Long range coupling between Spin Qubits

by

Simon Schaal

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The Faculty of Mathematics, Computer Science and Natural Sciences at RWTH Aachen University
Department of Physics, Institute II C

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supervised by
Prof. Hendrik Bluhm, PhD
Robert McNeil, PhD
Statement of authorship

Ich versichere, dass ich die Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt sowie Zitate kenntlich gemacht habe.

Aachen, den
Contents

1 Introduction 1
   1.1 Motivation ................................................. 1
   1.2 Outline ................................................ 3

2 Background 5
   2.1 Experimental background ............................... 5
      2.1.1 GaAs/AlGaAs heterostructure ................. 5
      2.1.2 Spin Qubits ...................................... 7
      2.1.3 Pre-existing work / Methods of coupling ...... 8
   2.2 Theory and Simulation .................................. 10
      2.2.1 Electrostatics .................................. 10
      2.2.2 Finite elements method ......................... 11
      2.2.3 COMSOL Multiphysics® .......................... 13

3 Simulations 15
   3.1 Simple toy model ..................................... 15
      3.1.1 Simple model .................................. 15
      3.1.2 Positioning the coupler with respect to the qubit . 17
      3.1.3 Coupler paddle size ............................. 19
      3.1.4 Height of the coupler ......................... 20
   3.2 Coupling two qubits .................................. 20
      3.2.1 Electrostatic gates ............................. 21
      3.2.2 The 2DEG and the GaAs substrate ............. 22
      3.2.3 Removal of the 2DEG and GaAs beneath the coupler ... 23
      3.2.4 Full model ..................................... 24
      3.2.5 Coupler paddle variations ..................... 25
      3.2.6 Induced 2DEG ................................. 26
3.3 Coupling multiple qubits ........................................... 27
  3.3.1 Two couplers per control qubit dot ......................... 27
  3.3.2 One coupler per control qubit dot ......................... 29
  3.3.3 Coupler paddle shape ....................................... 32
  3.3.4 Intercoupler coupling ....................................... 34
  3.3.5 Network of qubits ........................................... 39
  3.3.6 RF gates .................................................. 42

4 Summary ....................................................... 47

A Appendix ..................................................... 1
  A.1 Domain boundaries (COMSOL infinite elements) ............ 1
  A.2 Meshing in COMSOL .......................................... II
  A.3 Dependence of qubit coupling on the coupler area ........ III

Bibliography ..................................................... VII

List of Figures ................................................ XI

List of Tables .................................................. XIII
1 Introduction

1.1 Motivation

One of the most significant scientific developments in science of the 20th century is the theory of quantum mechanics. Over the last two decades, there has been remarkable experimental progress in the minimization and fabrication of solid state structures allowing to study and control quantum effects (such as superposition of states and entanglement).

Quantum bits (qubits), which are controllable quantum mechanical two level systems, form the fundamental basis of quantum information. In quantum computation the use of entanglement and superposition ($|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$) lead to enormous potential computational power through quantum parallelism allowing to store a complete $2^n$ dimensional Hilbert space in a system of $n$ qubits. This results in an exponential speed up with the number of qubits for quantum algorithms [1] and quantum simulations. Well-tailored quantum algorithms are needed that make use of the increased computational power and allow simultaneous extraction of information, as measurements of a qubit necessarily collapse the state from a superposition to a basis state ($|0\rangle$ or $|1\rangle$). Several quantum algorithms exist which fulfil these criteria (e.g. Shor Algorithm, Grover's search algorithm).

The spin of an electron localised in a quantum dot (in a GaAs/AlGaAs heterostructure for example) is one of the most promising realisations of a qubit for building a quantum computer. The electron spin interacts weakly with the environment, thus spin qubits show long decoherence times [2], which is the third of the five DiVincenzo criteria for universal quantum computation [3]. In addition to that, initialisation into a known state (II), universal quantum control via gates (IV), and a state readout with high fidelity is required (V). The spin of one electron can be used to form a single qubit, however singlet-triplet qubits ($S$-$T_0$ qubits) based of two quantum dots, each with one electron inside, show promising results. Fast electrical control and read-out is possible (no magnetic
fields are required) while the $S-T_0$ qubit still benefits from the long dephasing times of traditional spin qubits (see Sec. 2.1.2).

This work contributes to the first DiVincenzo criterion that has not been mentioned yet: scaling up the system to many reliably functioning qubits. A fundamental ingredient of any quantum computer is entanglement. Experiments so far have relied on nearest neighbour coupling only (see Sec. 2.1.3). Long-range coupling to distant dots (as suggested and modelled in the work of Trifunovic et al. [4]) could create two-dimensional (2D) arrays of qubits. This would give access to many benefits as an improvement in fault tolerant quantum computation and would enable entangling gate operations between distant qubits in one step, leading to more efficient algorithms. Error correction has to be considered during the computation to achieve fault tolerant quantum computation [5] as the qubit control is not free of noise. The detection of errors like a spin or phase flip can be done by copying the qubit information into other qubits. Quantum states cannot be copied (no-cloning theorem) but quantum error correction (reduction) is achieved by spreading the information of one qubit onto a highly entangled state of multiple qubits. Obviously, error correction increases the algorithm runtime since more qubits and gate operations are required but it does not grow exponentially with the problems size maintaining the quantum computation speed-up. Successful error correction requires the error rate to be below some constant threshold value (e.g, that no additional errors occur during the correction process). The most promising error correction codes make use of 2D arrays of qubits achieving error correction thresholds of $10^{-2}$ to $10^{-1}$.

The aim of this work is to further analyse and simulate the mediated electrostatic long-distance coupling via floating metal gates, introduced by Trifunovic et al. [4] which showed promising results. At first the work done by Trifunovic et al. [4] is confirmed while having a further look at every effect of the sample and setup. Then the coupling to multiple qubits is studied because this is an important step to build up two dimensional arrays leading to more efficient algorithms as described in the previous paragraph. Several variations are performed to find an optimal design.
1.2 Outline

The thesis is divided into three chapters. First experimental background about the sample (semiconducting heterostructure) and spin qubits is given, followed by theoretical background covering electrostatics and the simulation software.

The second chapter (body of the work) deals with the simulations and analysis of the coupling between two or more qubits via a floating metal gate (the coupler). This chapter shows a modular structure and where possible factors and trends are extracted to characterise the different effects.

The last chapter summarises the results and gives an outlook and suggestions for future work. An appendix gives further information and tips on the simulation software (COMSOL Multiphysics).
2 Background

In this chapter a description of the experimental and theoretical background is given.

2.1 Experimental background

In this work the coupling between spin qubits in a GaAs/AlGaAs heterostructure is simulated. Hence, this section introduces the experimental background of spin qubits and illustrates how they are generated in a GaAs/AlGaAs heterostructure.

2.1.1 GaAs/AlGaAs heterostructure

To create quantum dots as the basis of spin qubits, electrons have to be confined in all three dimensions (on a length scale comparable to their spread of wavefunction). To achieve this, the first step is to form a two dimensional electron gas (2DEG) where the electrons are only free to move in two directions. A 2DEG can be generated at the interface of two semiconductors with different band gaps. This is called a heterostructure and an example is shown Fig. 2.1b.

---

1 one of the first realisations was done by Petta et al. [6]
GaAs and AlGaAs are used because they have practically identical lattice constants that allows clean growth and electrostatic gates can easily be placed on top (electron beam lithography). The band gap of AlGaAs is bigger than the band gap of GaAs which results in a step of the conduction band at the interface. Introducing a (Si) donor in the AlGaAs layer results in a band bending and causes the conduction band the dip below the Fermi level \( E_F \) (dashed line) at the interface (with a proper choice of parameters) as seen in Fig. 2.1b. Being confined in the triangular potential below the Fermi level makes the electrons behave like two dimensional objects. Local depletion of electrons is achieved by applying a negative voltage (with respect to the 2DEG) to the electrostatic gates. This allows to create a double well potential as seen in Fig. 2.1c to confine electrons in the remaining directions. The confinement leads to discrete energy levels resulting in the quantum dot.

For the simulation typical dimensions of each part of the experimental setup are relevant. The dielectric constant (relative permittivity \( \varepsilon_r = 13 \)) of GaAs is also one important factor because it strongly influences the capacitive coupling strength.

From experimental setups [6, 9, 10] the following dimensions are taken.
2.1 Experimental background

<table>
<thead>
<tr>
<th>parameter</th>
<th>typical value</th>
</tr>
</thead>
<tbody>
<tr>
<td>dot diameter and centre to centre separation</td>
<td>100 nm</td>
</tr>
<tr>
<td>gate width and height</td>
<td>40 nm</td>
</tr>
<tr>
<td>2DEG position below the surface</td>
<td>100 nm</td>
</tr>
<tr>
<td>2DEG thickness</td>
<td>5 nm</td>
</tr>
</tbody>
</table>

Table 2.1: Typical heterostructure dimensions.

2.1.2 Spin Qubits

A single electron spin provides a two level system which can be used to form a qubit. Because of weak coupling to the environment, it shows long coherence times (compared to charge qubits). AC-magnetic fields are required to manipulate the spin. By splitting up the two spin states using a magnetic field (Zeeman splitting: \( H = -\mu \cdot B \)) a single shot readout can be performed (see [11] Fig. 15).

This work focuses on \( S-T_0 \) qubits consisting of two quantum dots motivated by several advantages. Two spins couple to a total spin of \( S = 0 \) or \( S = 1 \) which results in 4 spin states [12]. The \( M = 0 \) states are used as the computational basis resulting in further decoupling from the environment because they aren’t affected by changes in magnetic fields.

\[
|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \text{antisymmetric} \tag{2.1}
\]

\[
|T_0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad \text{symmetric} \tag{2.2}
\]

\[
|\psi\rangle = \cos \left( \frac{\theta}{2} \right) |S\rangle + e^{i\phi} \sin \left( \frac{\theta}{2} \right) |T_0\rangle \tag{2.3}
\]

As the \( M = \pm 1 \) states split off by an external magnetic field an effective two level system remains. The state of a qubit is usually visualised by a three-dimensional vector in a unit sphere called a Bloch sphere (2.3). The \( S-T_0 \) qubit allows quick electric manipulations and operations. Rotations along the \( z \) axis of the Bloch sphere are driven by the exchange splitting \( J(\varepsilon) \) and rotations along the \( x \) axis by a nuclear magnetic field gradient \( \Delta B_z \)\(^1\) leading to universal quantum control [13]. Furthermore, the state read-out is also done

\(^1\) \( S-T_0 \) subspace Hamiltonian: \( H = \frac{\Delta B_z}{2} \sigma_z + \frac{J(\varepsilon)}{2} \sigma_x \), where \( \sigma_i \) are the Pauli matrices
electrically and described in the following. Considering tunnel coupling between the quantum dots of the $S$-$T_0$ qubits, the two electrons could occupy both dots (1,1) or only one dot (0,2) where (left,right) denotes the occupancies in the double quantum dot. Because of Pauli’s exclusion principle the triplet will always stay in the (1,1) state (see Sec. 2.1.3). Applying a voltage $\varepsilon > 0$ (called detuning) to the RF gates (see Fig. 2.1a) controls the relative difference of the energy levels in the left and right dot and so the transition from the (1,1) to the (0,2) charge state. This enables measurements of the qubit state by a spin-to-charge conversion using either a simple tunnel barrier (quantum point contact, QPC) or a sensor quantum dot (SQD, shown in Fig. 2.1a) (see [14] for further details). The sensor conduction which depends on the charge distribution at the nearby dot directly reflects the qubit state. This is significantly easier than measuring the spin directly. Besides the read-out the detuning $\varepsilon$ also enables the preparation of the qubit in a known state ($|S\rangle$) by quickly applying a detuning $\varepsilon > 0$ and manipulations via quantum gates which are done while $\varepsilon < 0$ confining the subspace to the (1,1) charge states.

2.1.3 Pre-existing work / Methods of coupling

Spin qubits show promising results in scalability and miniaturisation for building a quantum processor, however the weak interaction with the environment makes interqubit operations challenging, while leading to long coherence times. This section summarises the effect of Coulomb and spin blockade followed by the different ways of coupling.

A quantum dot contains electrons and, via tunnel coupling, electrons can be exchanged. Capacitive coupling to gate electrodes can be used to tune the electrostatic potential (and energy levels) of the dot.

Coulomb blockade

There are discrete single-particle energy levels in the dot caused by confinement. Tunnelling from a source lead into the dot is only possible if there are empty dot states below the chemical potential at the source, and they can only leave the dot if there are empty states in a drain lead at the energy of the dot state. Using capacitively coupled gates, the levels in the dot can be pushed up and down showing peaks in conductance every time a new state falls within the source-drain tunnelling window $^1$.

---

$^1$ Coulomb blockade peaks, see [11] for more details
Spin blockade

In GaAs the spin states of an electron are degenerate in the absence of a magnetic field. The Zeeman splitting and Pauli’s exclusion principle lead to a spin blockade in a double quantum dot. Given a spin that cannot tunnel out of the dot, an anti parallel spin could tunnel into this dot and through to the reservoir. A parallel spin would have to move into a higher state (Pauli’s principle), and cannot enter the dot. The system remains spin blocked until a spin flip occurs [15].

Neighbouring dots

Intraqubit coupling between neighbouring dots can be achieved by the spin or charge degree of freedom. The exchange coupling between the electron spins in neighbouring dots was demonstrated to be successful in preliminary work [6, 16]. Exchange coupling involves the spin (and wavefunction) and is related to the Pauli exclusion principle and an output of the Fermi statistics: the total wave function for identical fermions is antisymmetric when exchanging the particles. This leads to an exchange energy where parallel spins for two electrons are energetically preferred because the electrons are further away from each other (Pauli repulsion, direct exchange interaction Hamiltonian in solids: \( H = \frac{J}{2} s_1 \cdot s_2 \)). The exchange interaction and the spin blockage allow the read-out mechanism described in Sec. 2.1.2 but these effects are short ranged therefore they are mostly used for single-qubit control or two qubit-gates for single spins.

Distant dots

Distant dots can only couple via charge states (capacitively), however the spins are not decoupled from the charge degree of freedom. The main feature is the spin-orbit interaction (SOI). A combination of SOI and long-ranged Coulomb interaction enables electrical control for both single- and two-qubit operations (where the state of one qubit is dependant on the state of the other) in the absence of tunnel coupling [17–19]. The spins are entangled and the coupling between them can be switched on and off without the need of overlapping wave functions.

Entanglement of electrostatically coupled S-T0 qubits has been experimentally shown by Shulman et al. [7] see Fig. 2.1a for their design. The different charge profiles of the \( |S\rangle \) and \( |T_0\rangle \) state allow a dipole-dipole coupling which can generate entangled states since
the $S$-$T_0$ qubit control is done via electric fields. At large distances, the Coulomb interaction is screened by electrons of the 2DEG and the metal gates, thus long-distance coupling cannot be achieved by direct Coulomb interaction. Strong capacitive coupling and control between quantum dots via a floating interdot metallic capacitor has been demonstrated [20]. Based on these experimental results Trifunovic et al. [4] presented a new approach of long-distance spin-spin coupling via a floating metal gate (coupler) where long-range coupling is achieved that shows coupling strengths above the spin-decay rates. They also present designs for future qubit arrays. Another approach [21] shows that two distant quantum dots can be directly tunnel coupled (tunnel coupling decreases exponentially) mediated by virtual occupation of an intermediate site over long distances but not nearly as long as seen with a electrostatic coupler.

2.2 Theory and Simulation

This section recaps the basics of electrostatics, and then explains how electrostatic problems are solved with the COMSOL Multiphysics software using the finite elements method (FEM). Although a qubit is a quantum system, the $S$-$T_0$ qubits can be controlled, manipulated, coupled and read out via electric fields only. This allows a purely electrostatic approach which is described in this chapter.

2.2.1 Electrostatics

The theory of electrostatics is the most relevant in this project as spin qubit control is achieved by electric fields and the qubit states are distinguished by different charge states. The Maxwell equations are a set of partial differential equations (PDE’s) that form the foundation of classical electrodynamics. The following shows the time independent macroscopic equations of electrostatics [22].

\[ \nabla \cdot D = \rho \]  \hspace{1cm} (2.4)

\[ \nabla \times E = 0 \]  \hspace{1cm} (2.5)

\[ D = \varepsilon_0 \varepsilon_r E = \varepsilon_0 E + P \]  \hspace{1cm} (2.6)
2.2 Theory and Simulation

\( D \) is the electric displacement, \( E \) is the electric field and \( P \) the dielectric polarization density. \( \varepsilon_0 \) and \( \varepsilon_r \) are the vacuum and the relative permittivity and \( \rho \) is the space charge density. The first equation forms Gauss’ law and the second equation yields to \( E = -\nabla V \) with the electrostatic potential \( V \). In this case, the potential can be considered to be static as the external time scale is very long compared to the charge relaxation times. The best approach is to solve the electrostatics using the potential \( V \) because the charge distribution can be considered as a given model input. Combining the two equations yields to the Poisson equation for the electrostatic potential \( V \) which is solved within the Electrostatics Interface of the AC/DC Module of COMSOL [23].

\[
-\nabla \cdot (\varepsilon_0 \nabla V - P) = \rho
\]

(2.7)

\[
\Delta V = -\frac{\rho}{\varepsilon_0 \varepsilon_r}
\]

(2.8)

It can be shown that the Poisson equation has an explicit solution for Dirichlet (where the potential is given at the boundaries of the domain: \( V = g \)) and Neumann boundary conditions (where the derivative in the normal direction of the boundaries is given: \( \frac{\partial V}{\partial n} = g \), in this case a irrelevant constant can be added) [24].

At a interface between two media (medium 1 and medium 2) the following field continuity condition has to be met [25],

\[
n_2 \cdot (D_1 - D_2) = \rho_s
\]

(2.9)

where \( n_2 \) is the unit vector normal to the interface pointing into medium 1 and \( \rho_s \) is the surface charge density. In the absence of surface charges (\( \rho_s = 0 \)) this turns into the natural boundary condition.

Because the Maxwell and Poisson equations consist of linear operators (derivatives), the electric field and the electric potential follow the principle of superposition. This allows to set the gates that confine the quantum dots to zero within the simulations.

2.2.2 Finite elements method

COMSOL uses the FEM to numerically solve a PDE problem. The FEM is associated with variational (Ritz), a functional has to be minimized, and residual (Galerkin) methods while both lead nearly to the same equations. Equation (2.8) with given boundary values is known as the strong form of an elliptical boundary value problem. To derive a functional
we want to introduce the weak form. Every problem in COMSOL is converted to the weak form in order to be solved using the FEM. Consider a stationary PDE problem (adapted from [26])

$$-\Delta u = f \quad \text{in } \Omega$$

(2.10)

where $\Omega$ is the domain in which the Poisson equation has to be solved. Let $v$ be an arbitrary test function. Multiplying the PDE by $v$ and integration and application of Green’s law results in

$$\int_{\Omega} fvdx = \int_{\Omega} -\Delta uvdx$$

(2.11)

$$= \int_{\Omega} \nabla u \cdot \nabla vdx$$

(2.12)

for all test functions $v$. Using the following notation shows the association to the linear functional $F$

$$F(v) := \int_{\Omega} fvdx, \quad a(u,v) := \int_{\Omega} \nabla u \cdot \nabla vdx.$$  (2.13)

The weak form requires less regularity of $u$ and the variation principle is more fundamental. Now we have to find the solution $u \in H$ that fulfils $a(u,v) = F(v)$ for every $v \in H$ ($H$ is a Hilbert space). The idea behind the FEM is to solve the variation problem in a finite dimensional sub-domain $H_h \subset H$ because it is very difficult to find test functions that approximately represent the true solution over the entire domain.

This discretisation relies directly on the fundamental variational principle and not on the PDE problem. The small regions (for example a triangle in 2D or a tetrahedral in 3D) are the finite elements and the points defining them are called nodes (degrees of freedom) while the assembly of the elements is called mesh [27]. As the solution often doesn’t vary much in a small sub domain polynomials are commonly used as

![Figure 2.2: Example mesh created by COMSOL (extra fine) for the model used in section 3.2.4.](image)
test functions. The solutions in the sub domains have to fulfil continuity conditions with the next element at the nodes or edges. Because the sub-domains have a finite dimension, a (nodal) basis can be chosen which leads to a system of \( m = \dim H_h \) equations and unknown variables. These can be solved for each element with respect to the given boundary conditions (e.g. Gauss algorithm). Solving each element gives the solution of the entire domain. With a finer mesh the solution becomes more accurate but it increases the degrees of freedom and hence the calculation time. The FEM allows the mesh to be adjusted to the model geometry which is necessary to acquire a good solution. Meshing can be difficult especially at sharp edges the (see Fig. 2.2). The following summarises the ideas behind the FEM.

\[
PDE \text{ problem (2.8) } \xrightarrow{weakform} \text{ variational problem (2.13) } \xrightarrow{FEM} \text{ system of linear equations } Kx = g
\]

2.2.3 COMSOL Multiphysics®

This work has been done with COMSOL Multiphysics 4.2a using the AC/DC Module which provides an environment which simulates electromagnetism in 2D and 3D. For the simulations only the Electrostatics Interface has been used. Charge conservation, zero charge and initial values (boundary condition) and associated properties as the relative permittivity \( \varepsilon_r \) are the main features.
3 Simulations

3.1 Simple toy model

3.1.1 Simple model

As an initial investigation of the parameters and their effect on the qubit coupling, a simple toy model has been used. This model consists of two discs representing the quantum double dots and a floating gate made of two metallic discs (paddles) connected by a thin wire. The coupling strength that comes from this toy model is not accurate but by getting closer to the experimental sample step by step the individual effect of each part can be shown. The effects can then be summarised in a final design to give more realistic values of the coupling strength (see Sec. 3.2.4).

![Diagram](image)

**Figure 3.1:** Simple toy model (a). Distance between the centres of the two coupler paddles (qubit separation $L$). Distance between the centre of the double dot and the centre of the paddle (qubit-paddle separation $a_x$). The radius of the coupler paddle disc $R$ and the height $d$ are indicated. One of the qubits acts as the control and the other as the target qubit. See Table 2.1 for dimensions. (b) Capacitive coupling sketch.
As introduced in [4], the coupling between two spin qubits is defined as the change of detuning $\varepsilon$ in one target qubit induced by the transfer of a full electron from one dot to the other dot in a control qubit. The discs representing the dots of the control qubit are set to have a $e^+$ and $e^-$ charge. The dots of the target qubit and the coupler are set to be floating with zero charge to measure the induced potential. Figure 3.1b shows a sketch of this capacitive coupling. In each qubit two electrons are trapped in the double-well potential and the qubits are coupled by a capacitor representing the coupler. The different charge states induce a detuning $\varepsilon$ at the coupled qubit.

The charged control dots induce an image charge of opposite sign in the coupler. An example of what this looks like at the simulation is shown Fig. 3.2. Figure 3.2a shows the potential at the level of the dots along the $x$-axis. One can easily identify the two dots with different charge on the left and how the coupler couples to the target dots on the right (see the enlarged view). Figure 3.2b shows the potential at the level of the coupler. A minimum caused by the left control dot is seen and followed by the constant potential of the coupler (as expected for metal).

For a simple parallel plate capacitor the following equations apply in general.
3.1 Simple toy model

\[ Q = C \cdot U \]  
\[ C = \varepsilon_0 \varepsilon_r \cdot \frac{A}{d} \]

Because the induced charge is fixed, the product of \( C \) and \( U \) is constant. That means that an increase in capacitance results in a decrease in voltage. The permittivity \( \varepsilon_r \), and the area \( A \), as well as the distance \( d \) affect the capacitance. These are the parameters that will be optimized in the upcoming sections. While strong coupling to the dots is required (high capacitance), the coupler should ideally have weak coupling to the other parts of the setup.

3.1.2 Positioning the coupler with respect to the qubit

The change in qubit coupling with respect to the relative \( x \) and \( y \) position of the coupler paddle was been confirmed to be a promising switching mechanism as shown by Trifunovic et al. [4]. A parametric sweep of the relative position of the control qubit is done while the rest of the setup stays fixed (see Fig. 3.3). The coupling strength to the target qubit is determined. This numerical analysis extends and confirms the analytical work done by Trifunovic et al. [4] by giving values for the coupling strength and by studying both \( x \) and \( y \) separations.
Figure 3.3: Parametric sweep of the qubit-paddle $x$- and $y$ separation taken from both the double dot and coupler paddle centre. The offset $a_{x,y}$ is normalised by the paddle radius $R = 90\,\text{nm}$.

The curve in Fig. 3.3a shows the sweep in the $x$ direction and it is not symmetrical because the centre of the dots is equal to the centre of the coupler paddle at the point $a_x/R = 0$. Thus, both of the dots induce an image charge at the coupler with different signs. The qubit qubit coupling does not reach zero at that point because the first dot also couples to the thin connection of the coupler (the thin connection alone provides a not insignificant coupling see Table 3.4). The curve reaches a maximum at approximately $a_x/R = 1.55$. At this point the coupler paddle ends at the edge of the close dot, thus the coupling of the second dot to the coupler is minimised while the coupling to the close dot is not reduced. With increasing $a_x/R$ the coupler moves away from the close dot. If the qubit coupler $x$ separation is increased from $1.5R$ to $2.5R$, the coupling is reduced by approx. 20%.

A similar parametric sweep in the $y$ direction is shown in Fig. 3.3b and gives as expected a symmetrical curve with a maximum at $a_y/R = 0$. Starting at the maximum at $a_y/R = 0$ the coupling first drops slowly and when the coupler is not directly above the dot any more the coupling drops more rapidly and seems to show a linear trend.

As suggested by Trifunovic et al. [4] this could be used as a switching mechanism if the dots are shifted by applying voltages to the surface gates.
3.1.3 Coupler paddle size

To show how the coupling depends on the change of the coupler paddle area, a parametric sweep of the coupler paddle disc radius has been performed. Besides an optimal coupler radius this analysis will give an understanding of how adjusting the paddle area may effects the qubit coupling for future multicouplers. Only the size of the control qubit paddle was changed during this variation to determine the change in coupling to the target qubit. With increasing radius, the coupler edge stayed fixed to the edge of the dot as shown in Fig. 3.4. This prevented a change of the qubit coupling caused by the paddle extending towards the second dot.

Increasing the area of the coupler paddle results in an increase in the capacitance. The qubit qubit coupling strength reaches a maximum for a paddle radius of 95 nm. Beyond this increasing the paddle area results in a decrease of the coupling because the additional area is far away from the coupler and so the main effect is due to an increase in the capacitance.

The following table summarises the results of the simple toy model parametric sweep optimisations.

<table>
<thead>
<tr>
<th>illustration</th>
<th>optimal separation $a_x$</th>
<th>optimal paddle disc radius $R$</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Illustration" /></td>
<td>140 nm</td>
<td>95 nm</td>
</tr>
</tbody>
</table>

Table 3.1: Results of the position and size parametric sweeps for the toy model.
3.1.4 Height of the coupler

A variation of the height $d$ of the the electrostatic coupler is the same as varying the 2DEG depth (distance to the heterostructure surface). A parametric sweep of the height $d$ has been performed and is shown in Fig. 3.5. Having the coupler close to the dots gives large coupling. Due to strain and defects close to the heterostructure surface the generation of the 2DEG and the dots inside could become more complicated and could result in increased noise. For $d > 50 \text{ nm}$ a reciprocal plot (which is not shown here) in $d$ is linear and gives the following proportionality for the qubit qubit coupling strength $C_{\text{QCQ}}$.

$$C_{\text{QCQ}} \propto 3.3 \cdot 10^4 \ \text{µeV nm} \cdot \frac{1}{d} \quad (3.3)$$

In typical experiments the 2DEG has been created at an interface approximately 100 nm below the surface. Figure 3.5 shows that moving the 2DEG closer to the surface could be one parameter to increase the mediated capacitive coupling where Eq. (3.3) indicates the trend.

3.2 Coupling two qubits

So far this toy model only consists of a simple coupler and two pairs of discs that represent the qubits. In the real sample the qubit qubit coupling will also be affected by a 2DEG and gates that define the quantum dots 100 nm below the surface of a GaAs sample. This section characterises the outcome of each of these parts of the real sample and gives a complete simulation at the end.
3.2.1 Electrostatic gates

Electrostatic gates on top of the sample create the double-well potential and hence the quantum dots. Here, simplified gates with respect to the ones seen in Fig. 2.1a has been added. First, the direct qubit to qubit coupling $C_{QQ}$ is measured. Then, the coupler is added to determine the mediated qubit qubit coupling $C_{QCQ}$ and finally simple grounded gates are included. A parametric sweep in the qubit separation (coupler length) has been done to see the long range coupling.

![Image](image-url)

**Figure 3.6:** Electrostatic gates. This graph shows the direct qubit to qubit coupling and the effect of adding a coupler and gates.

This repeats the work of Trifunovic et al. [4] but Fig. 3.6 additionally shows the effect of adding the gates. For separations greater than 1 µm $C_{QQ}$ is close to zero and confirms the work of Trifunovic et al. [4]. Adding the coupler has the desired effect of increasing the coupling between the qubits especially at large distance. The gates have an interesting effect. For short distances they reduce the coupling because they have finite capacitance to the coupler and shunt away some of the charge that would contribute to the qubit to qubit coupling [4]. We also note that for larger distances the gates screen the right dot of the target qubit from the coupler. This results in a ten times larger detuning of the target qubit in average for larger distances compared to the model without the gates. At
500 nm centre to centre separation the additional floating coupler increases the coupling about a factor of 4.5. This comes close to the factor of 3.5 presented by Trifunovic et al. [4] at 680 nm (this model does not include the GaAs dielectric yet and so the factors are being compared). At large separations (greater than 5 µm) there is still an appreciable coupling that allows long-range coupling between the qubits. In the experimental setup the electrostatic gates extend much further than in this simulation model. Because of the additional capacitance the coupling strength could be reduced by a small amount.

3.2.2 The 2DEG and the GaAs substrate

Adding the 2DEG as a grounded thin layer (5 nm) to the model with the coupler and gates has a similar effect to that of the gates. The 2DEG adds an additional capacitance to the setup, shunting away some of the charge as seen for the electrostatic gates.

As the 2DEG extends over the whole sample, strong coupling to the capacitive coupler is seen. The 2DEG at the area underneath the gates is removed in this simulation because the gates repel the electrons. Adding a dielectric between the dots and the coupler (for GaAs: $\varepsilon_r = 13$) increases the capacitance (see Eq. (3.2)). Therefore the measured voltage on the coupler is reduced by a factor of $\frac{1}{\varepsilon_r}$. This effect of dielectric constant is helpful in case of the dot-coupler coupling because we want strong capacitive coupling there, however $\varepsilon_r$ also increases the shunt capacitance of the coupler to the 2DEG.

![Figure 3.7: Adding the 2DEG and GaAs dielectric.](image)
3.2.3 Removal of the 2DEG and GaAs beneath the coupler

The numeric modelling in [4] already showed the approach of an etched coupler. Etching the GaAs sample in the locality of the coupler reduces the shunt capacitance between the coupler and the grounded 2DEG. Trifunovic et al. [4] compared the metallic coupler with a full 2DEG to the etched coupler with a trench of fixed depth beneath the coupler and found that removing the 2DEG and GaAs doubled the coupling strength. In order to identify each effect we start with the comparison between a model with a full 2DEG underneath the coupler and a second model with a removed 2DEG in the locality of the coupler. The depletion of the 2DEG results in an increase of the qubit qubit coupling strength by more than 100%. This shows the strong capacitive coupling between the coupler and the 2DEG. In addition, we determine the increase in qubit qubit coupling by etching a trench around the coupler with the same width as the depleted 2DEG (30 nm). The trench depth is varied at a fixed qubit separation of $L = 3 \mu m$ (see Fig. 3.9 to see how the GaAs is removed). At 90 nm the GaAs is removed up to the level of the 2DEG (see the dashed line in Fig. 3.8). The data shows a linear relation in this first section (data left to the dashed line). Close to zero and 90 nm the slope is different. This can be due to meshing problems or physical effects because of really sharp edges (see Sec. A.2).

Removing the GaAs beneath up to the level of the 2DEG (90 nm) increases the qubit qubit coupling about 12%. Further removal of the GaAs below the 2DEG level still increases the coupling but not as much as in the first section. This confirms the work of Trifunovic et al. [4] and shows that depleting the 2DEG underneath the coupler increases the qubit qubit coupling by more than 100% while additionally removing the GaAs beneath the coupler could increase the coupling by yet another 16%.

![Figure 3.8: Etching a trench around the coupler.](image-url)
3.2.4 Full model

After looking at every part of the setup individually a complete simulation that includes the coupler and gates as well as the 2DEG and the dielectric is done to determine realistic values of the qubit qubit coupling strength $C_{QCQ}$. As etching a trench and depleting the 2DEG underneath the coupler had the largest effect on qubit coupling a comparison with a depleted 2DEG and a trench underneath the coupler is shown in Fig. 3.10. This matches with the results seen in [4]. In our model the simulation gives slightly higher coupling (20%) which could be the result of the simplified electrostatic gates.

Figure 3.9: Full setup for the coupling of two qubits.

Figure 3.10: Results for coupling two qubits with a capacitive metallic coupler ($C_{QCQ}$). This realistic numerical model includes the characteristic of the heterostructure (GaAs dielectric), the 2DEG and the electrostatic gates. The coupling strength for a model with a full 2DEG underneath the coupler and additionally another model with a depleted 2DEG underneath the coupler and a trench around the coupler is shown (width: 30 nm, depth: 90 nm).
The following table summarises the outcome on the coupling of the effects discussed in the previous sections.

<table>
<thead>
<tr>
<th>parameter</th>
<th>effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>dot ↔ coupler</td>
<td>To achieve strong qubit qubit coupling it is important to determine the <strong>best position and size</strong> of the coupler paddle with respect to the qubit and the gates. Moving the coupler away from the qubit could be used as a switching mechanism.</td>
</tr>
<tr>
<td>gates</td>
<td>Adding gates decreases the coupling for short couplers because they add a shunt capacitance. A beneficial effect is seen for a larger coupler length where the gates significantly increase the qubit qubit coupling by <strong>screening the second dot of the target qubit</strong> from the coupler.</td>
</tr>
<tr>
<td>2DEG</td>
<td>The 2DEG adds a <strong>strong shunt capacitance</strong>. Removing the 2DEG underneath the coupler and doubles the qubit coupling.</td>
</tr>
<tr>
<td>GaAs</td>
<td>The GaAs dielectric is desirable for <strong>strong coupling between the coupler and the qubit</strong> but it also adds a large shunt capacitance which can be reduced by etching a trench underneath the coupler (coupling increased by 12% when etching up to the 2DEG level).</td>
</tr>
</tbody>
</table>

Table 3.2: Summary.

3.2.5 Coupler paddle variations

Before continuing to the coupling to multiple target qubits from one control qubit we have a look at the reduction of the qubit coupling when altering the shape of the coupler paddle to fit another coupler above the qubit. For this simulation the toy model with only the dots and a coupler is used (i.e. no 2DEG or gates), and so, the relative coupling strength is calculated. The separation between the qubits is fixed to 4 µm.
Table 3.3: Coupler variations with respect to a full circle. The red sections indicate the dot area being directly underneath the coupler.

These simple variations show that the area of a paddle can be reduced by a significant amount without reducing the coupling significantly. Reducing the area by half as shown in (III, IV) gives a larger coupling than shown in (II) which is an effect of a shorter average distance between the coupler and every part of the dot (more centred above the dot). The thin connection of the coupler (VI) still gives a large coupling.

3.2.6 Induced 2DEG

Figure 2.1b shows how a 2DEG is induced at the interface by dopants in the AlGaAs layer. The same result could be achieved by applying a positive voltage to a top gate that extends over the entire sample area.
A parametric sweep of the heterostructure and top gate distance $h$ is performed to show the effect on the qubit qubit coupling using the realistic model seen in Fig. 3.9. The dielectric between the top gate and the heterostructure is set to be air $\varepsilon_r = 1$. The sweep starts at a height of 50 nm just 10 nm above the coupler surface at which distance the coupling is reduced by 32% compared to the 1 $\mu$m value. For $h > 0.2 \mu$m the grounded top gate (Dirichlet boundary condition) reduces the coupling by less than 7% with respect to the coupling strength at $h = 1 \mu$m.

3.3 Coupling multiple qubits

In this section the analysis is extended to the coupling of multiple target qubits. This is an important step for building arrays of qubits. All subsequent models includes the GaAs dielectric.

3.3.1 Two couplers per control qubit dot

In order to be able to create an array of coupled qubits, each qubit has to couple to more than one target qubit. Thus, the model has to be extended. In these models, the gates are shrunk to be able to include more qubits without having large meshes. This should not make a significant difference because the qubits couple most strongly to the closest parts of the gates and to the coupler. The coupler paddle shape above the control qubit is reduced to the half paddle design (see II in Table 3.4) to fit two couplers with a separation of 10 nm between the paddles.
Figure 3.12: Coupling to a second target from one control qubit. (a) shows the setup with one coupler and gates at the control qubit only and in (b) a second coupler is added including an enlarged view of the gap between the couplers. In (c) & (d) gates at the target qubits and the 2DEG are added for a realistic model.

The coupling to the target qubit first with one target ($C_{QCQ}$) and then with two targets ($C_{QCQQ}$) using the same model (Fig. 3.12) is determined and the fraction of the remaining coupling is calculated $\frac{C_{QCQQ}}{C_{QCQ}}$ and shown in Fig. 3.13. Adding the second coupler increases the total coupler area. The fraction of the coupler area seen in Fig. 3.12.a with respect to the total area of both couplers seen in Fig. 3.12.b is 0.58. The same fraction is seen for the remaining coupling in Fig. 3.13 (black curve) and this result implies a linear trend seen for the remaining qubit coupling when increasing the coupler length since there is no screening effect or strong shunt capacitance because of the missing target gates and 2DEG. More realistic values are determined by adding gates to the target qubits and by adding the 2DEG to the model.
3.3 Coupling multiple qubits

Adding the gates to the target qubits shows again a screening effect which increases the target detuning. The fraction of the remaining coupling is increasing with the coupler length while having gates at the targets. This shows that the screening effect is increased when the voltage on the coupler drops. The blue data shows that the 2DEG adds a shunt capacitance which decreases the qubit coupling. This effect is especially important for a long couplers which is shown by the decrease of the fraction for large separations. These simulations show that a fraction above 50% (in comparison to the coupling to one target qubit) can be achieved in the realistic model when coupling to multiple target qubits.

3.3.2 One coupler per control qubit dot

Instead of adjusting the coupler paddle to make space for a second coupler one can also place another full coupler above the control qubit in order to couple to a second target qubit. However to create a two dimensional array (allowing more efficient algorithms) coupling of a control qubit to at least three other qubits is necessary.
This approach should have a beneficial effect on the qubit qubit coupling. Putting a second coupler above the qubit next to the first coupler screens the second dot from the first coupler and vice versa. At first, a simulation with only one coupler is performed (see Fig. 3.14a). After adding a second coupler above the second control dot, as shown in Fig. 3.14b, the increase in qubit qubit coupling strength is determined while doing a sweep of the $x$ separation. As expected, the coupling to the target qubits increases when adding a coupler above the second control dot (see Fig. 3.15) starting at 9% and going up to 10.5%. This shape of the curve can be explained by a change in the intercoupler coupling between the two couplers when increasing the coupler length. We now take a deeper look at the intercoupler coupling for this setup because it will also be relevant when building qubit arrays. One of the target qubits is now set to be the control qubit (the old control qubit turns into a target qubit) and the voltages on the first and second (intercoupled) coupler are being measured to determine the intercoupler coupling $C_{CC}$ by the fraction of the induced voltages on the couplers. The setup is shown in Fig. 3.14c.
The intercoupler coupling decreases with the qubit separation (coupler length) caused by a dropping voltage on the couplers. In general the couplers couple extremely weak in the design seen in Fig. 3.14c, only 4.5% for the shortest separation of 1 µm, because the distance to the gates and the dot (90 nm) is less than the distance to the next coupler (160 nm).

Furthermore a decrease of the intercoupler coupling can be achieved by altering the paddle shape at the point where the couplers are closest. This is done by circularly cutting off the edges at a fixed qubit separation of 2 µm and the result is shown in Fig. 3.17. A parametric sweep in the cut off circle radius for the setup shown in Fig. 3.14c is performed.

A linear decrease of the intercoupler coupling with respect to the circle radius is seen. The induced detuning at the first (direct coupled) target qubit ($C_{QCQ}$) and at the second (intercoupled) target qubit ($C_{QCCQ}$) is measured and shown in Fig. 3.17b. Altering the coupler shape always affects the coupling to the dot underneath. Because the coupler is still the closest object to the dot, this doesn’t affect the coupler qubit coupling $C_{CQ}$ much (as already seen in Table 3.3). $C_{QCCQ}$ directly depends on the voltage seen on the second coupler, thus it shows the same linear trend as the intercoupler coupling. The largest radius (100 nm) reduces the intercoupler coupling $C_{CC}$ by nearly 50% while the coupling to the first qubit $C_{QCQ}$ remains above 90% of its initial value.
3.3.3 Coupler paddle shape

In this section different coupler paddle shapes are presented in order to find an optimal shape with respect to the electrostatic gates used in this chapter. For each shape the size and the relative position is optimised as seen in Sec. 3.1.2 to achieve the best qubit qubit coupling. The result is shown in Table 3.4 for a fixed separation of 2 µm. Simulations include the gates and 2DEG.
3.3 Coupling multiple qubits

The variation of the shape of the coupler paddle shows only a small difference in the
coupling strength provided that it is positioned well (maximum difference is 4.5% with respect to the circular shape). Because a circular paddle should be easy to fabricate and because it shows good coupling to the qubit and weak coupling to the gates it could be the preferred choice.

3.3.4 Intercoupler coupling

The intercoupler coupling $C_{CC}$ between the couplers introduced in Fig. 3.12 is analysed in this section. When coupling to two qubits per control qubit dot the couplers are quite close. This results in a higher intercoupler coupling rate than seen in Sec 3.3.2. The intercoupler coupling $C_{CC}$ is defined by the fraction of the induced voltage on a second coupler with respect to the voltage on the first (inducing) coupler. Both strong and weak intercoupler coupling would be desirable in different situations e.g., strong coupling to a first and a second target but weak cross coupling to further targets.

The size of the gap between the couplers is one parameter to consider because it is the place where the couples have the smallest separation as shown in Fig. 3.12b. Therefore a sweep of the gap size is performed while keeping the area of the coupler paddles constant, which also means that the couplers are moving slightly closer to the gates.

![Figure 3.19: Adjusting the gap between coupler paddles. The intercoupler coupling can be reduced to 15% without reducing the qubit qubit coupling. (a) shows the intercoupler coupling and (b) the target qubit coupling. The qubit separation is 2 µm.](image)

For a parallel plate capacitor (Eq. (3.2)) we expect the intercoupler coupling to decrease
as the reciprocal of the gap size. Figure 3.19a shows this trend but the four data points are not enough to make a certain decision. The coupling strength reaches a maximum at 30 nm. With increasing gap size the couplers move closer to the gates and intercept some of the field that previously went to the gates. This increase continues until the coupler to gate coupling dominates and causes a decrease in coupling to the dot. By setting the gap size to 30 nm the intercoupler coupling can be reduced by 15% without loosing any coupling strength to the qubit.

The connecting wires of the couplers are very close to each other near the control qubit. This is another parameter which should be optimised. Therefore a parametric sweep of the coupler length (qubit x separation) is done and the intercoupler coupling $C_{CC}$ and the qubit-qubit coupling $C_{QQ}$ is determined for a variation of the path of the wires. This simulation includes the gates but it does not include the 2DEG in order to isolate the intercoupler coupling.
Figure 3.20: The intercoupler coupling $C_{CC}$ (a) and the qubit qubit coupling $C_{QCQ}$ (b) is shown for different connection wire paths. (c) shows the in previous sections introduces Y shape. The V shape connection shown in (b) reduces $C_{CC}$ by up to 25% without decreasing the qubit coupling. The short variation of the Y shape shown in (e) reduces $C_{CC}$ by up to 28% and $C_{QCQ}$ by 7%. Grounded screening gates shown in (f) reduce $C_{CC}$ by up to 58% but also reduce $C_{QCQ}$ by up to 42%. Red: high electrostatic potential, blue: zero potential. The intercoupler coupling rates are higher in this simulations because of the not included 2DEG.
The intercoupler coupling in Fig. 3.20 is increasing with the coupler length for every design as expected and it tends to a extreme value. This can be explained by the fact that a constant change in length of a long coupler wire has a weaker effect than applying the same change to a short coupler wire. The Y shape design (Fig. 3.20c) shows the strongest intercoupler coupling.

With the V shape design (Fig. 3.20d) the wires are separated earlier. This path variation looks promising because the intercoupler coupling is reduced from 15% (6 µm) through to 25% (2 µm) while the qubit qubit coupling strength remains the same with respect to the Y shape design.

The short Y shape (Fig. 3.20e) has a fixed length close to the control qubit until the connection wires of both couplers are separated. Therefore the intercoupler coupling is approximately reduced by a constant amount with respect to the Y shape as only the well separated part is extended when increasing the coupler length. This short Y shape reduces the intercoupler coupling by between 21% and 28%. Possibly due to the coupling to the close control qubit gates the qubit qubit coupling is reduced by constantly 6% for the short Y design.

To further reduce the intercoupler coupling a grounded screening gate is introduced at the short Y shape and shown in Fig. 3.20f. The intercoupler coupling is decreased by between 45% and 58% with respect to the Y shape design. At the same time the qubit qubit coupling is reduced by between 16% and 42% which is quite significant especially for large qubit separations because nearly only half of the qubit qubit coupling remains.

The V shape design shows promising results in terms of intercoupler coupling and qubit qubit coupling. An additional variation of the opening angle $\alpha$ of the wires is done. The $x$ separation between the left and right qubit seen in Fig. 3.20d is fixed to 3 µm while a parametric sweep of the $y$ separation of the two qubits on the right is done to increase the

![Figure 3.21: Increasing the opening angle $\alpha$ of the V shape design seen in Fig. 3.20d further decreases the intercoupler coupling. The angle is increased by increasing the $y$ separation between the qubits on the right while having a fixed $x$ separation between the left and right qubits.](image-url)
opening angle. This results in a further decrease of the intercoupler coupling $C_{CC}$ which is shown in Fig. 3.21.

Another approach to reduce the intercoupler coupling would be to adjust the coupler shape. Parts of the coupler paddle could be removed, especially the sections further from the qubit dot as these do not contribute much in terms of the coupling to the qubit dot underneath. Figure 3.22 shows the double paddle design (from Fig. 3.20c) with a cut away area between the coupler paddles.

![Figure 3.22: Remaining fraction when removing a circular section from the coupler paddle disc. Both the qubit qubit coupling and the intercoupler coupling are reduced but the qubit coupling drops more quickly.](image)

Removing a circular section at the end of the coupler paddles reduces both the qubit qubit coupling and the intercoupler coupling between the couplers. A further increase of the radius removes the coupler directly above the dot. Thus, the coupling reduces more quickly after reaching the radius of 40 nm as seen in Fig. 3.22. This shows that only removing areas of the coupler paddle that are not directly above the qubit dot are useful. Hence, a doughnut shape as seen in Table 3.3 shows a worse qubit coupling because area
directly above the qubit dot is removed which has been confirmed by a similar simulation which isn’t shown here.

Figure 3.22 shows that shrinking the coupler paddle to decrease the intercoupler coupling always reduces the qubit qubit coupling strength. It might also be more complicated to fabricate such coupler shapes. Therefore one should focus on adjusting the gap size and the wire path because the related results in the previous sections showed that the intercoupler coupling is reduced by a significant amount while the qubit qubit coupling is only reduced by a few percent.

Combining the results (factors) of the gap size variation (Fig. 3.19), the coupler path variations (Fig. 3.20), and the coupler paddle adjustment (Fig. 3.22) with the different coupler shapes seen in Table 3.4 and Table 3.3 gives many possible coupler variations with different properties in qubit and intercoupler coupling. For strong intercoupler coupling the Y shape design can be chosen with a small gap size and no removal of coupler paddle area. Weak intercoupler coupling and strong qubit coupling can be achieved with the V shape design. Then the intercoupler coupling can be additionally adjusted by the gap size. Especially weak intercoupler coupling and strong qubit coupling is seen when coupling with one coupler per control qubit dot only.

3.3.5 Network of qubits

In this section shows how the qubit qubit coupling propagates through a network of qubits. Therefore we verify if a simple multiplication model that depends on the intercoupler coupling can be applied. Here, we focus on the voltage on the couplers. One coupler is set to a fixed voltage and the voltages on the neighbouring couplers or the target qubits is measured. The ratio of the voltages gives multiplication factors that can be used to predict how the coupling strength changes from one coupler or qubit to the next which depend on the chosen coupler paddle and connection design.

As seen in Table 3.5, we extend the analysis seen in section 3.3.1 to an additional double half paddle coupler that will be needed to create a large network. A simulation with two couplers above both the control and the target qubit is performed for large qubit separations because there the qubit coupling $C_{Q_{QCQ}}$ tends to a constant value as seen in Fig. 3.13.
Coupling to two target qubits by replacing the full paddle on top of one control dot with two half paddles results in a remaining qubit coupling fraction of 0.61 (Table 3.5.II). Additionally replacing the paddle above the target qubits (Table 3.5.III) gives a fraction of 0.37 of the effect of a simple coupler (Table 3.5.I). This suggests that multiplication law may apply because going step by step from two full paddles to two half paddles results in a fraction of $0.61^2 = 0.37$. Before continuing to verify the multiplication law the linear dependence of the qubit detuning on the voltage which is applied to a coupler above is shown in Fig. 3.23. A full coupler paddle induces a larger detuning than a half paddle and both increase linearly with the coupler voltage. As a result of this linearity the propagation of the qubit qubit coupling in a network should only depend on the intercoupler coupling given that all couplers are the same. In this way we should be able to take the detuning at one qubit and multiply it by the intercoupler

Table 3.5: Remaining qubit qubit coupling when having half and full paddles.

<table>
<thead>
<tr>
<th>Coupler Design</th>
<th>Fraction of the Remaining Qubit Qubit Coupling</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
</tr>
<tr>
<td>II</td>
<td>0.61</td>
</tr>
<tr>
<td>III</td>
<td>0.37</td>
</tr>
</tbody>
</table>

Figure 3.23: Detuning induced by a full (slope: 0.0267) and half (slope: 0.0169) coupler paddle with respect to the voltage set on a coupler.
coupling to the \( n \)-th power (where \( n \) is the number of inter coupling steps) to calculate the detuning at a distant target qubit.

\[
\varepsilon_n = \varepsilon_0 \cdot f_{ic}^n
\] (3.4)

Figure 3.24 illustrates the multiplication law. The model for the figure has been reduced to three qubits and the outer couplers are cut off for reasons of simplicity. In the simulations the couplers have all the same length and equal paddles. The simulation includes a 2DEG and the separation is fixed at 2 \( \mu \)m with a fixed gap between the paddles of 10 nm. A parametric sweep of the coupler voltage of the first coupler (red) is performed. This causes a detuning \( \varepsilon_0 \) at the first directly coupled qubit and a detuning at distant qubits \( \varepsilon_1 \) and \( \varepsilon_2 \). The detuning at the three qubits is measured and the fraction \( f_{ic}^{nm} = \frac{\varepsilon_m}{\varepsilon_n} \) (see Table 3.6) is calculate to verify if the simple multiplication model applies.

<table>
<thead>
<tr>
<th>fixed coupler voltage [( \mu )V]</th>
<th>( \varepsilon_0 ) [( \mu )V]</th>
<th>( \varepsilon_1 ) [( \mu )V]</th>
<th>( \varepsilon_2 ) [( \mu )V]</th>
<th>( f_{ic}^{01} )</th>
<th>( f_{ic}^{12} )</th>
<th>( f_{ic}^{02} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>8.47</td>
<td>2.01</td>
<td>0.49</td>
<td>0.237</td>
<td>0.244</td>
<td>0.058</td>
</tr>
<tr>
<td>100</td>
<td>16.95</td>
<td>4.02</td>
<td>0.98</td>
<td>0.237</td>
<td>0.244</td>
<td>0.058</td>
</tr>
</tbody>
</table>

Table 3.6: Verifying the applicability of a simple multiplication law for the propagation of the qubit coupling in a network.

This multiplication law should not depend on the fixed coupler voltage because of the linearity seen in Fig. 3.23 which is shown by \( f_{ic}^{nm} \) being constant for different coupler voltages. \( f_{ic}^{01} \) is exactly the same as the intercoupler coupling for the gap size of 10 nm seen in Fig. 3.19a showing that the propagation depends only on the intercoupler coupling. We expect the fraction \( f_{ic}^{12} \) to be equal to \( f_{ic}^{01} \). Table 3.6 shows that \( f_{ic}^{12} \) is increased...
by 5% with respect to $f_{ic}^{01}$. The separation of the first and the second qubit is 2µm while the separation of the first and the third qubit is only approx. 1µm. This shorter separation could cause this 5% increase because of the direct qubit to qubit coupling (see Fig. 3.6) which quickly tends to zero for separations greater than 1µm but still remains for separations less than 1µm. The simulation mesh also always has a small effect on the coupling values but the error is less than 1% (see Sec. A.2). $f_{ic}^{02}$ is equal to the product of $f_{ic}^{01} \cdot f_{ic}^{12}$ as expected.

In summary this analysis shows that a simple multiplication law can approximately be applied and the law is defined by the intercoupler coupling. The intercoupler coupling depends on the qubit separation (coupler length and path), the coupler paddle shape and gap size. For this specific choice of the Y shape connection and half circle paddles with a 10 nm gap one could use the average of $f_{ic} = 0.24$ to describe how the coupling decays across the network.

### 3.3.6 RF gates

This section looks at the interaction of the couplers and the RF gates, often called crosstalk. The RF gates are the gates creating the detuning ($\varepsilon$) (see Fig. 2.1a). So far we neglected these gates in the simple gate model. Placing the RF gates as shown Fig. 2.1a means that they are in close proximity to the coupler. Because of the linearity of the model the detuning induced by varying the RF gate voltage follows a similar linear trend as seen for the couplers in Fig. 3.23.

Firstly, the gates are modelled at a position similar to the one of the experimental design. Then two couplers are added to the qubit and the coupler paddle shape is varied in order to characterise the coupling to the RF gates. In each case the induced detuning at the control qubit ($\varepsilon_0$) is measured with respect to the coupler paddle shape and a fixed RF gate voltage ($\varepsilon_{rf}$) showing how the coupler screens the effect of the RF gates. Then the crosstalk to the neighbouring qubit ($\varepsilon_1$) is measured and normalised by the control qubit detuning ($\varepsilon_0$).
3.3 Coupling multiple qubits

<table>
<thead>
<tr>
<th>design</th>
<th>fraction of voltage seen on the control qubit $\frac{\varepsilon_0}{\varepsilon_0}$</th>
<th>fraction of voltage seen on a neighbouring qubit (crosstalk) $\frac{\varepsilon_1}{\varepsilon_0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.05</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>0.025</td>
<td>0.115</td>
</tr>
<tr>
<td></td>
<td>0.029</td>
<td>0.068</td>
</tr>
<tr>
<td></td>
<td>0.035</td>
<td>0.032</td>
</tr>
</tbody>
</table>

Table 3.7: Applying a 1V difference (±0.5V) to the RF gates $\varepsilon_0^0$ results in a detuning $\varepsilon_0$ of the control qubit. The fraction of these voltages is shown in the second column and describes how the couplers screen the effect of the RF gates. The crosstalk to a target qubit $\varepsilon_1$ via the coupler is shown in third column with respect to the control qubit detuning. Qubit separation: 2 µm.

Only 5% of the voltage applied to the RF gates is seen at the qubit underneath without having a coupler. Adding full coupler paddles decreases the effect of the RF gates on the control qubit by 50% because of the screening effect of the couplers. Removing half of the coupler paddle results in a reduction of only 30% rather than the 50% seen for a full coupler. The couplers couple to the RF gates in the control qubit and so they detune the neighbouring qubit. The fraction of the detuning induced by the couplers on the target
qubit normalised by the control qubit is measured and shown in the third column of Table 3.7. From experimental setups we know that applying a voltage to the RF gates of a control qubit causes a detuning at neighbouring target qubit which is equal to applying 5% of the control qubit RF gate voltage to the target qubit RF gates (crosstalk). This value of 5% is comparable with the measured crosstalk of $\frac{24}{20}$ but our values are for a separation of $2 \mu m$ with a capacitive coupler. With a full coupler paddle the crosstalk is 11.5%. With a half paddle a crosstalk of only 3.2% is seen while also increasing the detuning to the control qubit by 40%.

Now the RF gates are set to be closer to the dots to achieve stronger detuning of the control qubit. This means that a section is removed from the coupler paddles. The results are shown in Table 3.8.
### 3.3 Coupling multiple qubits

<table>
<thead>
<tr>
<th>design</th>
<th>fraction of voltage seen on the control qubit $\varepsilon_{0}$</th>
<th>fraction of voltage seen on a neighbouring qubit (crosstalk) $\varepsilon_{1}$</th>
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<tr>
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<td>0.112</td>
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<tr>
<td></td>
<td>0.077</td>
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Table 3.8: Applying a 1V difference ($\pm 0.5V$) to the RF gates $\varepsilon_{0}$ results in a detuning $\varepsilon_{0}$ of the control qubit. The fraction of these voltages is shown in the second column and describes how the couplers screen the effect of the RF gates. The crosstalk to a target qubit $\varepsilon_{1}$ via the coupler is shown in third column with respect to the control qubit detuning. Qubit separation: 2 $\mu$m.

Placing the RF gates closer to the dots nearly doubles the control qubit detuning without a coupler (see Table 3.7, 3.8). Because the RF gates now reach inside the coupler paddle the coupling to the coupler and therefore the coupling to the neighbouring target qubits is increased (crosstalk).

This analysis shows that the full coupler paddle halves the effect of the RF gates. Placing the RF gates closer above the dots is one solution to increase the RF gate and control qubit coupling but it also increases the crosstalk. Removing sections of the coupler paddle reduces the crosstalk and increases the control qubit detuning.
4 Summary

This work numerically analysed the approach of long-distance spin qubit coupling via a floating metal gate.

The effect of different aspects of the experimental setup have been studied. The 2DEG and the electrostatic gates add a shunt capacitance to the coupler resulting in a reduced qubit coupling. However the gates also have a screening effect which increases the detuning of the target qubit. With a complete design, realistic values of the qubit coupling have been determined for the coupling between two qubits. There is still noticeable qubit coupling for qubit separations larger than $8 \mu m$ with the coupler allowing approximately ten times larger separations in comparison to the direct qubit to qubit coupling. Removing the 2DEG beneath the coupler increases the coupling by more than 100% by reducing the shunt capacitance between the coupler and the 2DEG. Further reduce of the shunt capacitance can be done by etching the GaAs sample beneath the coupler which increases the qubit coupling up to 16%. These results confirm similar work done by Trifunovic et al. [4].

In order to study the coupling in qubit arrays the coupling to multiple qubits has been shown. When coupling to two target qubits with one coupler per control qubit dot (1-dimensional arrays) a slightly increased coupling strength is seen due to screening effects of the second coupler. Replacing one complete coupler paddle above the control qubit with two half paddles, to couple to more than two qubits in order to create a 2-dimensional array, reduces the qubit qubit coupling to 61% of the complete paddle coupling strength. Additionally there is a coupling between neighbouring couplers. Maximum intercoupler coupling rates of 24% are seen. Parameters as the gap size and the wire path as well as removing sections of the coupler paddles allow to reduce the intercoupler coupling. Strong intercoupler coupling and qubit qubit coupling was seen for a Y shape wire design. Changing to a V shape design reduced the intercoupler coupling by 20% and it can be
further reduced by 15% by adjusting the gap size while strong qubit qubit coupling via the coupler remains. Further variations of the coupler paddles and wires are shown but a decrease of the qubit qubit coupling is always seen when removing sections of the coupler paddle or when adding screening gates which add shunt capacitance to the setup. This also means that it might be beneficial to shrink the qubit control wiring to a minimum to reduce the shunt capacitance to the wiring. The couplers at a qubit come close to the controlling gates. Thus, the couplers screen the effect of the RF gates creating the detuning $\varepsilon$ of the qubit. Removing sections of the coupler paddle and moving the RF gates closer to the middle of the qubit increases the induced voltage on the control dots. The crosstalk to neighbouring qubits via the coupler goes up to 11% and can be reduced to 3% by removing paddle sections.

There are still many other parameters that could be analysed. An optimisation of the controlling gate wiring for a multi qubit design would be an interesting aspect. It should be beneficial to reduce the wiring to a minimum to achieve strong qubit coupling since every material adds a shunt capacitance to the coupler. This work shows that the approach of a floating coupler that extends the qubit coupling over long distances between two qubits should be extendable to networks of coupled qubits whilst maintaining a reasonable level of coupling. The coupler crosstalk can be minimised where desired.
A Appendix

A.1 Domain boundaries (COMSOL infinite elements)

To limit the required computation source it is important to use efficient boundary conditions. This may be done by creating an object around the model on which one can define the boundaries.

Figure A.1: Small domain. Also used for the infinite elements method.

Figure A.2: Medium domain which comes close to the dimensions of the GaAs heterostructure.

To check the effect of the boundaries (errors by truncating the geometry) the qubit coupling for different box sizes is determined and compared to the infinite elements option where COMSOL sets the boundaries mathematically to infinity [23]. The edges are shown to illustrate the size of the simulation box and they always have the same width. By using the infinite elements method unnecessary mesh elements are avoided as one do not have to include large empty regions in the simulation to avoid the

Figure A.3: Large domain.
boundary affecting the region of interest. Additionally, the difference between the biggest and the smallest object is reduced, what makes the meshing more efficient and produces less meshing errors. A parametric sweep in the paddle-centre to paddle-centre separation \( L \) allows to compare the effect of the boundaries and the result is shown in Fig. A.4.

![Figure A.4: The qubit qubit coupling for different box sizes is shown to demonstrate the coupling to outer boundaries.](image)

As seen in Fig. A.4 the infinite elements method gives the same results as a large box in comparison to the size of the model. The qubit coupling decreases with increasing \( L \) due to the increase in coupler length and shunt capacitance (see Sec. A.3).

### A.2 Meshing in COMSOL

COMSOL provides a default automatic meshing although it allows many adjustments. This section describes some adjustments which helped avoiding meshing errors.

Firstly, COMSOL provides preset mesh element sizes. The default Normal mesh is not fine enough for most of the simulations. A model which includes both small and large dimensions can cause problems in the default meshing process.

In addition to the infinite elements method the Scale Geometry option is also helpful for thin objects because it allows separate scaling of the mesh in each direction. In particular creating Free Tetrahedral nodes under Mesh and adjusting the z-direction scale for each
object e.g., 3 or 5 was a good value for the thin 2DEG or the dots, allows reducing mesh elements where they aren’t needed.

When performing deformations of the simulation model (e.g. in a parametric sweep) the mesh is recreated at every step. COMSOL offers a *Moving Mesh* method under

Add Physics → Mathematics → Deformed Mesh → Moving Mesh(ale)

which allows the creation of a smoothly deformable mesh using an Arbitrary Lagrangian-Eulerian technique (ALE).

A meshing discretisation error has been estimated within the multiple qubit simulations. For the symmetric design (see Fig. 3.12d) the same coupling strength should be measured on the two target qubits. Taking the average difference in the coupling strength to the two targets of several simulations gives an indication of a typical error of approx. 0.5%.

Slightly increased meshing errors have been determined for simulations with a 2DEG, as a thin 2DEG which extends over the whole sample makes the meshing more difficult. The maximum error in these cases was approx. 1%.

**A.3 Dependence of qubit coupling on the coupler area**

In this work a parametric sweep of the qubit separation (coupler length) is often performed. According to Eq. (3.2) the change in the qubit qubit coupling should be caused by a change in area of the coupler. If the coupler can be approximated by a parallel plate capacitor, then the coupling strength should show a reciprocal \( \frac{1}{A} \) trend. To verify the dependence on the area ‘wings’ are added (in the y direction) in the middle of a coupler, which has a fixed coupler length in the x direction, to avoid direct coupling to the added material (see Fig. A.6). A parametric sweep of the ‘wing’ length is done to increase the coupler area by the same amount as seen at the coupler length sweep. The simulations are done with the *infinite elements* method.
Figure A.5: The dependency of the qubit qubit coupling on the coupler area shown by a sweep of the coupler length and by adding ‘wings’ to the coupler. Enlarged and reciprocal plot for a coupler area greater than $0.15 \mu m^2$ (b).

The curves with the wings (red & blue) start at zero wing length where they share a data point with the curve that shows the coupling for the sweep in coupler length (black). As the length of the wings increases the curves show a bump with increased coupling compared to the wing free curve (black). This is due to direct coupling from the qubit to the closest parts of the wings. Thus, the curves with the wings show an offset compared to the one without but they should have nearly the same slope in the $1/\text{area}$ plot for a large area (see Fig A.5) if the change in qubit coupling depends on the area. The curves show similar slopes but they are not exactly linear as the thin connection can not be approximated by a parallel plate capacitor model only (for a parallel plate we would expect a linear shape), i.e. seeing deviations from the parallel plate capacitor model.

This shows that a simulation with thinner wings and paddles connected to the wings far away from the qubits (with increasing area) would be a preferable model to show the dependence on the area. In addition to that a sweep of the coupler wire thickness without ‘wings’ could also give another view of the dependence on the coupler area.

Figure A.6: Adding ‘wings’ to the coupler to increase the area.
Acknowledgement

At first I want to thank Prof. Hendrik Bluhm for giving me the opportunity to work on this interesting project on spin qubits and to be part of the group.

Especially I also want to thank my advisor Rob McNeil, who always showed much interest in my work. The discussions on physical questions have always been fun and helpful. I also want to thank him for proofreading this work and all the helpful suggestions.

I would like to thank every member of this group for the great working atmosphere which made all the days of this project pass by very quickly.
Bibliography


## List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Qubits in a GaAs heterostructure</td>
<td>6</td>
</tr>
<tr>
<td>2.2</td>
<td>COMSOL example mesh</td>
<td>12</td>
</tr>
<tr>
<td>3.1</td>
<td>Simple toy model</td>
<td>15</td>
</tr>
<tr>
<td>3.2</td>
<td>How the capacitive coupling works</td>
<td>16</td>
</tr>
<tr>
<td>3.3</td>
<td>Sweep of the relative control qubit position</td>
<td>18</td>
</tr>
<tr>
<td>3.4</td>
<td>Sweep of the coupler paddle disc radius</td>
<td>19</td>
</tr>
<tr>
<td>3.5</td>
<td>Height of the coupler</td>
<td>20</td>
</tr>
<tr>
<td>3.6</td>
<td>Electrostatic gates</td>
<td>21</td>
</tr>
<tr>
<td>3.7</td>
<td>Adding the 2DEG and GaAs dielectric</td>
<td>22</td>
</tr>
<tr>
<td>3.8</td>
<td>Etching a trench around the coupler</td>
<td>23</td>
</tr>
<tr>
<td>3.9</td>
<td>Full setup</td>
<td>24</td>
</tr>
<tr>
<td>3.10</td>
<td>Realistic coupling strength</td>
<td>24</td>
</tr>
<tr>
<td>3.11</td>
<td>Top gate induced 2DEG</td>
<td>27</td>
</tr>
<tr>
<td>3.12</td>
<td>Add a second target to one control dot</td>
<td>28</td>
</tr>
<tr>
<td>3.13</td>
<td>Fraction when coupling to two targets</td>
<td>29</td>
</tr>
<tr>
<td>3.14</td>
<td>One coupler above each control dot</td>
<td>30</td>
</tr>
<tr>
<td>3.15</td>
<td>Increased coupling having couplers above each control dot</td>
<td>30</td>
</tr>
<tr>
<td>3.16</td>
<td>Intercoupler coupling between left &amp; right coupler</td>
<td>31</td>
</tr>
<tr>
<td>3.17</td>
<td>Reducing the intercoupler coupling between the left &amp; right coupler</td>
<td>32</td>
</tr>
<tr>
<td>3.18</td>
<td>Adding a gate between couplers</td>
<td>32</td>
</tr>
<tr>
<td>3.19</td>
<td>The gap between coupler paddles</td>
<td>34</td>
</tr>
<tr>
<td>3.20</td>
<td>Different coupler wire path designs</td>
<td>36</td>
</tr>
<tr>
<td>3.21</td>
<td>Opening angle of the V shape design</td>
<td>37</td>
</tr>
<tr>
<td>3.22</td>
<td>Removing a circular section from the paddle</td>
<td>38</td>
</tr>
<tr>
<td>3.23</td>
<td>Coupler induced detuning</td>
<td>40</td>
</tr>
<tr>
<td>3.24</td>
<td>Multiplication law</td>
<td>41</td>
</tr>
</tbody>
</table>
A.1 Small domain .......................................................... I
A.2 Medium domain ..................................................... I
A.3 Large domain .......................................................... I
A.4 Coupling to boundaries and infinite elements ................ II
A.5 Dependence of coupling on the area .............................. IV
A.6 Adding wings to the coupler ....................................... IV
List of Tables

2.1 Typical heterostructure dimensions ........................................ 7
3.1 Position & size results for the toy model ............................... 19
3.2 Summary ................................................................. 25
3.3 Coupler variations ...................................................... 26
3.4 Coupler paddle shape variations for the simplified gates .......... 33
3.5 Remaining qubit coupling for half paddles ............................ 40
3.6 Multiplication law ....................................................... 41
3.7 RF gates effect with couplers I ........................................ 43
3.8 RF gates effect with couplers II ....................................... 45