -t & -t & 0 & V_1 & 0 & 0 \\ -t & -t & 0 & 0 & V_1 & 0 \\ -t & -t & 0 & 0 & 0 & V_1 \end{array} \right) \\
 &= \begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix}
 \end{aligned} \tag{1.4}$$

Here, we have partitioned the Hamiltonian into four blocks, H_{PP} , H_{QQ} , H_{PQ} , and H_{QP} , corresponding to the low-energy subspace $|\psi_P\rangle$, the high-energy subspace $|\psi_Q\rangle$, and transitioning between the subspaces. With a this partitioned Hamiltonian the time-independent Schrödinger equation is

$$\begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix} \begin{pmatrix} \psi_P \\ \psi_Q \end{pmatrix} = E \begin{pmatrix} \psi_P \\ \psi_Q \end{pmatrix} \tag{1.5}$$

Writing out the matrix equation as two equations explicitly and eliminating $|\psi_Q\rangle$ yields

$$H_{PP} |\psi_P\rangle + H_{PQ} \frac{1}{E - H_{QQ}} H_{QP} |\psi_P\rangle = E |\psi_P\rangle \tag{1.6}$$

and therefore

$$\tilde{H}^c = H_{PP} + H_{PQ} \frac{1}{E - H_{QQ}} H_{QP}. \tag{1.7}$$

Assuming that the system is predominantly in the subspace spanned by $|\psi_P\rangle$ and additionally that the hopping is very small, $t \ll V_0$, we can approximate $E \approx V_0$. We write out the matrix multiplications and use $H_{PP} = (V_0)_{ii} \delta_{ij}$, $H_{PQ} = (-t)_{ij}$, and so on. The effective Hamiltonian becomes

$$\begin{aligned}
 \tilde{H}_{ij}^c &= (V_0)_{ii} \delta_{ij} + (-t)_{ik} (V_0 - V_1)_{kk}^{-1} (-t)_{kj} \\
 &= (V_0)_{ii} \delta_{ij} - \left(\frac{4t^2}{\Delta V} \right)_{ij}.
 \end{aligned} \tag{1.8}$$

As the system remains unchanged upon adding a constant term to the Hamiltonian, we can subtract the constant diagonal term $\tilde{H}_{ii} = V_0 - \frac{4t^2}{\Delta V}$, and arrive at

$$\tilde{H}^c = \begin{pmatrix} 0 & -\frac{4t^2}{\Delta V} \\ -\frac{4t^2}{\Delta V} & 0 \end{pmatrix}. \tag{1.9}$$

The off-diagonal matrix elements are the effective hopping, transitioning the system between its two states $|1\rangle \leftrightarrow |2\rangle$. If we now compare this matrix with the transverse field term of the Ising model, where we use the basis $|\downarrow\rangle \doteq |1\rangle$ and $|\uparrow\rangle \doteq |2\rangle$,

$$\begin{aligned}\tilde{H}^c &= -\gamma S_k^x \\ &= -\frac{1}{2}\gamma (S_k^+ + S_k^-) \\ &= \begin{pmatrix} 0 & -\frac{1}{2}\gamma \\ -\frac{1}{2}\gamma & 0 \end{pmatrix},\end{aligned}\tag{1.10}$$

we identify the effective hopping as the transverse field γ

$$\gamma = \frac{8t^2}{\Delta V}.\tag{1.11}$$

The effective hopping γ is a virtual process, involving two hopping processes in the original bond model, yielding the t^2 in the numerator of the expression for γ , and an interim high-energy state gapped out by ΔV , hence the ΔV in the denominator. To arrive at the expression for the effective hopping we used the assumptions $\Delta V \gg T$ and $t \ll \Delta V$. As a reminder, $\Delta V = V_1 - V_0 = \frac{2-\sqrt{2}}{2}\frac{1}{a} \approx 0.3V_1$. Notably, the energy gap is independent of the compensation charge q . As the derivation used only a single cell, it is also implicitly assumed that the perturbations from other cells in the system are small, at least as far as the effective hopping is concerned. If the hopping depended on nearby cells' state, then the effective Hamiltonian would be much more involved and certainly could not be mapped to an Ising-like model.

We have successfully derived an effective hopping term and therefore also an effective two-state model for the QCA Hamiltonian. With only two states per cell the Hilbert space scales as $N_s = 2^{N_c}$ (N_c the number of cells) and up to 14 cells are computationally feasible, with memory requirements of 2GB. In practice we restrict the calculations to a maximum of 12 or 13 cells. For our calculations we can use the two-state approximation with the effective hopping term, but still retain the original cell-cell interaction term H_{kl}^{cc} . Summing up all cell-cell interactions exactly is no problem for the relatively small system sizes accessible with exact diagonalization. Thus, from a computational point of view, nothing is gained by expressing the cell-cell interaction as an Ising interaction. However, deriving J_{kl} from H_{kl}^{cc} is very rewarding conceptually and enables us to properly map the QCA approach to an Ising model. Additionally, an analytical expression for J_{kl} will already allow some key insights into the characteristics of QCA devices. Therefore, we now undertake the derivation of an approximate expression for J_{kl} via a multipole expansion. The obvious

starting point is the cell-cell interaction term H_{kl}^{cc} ,

$$\begin{aligned} H_{kl}^{cc} &= \sum_{\substack{i \in k \\ j \in l}} V_{ij} (n_i - q) (n_j - q) \\ H_{kl}^{cc} &= \sum_{\substack{i \in k \\ j \in l}} \frac{(n_i - q) (n_j - q)}{|\mathbf{R}_{kl} + \mathbf{r}_j - \mathbf{r}_i|} \\ &= \sum_{\substack{i \in k \\ j \in l}} \frac{n_i n_j - q(n_i + n_j)}{|\mathbf{R}_{kl} + \mathbf{r}_{ij}|}, \end{aligned} \quad (1.12)$$

where i and j sum over the four dots $1 \dots 4$ of cell k and l , respectively, \mathbf{R}_{kl} denotes the vector between the centres of the cells, see Fig. 1.2(a). We have introduced $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ and dropped the constant q^2 term. There are only four possible configurations for two interacting cells, $\uparrow\uparrow$, $\downarrow\downarrow$, $\uparrow\downarrow$, and $\downarrow\uparrow$, and we can calculate their energies explicitly. For example, with the shorthand notations $V_{ij} = \frac{1}{|\mathbf{R}_{kl} + \mathbf{r}_{ij}|} + \frac{1}{|\mathbf{R}_{kl} - \mathbf{r}_{ij}|}$ and $V_{00} = \frac{1}{|\mathbf{R}_{kl}|}$, the Coulomb energy for two spin-up cells is written

$$E^{\uparrow\uparrow} = 2(1 - 2q)[V_{00} + V_{24}] - 2q[V_{12} + V_{14}]. \quad (1.13)$$

The energy for two spin-down cells can be obtained simply by rotating the system by 90° and thus by permutating the dot numbering in the expression above, $2, 3, 4, 1 \rightarrow 1, 2, 3, 4$. Using symmetries, for example $V_{43} = V_{12}$, we arrive at

$$E^{\downarrow\downarrow} = 2(1 - 2q)[V_{00} + V_{13}] - 2q[V_{12} + V_{14}]. \quad (1.14)$$

The remaining two configurations' energies can be calculated similarly and we find $E^{\uparrow\downarrow} = E^{\downarrow\uparrow}$, which, given the highly symmetric geometry of the cell arrangement, does not come as a surprise. But crucially, in general we have $E^{\uparrow\uparrow} \neq E^{\downarrow\downarrow}$. Therefore we have a system with three distinct energy levels which we cannot hope to represent with the solely two-level Ising term $J_{kl} S_l^z S_l^z$. Instead, let us try to map to a *modified* Ising model with a three-level cell-cell interaction term of the form

$$\tilde{H}_{kl}^{cc} = J_{kl} S_k^z S_l^z + J'_{kl} (S_k^z + S_l^z). \quad (1.15)$$

For this Hamiltonian we have the energies

$$\tilde{E}^{\uparrow\uparrow} - \tilde{E}^{\uparrow\downarrow} = 2J_{kl} + 2J'_{kl} \quad (1.16)$$

$$\tilde{E}^{\downarrow\downarrow} - \tilde{E}^{\uparrow\downarrow} = 2J_{kl} - 2J'_{kl} \quad (1.17)$$

which yields

$$J_{kl} = \frac{1}{4} (\tilde{E}^{\uparrow\uparrow} + \tilde{E}^{\downarrow\downarrow} - 2\tilde{E}^{\uparrow\downarrow}) \quad (1.18)$$

$$J'_{kl} = \frac{1}{4} (\tilde{E}^{\uparrow\uparrow} - \tilde{E}^{\downarrow\downarrow}). \quad (1.19)$$

To map the bond cell-cell interaction H_{kl}^{cc} to the modified Ising interaction term we identify $E^{\uparrow\uparrow} = \tilde{E}^{\uparrow\uparrow}$, $E^{\downarrow\downarrow} = \tilde{E}^{\downarrow\downarrow}$, and so on. The newly introduced J'_{kl} term tracks the difference between $E^{\uparrow\uparrow}$ and $E^{\downarrow\downarrow}$. Going back to the expressions (1.13) and (1.14) we realize that for $q = \frac{1}{2}$ —charge neutral cells—they *do* become equal, $E^{\uparrow\uparrow} = E^{\downarrow\downarrow}$, and therefore $J'_{kl} = 0$. This is an important result: Only for charge neutral cells does the QCA model map to a genuine, unmodified transverse field Ising model.

To obtain concrete expressions for J_{kl} and J'_{kl} we do a multipole expansion of $E^{\uparrow\uparrow}$, $E^{\downarrow\downarrow}$, $E^{\uparrow\downarrow}$, and $E^{\downarrow\uparrow}$. Specifically,

$$\begin{aligned} \frac{1}{|\mathbf{R}_{kl} \pm r_{ij}|} &= \frac{1}{R} \left(1 \pm 2 \frac{\mathbf{r}_{ij} \cdot \hat{\mathbf{R}}}{R} + \frac{r_{ij}^2}{R^2} \right)^{-1/2} \\ &= \frac{1}{R} (1 \pm x + y)^{-1/2} \end{aligned} \quad (1.20)$$

is Taylor-expanded in x and y , keeping all terms up to $\mathcal{O}\left(\frac{a^4}{R^5}\right)$ which corresponds to quadrupole-quadrupole interactions. Plugging the multipole-expanded energies into Eq. (1.18) yields the final expressions

$$J_{kl} = \frac{1}{32} (9 - 105 \cos 4\theta) \frac{a^4}{R_{kl}^5} \quad (1.21)$$

$$J'_{kl} = (1 - 2q) \left(\frac{3}{2} \sin 2\theta \frac{a^2}{R_{kl}^3} + \frac{5}{4} \sin 2\theta \frac{a^4}{R_{kl}^5} \right). \quad (1.22)$$

We have successfully mapped the QCA bond Hamiltonian (1.1) to a modified transverse field Ising model

$$\tilde{H} = - \sum_k \gamma S_k^x + \sum_{k < l} [J_{kl} S_k^z S_l^z + J'_{kl} (S_k^z + S_l^z)], \quad (1.23)$$

which reduces to a genuine Ising model, $J'_{kl} = 0$, in the case of charge neutral cells, $q = 0$.

These results are remarkable in two ways. First, J_{kl} does not depend on the compensation charge q . In turn, the Ising interaction $J_{kl} S_k^z S_l^z$ is independent of the cell net charge and represents only the quadrupole-quadrupole interaction, falling off as $J_{kl} \sim R_{kl}^{-5}$. Second, the J'_{kl} term does depend on the compensation charge but vanishes for $q = \frac{1}{2}$, that is, charge neutral cells. For charge neutral cells QCA therefore maps directly to a normal (unmodified) Ising model.

We can also look at the angle dependence of the interactions. The J_{kl} term is symmetric under rotations by 90° —which is what we expect intuitively—whereas the J'_{kl} is symmetric under rotations by 180° . Thus, by slowly turning on J'_{kl} (by, for example, going from charge neutral to effectively negatively charged cells $q = \frac{1}{2} \rightarrow q = 0$), we break the 90° rotational invariance. It is important to note that the J'_{kl} term also breaks the symmetry between

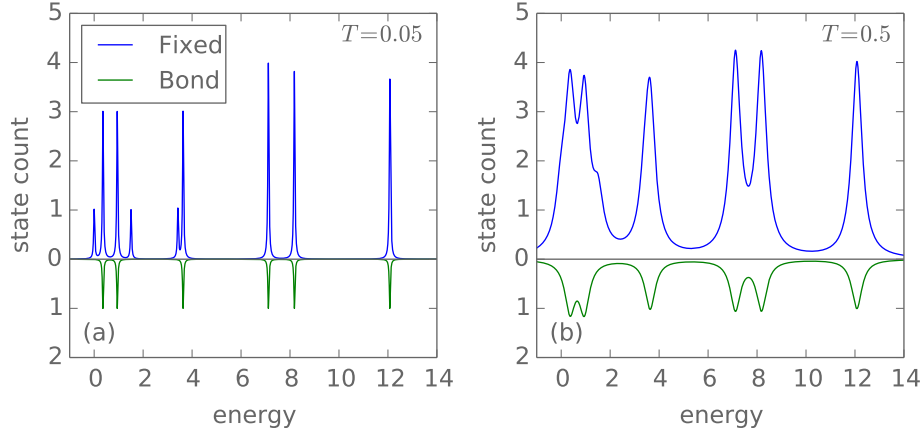


Figure 1.3: Low-energy density of states of a one cell QCA system for both the *fixed charge* and the *bond* model. The *bond* approximation does not reproduce the singlet-triplet splitting.

spin up and spin down cells. For $J'_{kl} \neq 0$, $\uparrow\uparrow$ and $\downarrow\downarrow$ have different energies and therefore also different polarization responses. For a practical implementation this is definitely not what we want! At the angles $0^\circ, 90^\circ$, and 270° J'_{kl} vanishes, so here we have a pure Ising interaction even for $q \neq 0$. Conversely, J_{kl} also vanishes at select angles, rendering the system bare any interaction for charge neutral cells, at least within the limits of our multipole expansion.

1.4 Validity of the approximations

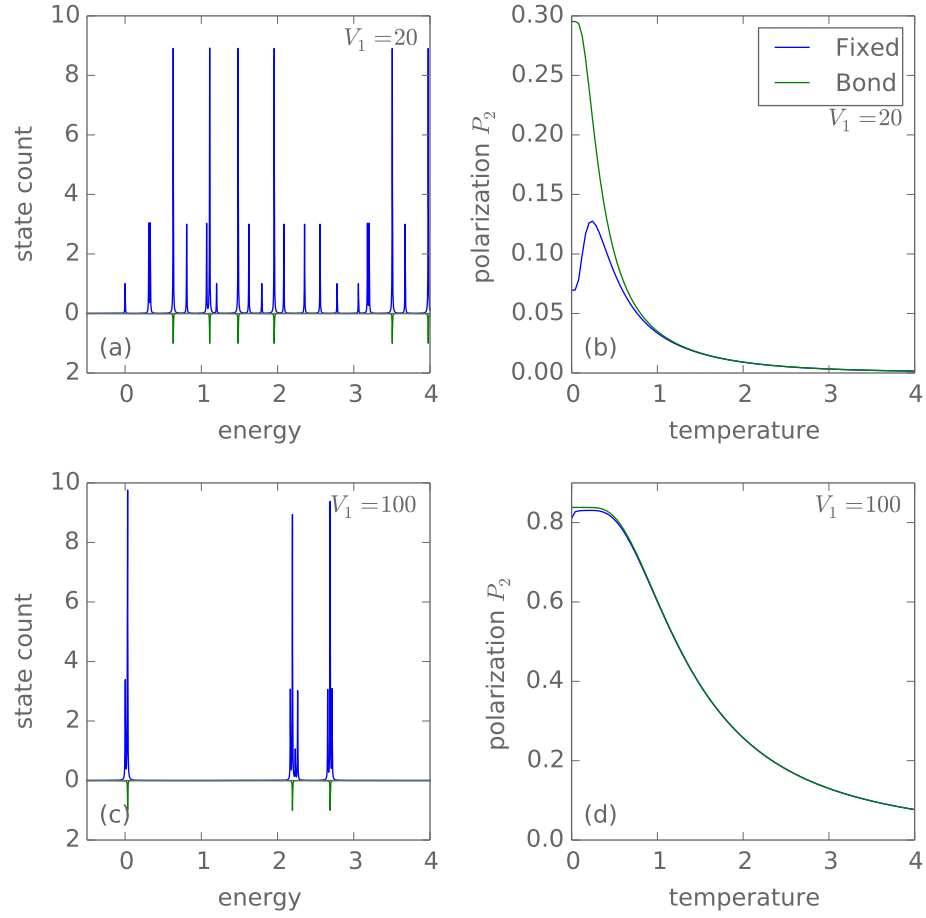


Figure 1.4: The two cell *fixed charge* and *bond* systems at $V_1 = 20$ and $V_1 = 100$. (a)(c) Low-energy density of states. (b)(d) Output polarization P_2 over temperature. For a small Coulomb repulsion the density of states curves look qualitatively very different (a) and the *bond* approximation does not work very well (b). At a larger Coulomb repulsion the density of states curves look much more alike (c) and the *bond* approximation works much better (d).

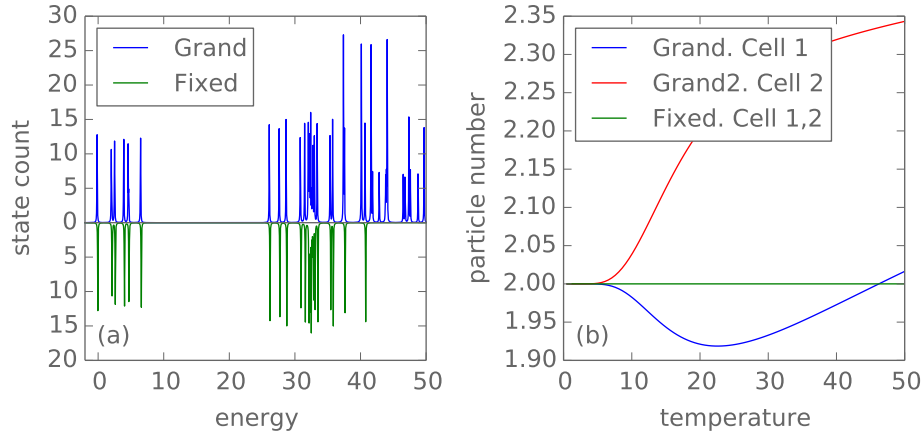


Figure 1.5: (a) Low-energy density of states of the exact *grand canonical* and the approximate *fixed charge* two cell QCA system. For small energies the curves agree perfectly (up to $E \lesssim 35$). (b) Particle number per cell over temperature for the same two cell system. The curves diverge for $T \gtrsim 5$.

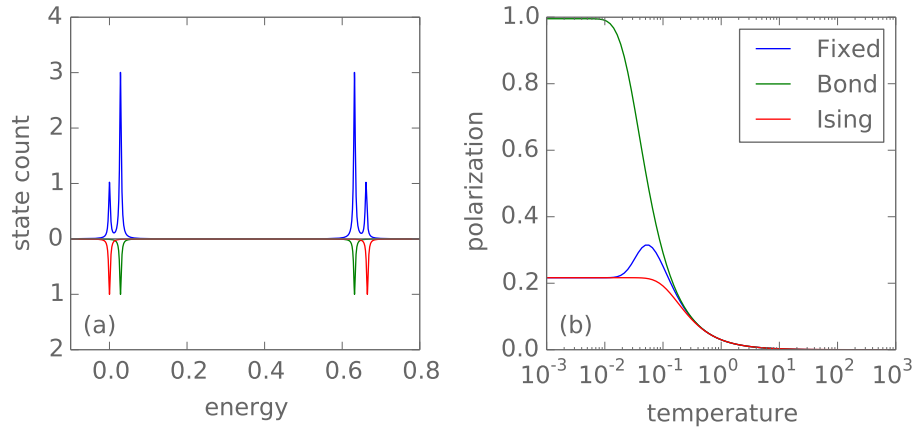


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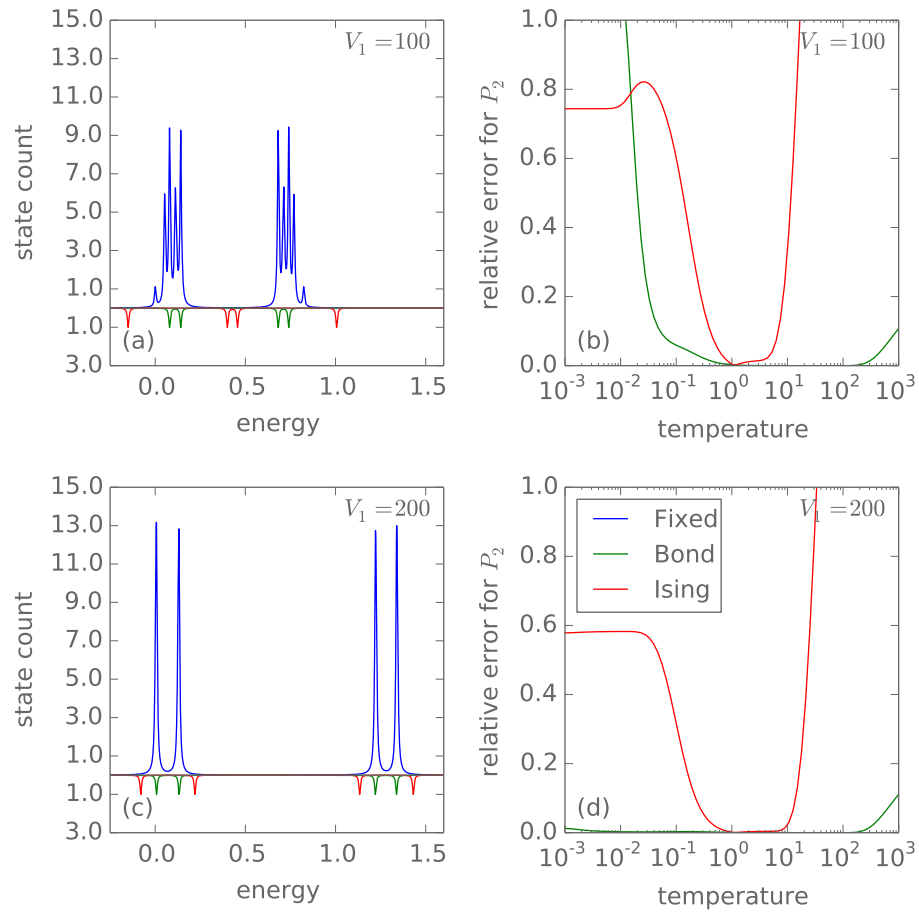


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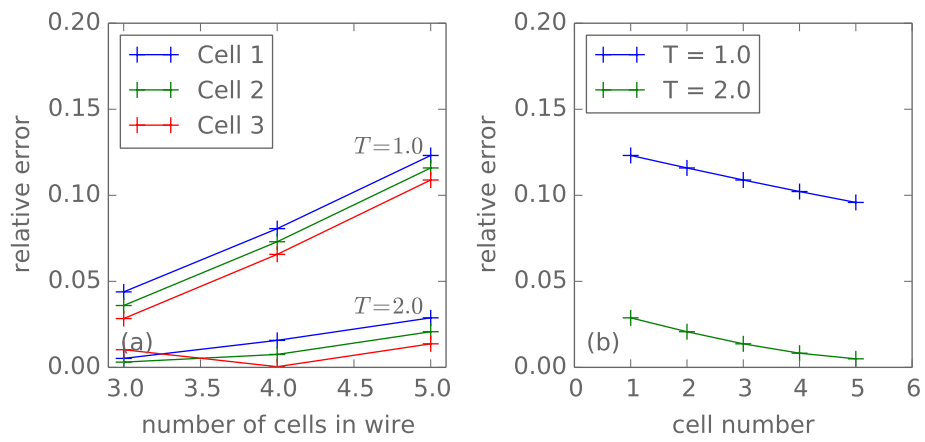


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