Multiqubit Coupling Dynamics and the Cross-Resonance Gate
Nonlocal Properties of High Fidelity Qubit Operations

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Abstract

The cross-resonance gate is implemented by applying a microwave drive to a system of two coupled qubits. I study the nonlocal properties of the driven and undriven system induced by this coupling. In the undriven case, entanglement is still being generated, but it is periodic and bounded linearly by the ratio of coupling strength and qubit frequency detuning. Specifically I derive an upper bound for the concurrence as a measure of entanglement.

When driving the system cross-resonantly the nonlocal properties of the resulting gate are supposed to coincide with those of the controlled NOT gate. Applying the theory of the Makhlin invariants provides a new way to quantify this statement, which I do for several different possible implementations.

A core difference of the aforementioned multiple possible implementations is the chosen qubit basis. By using a nonlocal qubit basis that is the eigenbasis of the undriven system the entanglement generation in the absence of a drive may be circumvented. But this might create further problems for supposedly single-qubit actions, like single-qubit measurements, which only couple to the physical degrees of freedom instead of nonlocally redefined qubits. This thesis collects the groundwork for examining this problem more thoroughly, building several simple models to describe the nonlocal action of a single-qubit measurement on a system of coupled qubits.
1 Introduction

There are still many steps to take on the quest for a fault tolerant quantum computer running a wealth of exponentially sped-up algorithms, both in the hardware and in the software department. Quantum software development I understand as studying and developing algorithms that ideally tackle interesting but hard problems and solve them by making full use of the unique power of a quantum computer. The hardware problem is building that quantum computer. And that again can be split up in myriad smaller problems.

The quantum power mentioned above mostly stems from the principles of superposition and entanglement allowing the probing of many different states at once. Harnessing that power requires isolating and manipulating individual quantum systems to extremely high accuracy. In particular unwanted interaction with the environment must be avoided at all cost, lest precious entanglement be lost to the claws of equilibration.

No system is perfect though, so to be able to deal with flaws to a certain degree, to become “fault-tolerant”, is the mission statement of the field of quantum error correction (QEC). QEC seeks to encode quantum information to protect it against noise, faulty gate or measurement operations, and generally errors of all kinds. But not every error can be detected and corrected. It is easy to imagine e.g. that if an error is so severe as to map one encoded state onto a different encoded state, it probably cannot be detected. Thus QEC is often concerned with finding thresholds for elementary error rates promising that if experimentalists operate within these threshold QEC will work.

The quality of state preparation, gates and other constituents is often measured in terms of fidelity, which basically is a measure for how close two quantum states (say the actual and ideal state after a certain operation) are. Fidelity ranges from zero to one with maximum fidelity corresponding to perfectly equal states. The above mentioned thresholds can then be translated more or less into a minimum required fidelity. Improvements in this regard are quite formidable. For example considering the cross-resonance (CR) gate, when it was first implemented in 2011, Chow et al. reported a gate fidelity of 81\% [4] which has since been improved to an average fidelity of 99\% achieved by Sheldon et al. in 2016 [19].

A common framework for exploring quantum computation is the circuit model. In it we graphically represent a quantum computation as a sequence of operations acting on a number of qubits, beginning by having the qubits initialised in a certain state, followed by unitary operations and possibly noise and usually ending in a measurement of the qubits.

Often the unitary gates in such a circuit are already chosen from a finite “univer-
sal” set, i.e. one that can approximate any unitary to any desired precision, where according to the Solovay-Kitaev theorem the number of required gates scales polynomially with the precision (p. 617 of [12]). A popular choice for this set are Clifford gates together with the T gate. The Clifford group, which is the normalizer of the Pauli group, is spanned by the single-qubit Hadamard and S gates, and a single maximally entangling two-qubit gate, the controlled NOT (CNOT) gate which will be the focus of this thesis.

More specifically we will look at the cross-resonance gate, an implementation of the CNOT gate, which will be derived and analysed (w.r.t. e.g. the aforementioned fidelity) in Chapter 3. Before we get to this main part though we will have a look at the system which is required for the CR gate to work and some of its properties. Chapter 4 examines the measurement process in this system and how that may resolve some questions concerning our qubit basis.

We will seek to better understand the dynamics of systems incorporating the CR gate and the limiting factors when fidelities beyond 99% are approached.

1.1 Superconducting Multiqubit Devices

A current superconducting qubit architecture, pictured in Fig. 1.1, consists of a number of qubits (squares 0 to 4), bus resonators (B0, B1) and readout resonators (R0 to R4). Typically each qubit comes with its own readout resonator which in turn is connected to a transmission line where microwave drive tones can be injected. This is used to measure the qubit and drive gates. The bus resonators are connected to two or more qubits to induce a coupling between them which forms the basis for performing multiqubit gates.

In this thesis we are mostly interested in finding simple models that nevertheless capture the essential multiqubit dynamics. To that end the resonators are assumed as simple harmonic oscillators

$$H_{\text{res}} = \omega_r a_r^\dagger a_r$$

with some resonance frequency $\omega_r$ and annihilation (creation) operators $a_r^{(\dagger)}$, where we will generally omit any constant (and thus inconsequential) energy contributions. We will not model the transmission lines explicitly but instead just add drives directly on the resonators (or even on the qubits) to the Hamiltonian where necessary.
1.1 Superconducting Multiqubit Devices

e.g.

\[ H_{\text{drive}} = \varepsilon_{\text{res}} \left( e^{i\omega_{\text{d,r}} t} a_r + e^{-i\omega_{\text{d,r}} t} a_r^\dagger \right) + \varepsilon_{\text{qbt}} \cos (\omega_{\text{d,q}} t) X_q. \]

This is a lab frame example, assuming we are driving at frequencies \( \omega_{\text{d,r}}/q \) respectively. To actually solve the Schrödinger equation, a time-independent Hamiltonian would be most convenient. A simple “trick” to achieve this is going to a frame rotating at the driving frequency. For example, if our system consisted only of a resonator driven at its resonance frequency

\[ H = \omega_r a^\dagger a + \varepsilon \left( e^{i\omega_{\text{d,r}} t} a + e^{-i\omega_{\text{d,r}} t} a^\dagger \right) \]

we go to a rotating frame with respect to \( V = \exp \left( -it\omega_r a^\dagger a \right) \) so that we are left with the drive term in its most simple (time-independent) form

\[ H_{\text{rot}} = V^\dagger HV - iV^\dagger \frac{\partial V}{\partial t} = \varepsilon \left( a + a^\dagger \right). \]

A possible qubit implementation is the transmon qubit [9]. A transmon has circuitry similar to a Cooper Pair Box (Josephson junction in parallel to a capacitance), but uses a significantly different parameter regime, where the Josephson energy \( E_J \) is much greater than the charging energy \( E_C \). In this regime the charge dispersion is basically flat which translates to a low susceptibility to charge noise.

A quantised transmon can then be described by an anharmonic oscillator

\[ H_{\text{tr}} = \omega_q b^\dagger b + \frac{\delta}{2} b^\dagger b \left( b^\dagger b - 1 \right) \]

with annihilation (creation) operators \( b^{(1)} \). The \(|0\rangle\) and \(|1\rangle\) levels, separated in energy by \( \omega_q \), are the qubit levels. When we drive the qubit at its transition frequency \( \omega_q \), a finite anharmonicity \( \delta \) makes transitions to higher levels off-resonant. The anharmonicity of the transmon is fairly small though as another consequence of the large \( E_J/E_C \) ratio. The higher levels thus cannot be neglected by default. And the size of the anharmonicity imposes constraints on some parameters and limits gate speed.

In this thesis we will nevertheless assume a pure qubit model (sending \( \delta \to \infty \))

\[ H_{\text{qubit}} = -\frac{\omega_q}{2} Z_q \]

since this already exhibits nontrivial coupling effects.

The transmon qubits are capacitively coupled to the resonators, as commonly described by a Jaynes-Cummings interaction

\[ V_{\text{tr-res}} = g_{qr} \left( b^\dagger a_r + ba_r^\dagger \right), \quad V_{\text{qu-res}} = g_{qr} \left( \sigma_q^+ a_r + \sigma_q^- a_r^\dagger \right). \]

Here we only consider the dispersive regime of this interaction, i.e. \( |g_{qr}| \ll |\omega_r - \omega_q| \). This means that we can often eliminate resonator degrees of freedom and get a qubit-only description; details on that follow in the main text.
With this information we can now write down a simple model of the Quantum Experience five qubit chip

\[
H_{QX} = \sum_{i=0}^{4} \left[ -\frac{1}{2} \omega_i Z_i + \omega_i a_i^\dagger a_i + g_{q_i r_i} \left( \sigma_i^+ a_i + \sigma_i^- a_i^\dagger \right) \right] \\
+ \sum_{i=0}^{1,2} g_{q_i b_0} \left( \sigma_i^+ a_{b_0} + \sigma_i^- a_{b_0}^\dagger \right) + \sum_{i=2,3,4} g_{q_i b_1} \left( \sigma_i^+ a_{b_1} + \sigma_i^- a_{b_1}^\dagger \right).
\]

As mentioned above, a universal gate set need only contain a single two-qubit gate, the most common choice for which is the CNOT gate. On the IBM Quantum Experience chip the CNOT is implemented via a CR gate. This is where the bus resonators come in. A direct two-qubit gate can only be performed between pairs of qubits that are connected to the same bus resonator. And even then, conditions on parameters like the qubits’ frequencies may not be symmetric between two suitably coupled qubits, thus dictating which of them needs to be the control and which the target qubit. For example, the CR gates possible on the Quantum Experience five qubit chip (as of September 2017) are indicated in Fig. 1.1.

**Preliminary Remarks on Notation**

**Paulis** Throughout the thesis operators \(X, Y, Z\) designate the Pauli matrices

\[
X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

which are most often acting on qubit states. Unless otherwise specified or clear from context, matrices will be given in the computational basis, defined by \(Z = |0\rangle \langle 0| - |1\rangle \langle 1|\). For qubits \(|0\rangle\) is the ground and \(|1\rangle\) the exited state. This is why \(Z\) appears with a negative sign in the Hamiltonian. As a consequence, the raising and lowering operators have to be defined as \(\sigma^\pm = \frac{1}{2} (X \mp iY)\) so that \(\sigma^+ |0\rangle = |1\rangle\) and \(\sigma^- |1\rangle = |0\rangle\). Where necessary, subscripts indicate which qubit(s) an operator acts on, e.g. \(X_1 |00\rangle = |10\rangle\), or which qubit(s) a state describes, e.g. \(X_1 |1\rangle_1 = |0\rangle_1\) or \(|1\rangle (|01\rangle + |10\rangle) = |10\rangle\).

**Units** The reduced Planck constant is set to \(\hbar = 1\). Thus energies are given in units of angular frequencies.

**Reusing Parameter Names** A note of warning: Throughout the thesis we will examine problems from different angles and different frames. Along this way parameters (like qubit transition frequencies) will get shifted and renormalised. To keep the narrative readable and concise though they will often not be renamed. More specifically, different labels will be used when talking about the transformation directly. But when the transformation is not the focus of attention any more
we will switch to a minimalistic labelling that does not necessarily reflect a parameter’s history of transformations, but only focuses on describing the current problem clearly. This also means that the same symbol does not always describe the same quantity. Though renamings will always be mentioned and should be clear when reading the sections of this thesis consecutively, it is something that should be kept in mind when just skipping through.

**Other** Unless otherwise specified, angle brackets indicate expectation values, i.e. taking the trace with the density matrix $\rho$ (\(= |\psi\rangle \langle \psi|\) for a pure state), \(\langle x \rangle = \text{tr} (\rho x)\) (\(= \langle \psi | x | \psi \rangle\) for a pure state), where the density matrix may depend on time \(\langle x \rangle (t) = \text{tr} [\rho (t) x]\).
2 Undriven System

We consider a system of two qubits, with transition frequencies \( \omega_{qi} \), and a resonator, with resonance frequency \( \omega_r \) and ladder operators \( a^{(i)} \),

\[
H_0 = \omega_r a^\dagger a - \sum_{i=1}^{2} \frac{\omega_{qi}}{2} Z_i
\]

where both qubits couple to the resonator via a Jaynes-Cummings type interaction of strength \( g_i \)

\[
V = \sum_{i=1}^{2} g_i \left( a^\dagger \sigma_i^- + a \sigma_i^+ \right).
\]

The resonator coupling can be eliminated with a Schrieffer-Wolff transformation yielding the effective Hamiltonian

\[
H_{\text{eff}} = \omega_r a^\dagger a - \frac{1}{2} \sum_{i=1}^{2} \left( \omega_{qi} - \frac{g_i^2}{\Delta_i} \left( 2a^\dagger a + 1 \right) \right) Z_i - \frac{g_1 g_2 (\Delta_1 + \Delta_2)}{\Delta_1 \Delta_2} \left( \sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+ \right),
\]

where \( \Delta_i = \omega_r - \omega_{qi} \).

The Schrieffer-Wolff transformation is a perturbative technique for block diagonalisation. It can be used when there are two blocks in a Hamiltonian, here \( H_0 \), that are sufficiently separated in energy and a coupling between those blocks, here \( V \), which is weak compared to the energy gap. The two blocks can be chosen as even and odd qubit parity states. Here we assume that we are in the dispersive regime, i.e. \( |g_i| \ll |\omega_{q1} - \omega_{q2}| \) so that the coupling is sufficiently weak and the transformation is a valid approximation.

An introduction to the Schrieffer-Wolff transformation can be found in [20], extensive applications in the perturbative analysis of two-qubit gates for transmon qubits are provided in [17] and [2] gives a more mathematically rigorous discussion. An extension to multiple energy sectors and thus possibly full diagonalisation is offered in the appendix of [7].

Neglecting the resonator dynamics in favour of our effective interaction and simplifying notation, in the following we consider the Hamiltonian

\[
H = -\frac{\omega_1}{2} Z_1 - \frac{\omega_2}{2} Z_2 + J \left( \sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+ \right),
\]

which, as is the desired result of the Schrieffer-Wolff transformation, is block-diagonal
in the \{\ket{00}, \ket{11}, \ket{01}, \ket{10}\}-basis
\[
H = \begin{pmatrix}
\frac{-\omega_1+\omega_2}{2} & \frac{-\omega_2-\omega_1}{2} \\
\frac{\omega_1+\omega_2}{2} & \frac{\omega_2-\omega_1}{2} \\
\frac{\omega_2-\omega_1}{2} & \frac{-\omega_2-\omega_1}{2}
\end{pmatrix} = \begin{pmatrix}
-\omega Z & JX + \delta Z
\end{pmatrix},
\]
with \(\omega = (\omega_1 + \omega_2)/2\) and \(\delta = (\omega_2 - \omega_1)/2\).
This is time-evolved easily as
\[
U(t) = e^{-iHt} = \begin{pmatrix}
e^{i\omega t} & e^{-i\omega t} \\
\cos \tilde{t} - i\frac{\delta}{\sqrt{J^2+\delta^2}} \sin \tilde{t} & -i\frac{J}{\sqrt{J^2+\delta^2}} \sin \tilde{t} \\
-i\frac{J}{\sqrt{J^2+\delta^2}} \sin \tilde{t} & \cos \tilde{t} + i\frac{\delta}{\sqrt{J^2+\delta^2}} \sin \tilde{t}
\end{pmatrix},
\]
with \(\tilde{t} = \sqrt{J^2+\delta^2} t\), since \(\exp(i\phi A) = \cos \phi + iA \sin \phi\) for an operator \(A\) with \(A^2 = I\), such as (normalised linear combinations of) Pauli matrices.

We thus have a complete description of the effective two-qubit system given an initial state and a time, enabling us to examine whatever system property we want to know about.

### 2.1 Entanglement Generation

Starting in a product state \(\ket{\psi(t=0)}\), one can analytically compute the concurrence \(C(\ket{\psi(t)}) = |\langle \psi(t)|Y_1Y_2|\psi^*(t)\rangle|\) of the time-evolved state \(\ket{\psi(t)} = U(t)\ket{\psi(0)}\) as a measure for the entanglement between the two qubits. Here the * refers to complex conjugation with respect to the standard basis. For a pure state the concurrence is closely related to the von-Neumann entropy \(S(\rho_1)\) which can be seen by noting that the eigenvalues of the reduced density matrix \(\rho_1(t) = \tr_2\ket{\psi(t)}\bra{\psi(t)}\) are given by
\[
\lambda_{\pm} = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - C^2(\ket{\psi(t)})}.
\]
The concurrence is bounded and periodic in time, as can be seen in Fig. 2.1. In this example the initial state is chosen as \(\ket{\psi(0)} = \ket{01}\). This is one of the initial states where maximum entanglement, corresponding to a concurrence of 1, can be reached for small enough \(\delta/J\).

#### 2.1.1 Upper Bound

Maximizing the concurrence squared over time and initial conditions, I find the upper bound
\[
C^2(\ket{\psi(t)}) \leq \begin{cases}
\frac{4(\delta/J)^2}{(1+(\delta/J)^2)^2} & \text{for } |\delta/J| \geq 1 \\
1 & \text{for } |\delta/J| \leq 1
\end{cases},
\]
showing how the entanglement generation (at all times) is suppressed by large detuning \(\delta = (\omega_2 - \omega_1)/2\) between the qubits. The maximum is reached by \(\ket{\psi(0)} \in \{\ket{01}, \ket{10}\}\).
Equation (2.3) was produced by visualizing the full result for $C^2(\psi(t))$ as a function of $\delta/J$ and $t$ for varying initial conditions, thus finding strong evidence that it is maximised by $|\psi(0)\rangle \in \{|01\}, \{|10\}\}$, substituting which into $C^2$ yields Eq. (2.3). This result is further confirmed by a numeric maximisation with respect to time and initial conditions which perfectly matches a plot (see Fig. 2.2) of Eq. (2.3).

For large $\delta/J$ the concurrence squared is proportional to $(\delta/J)^{-2}$ in leading order, independent of initial conditions (apart from starting in a product state), which can be seen by expanding the full result into a series for $\delta/J \to \infty$.

Qualitatively the concurrence is expected to vanish for large qubit detuning. In this case one would usually perform a rotating wave approximation (RWA) on the
Hamiltonian Eq. (2.1), eliminating the single-qubit terms by going to the respective rotating frame and then also dropping the interaction term which becomes fast rotating, thus being left with no two-qubit dynamics at all. We would always remain in a product state if we start in one, not generating any entanglement.

The above bound quantifies this approximation. And while we indeed find that the concurrence vanishes for infinite detuning, the suppression is only linear in $J/\delta$, so not that strong.

2.2 Canonical Decomposition of Two-Qubit Unitary

The framework for analysing entanglement capabilities extends beyond computing different entanglement measures for specific experiments.

When seeking to determine the maximum entanglement a given unitary can create, it often makes sense to only look at the entangling part of a unitary separating off single-qubit gate contributions [11, 22, 10]. In the same spirit single-qubit terms in the Hamiltonian are often neglected. However while I do want to make use of the former paradigm, the Hamiltonian remains unchanged.

One tool to separate off the single-qubit dynamics and extract a purely nonlocal unitary is given by what is sometimes called the canonical decomposition. The transformation demonstrated in the appendix of [10] is applied to Eq. (2.2). That means the single-qubit terms in the Hamiltonian $(\propto Z_{1/2})$ are explicitly included in the calculation to determine the effect of the detuning between qubit frequencies on the potential entanglement between them in this framework.

The result has the same structure as the original interaction, but is renormalised

$$U(t) = U_A \otimes U_B e^{i\alpha(X_1X_2+Y_1Y_2)}V_A \otimes V_B,$$

where $U_{A/B}$, $V_{A/B}$ are single-qubit gates on qubit 1/2 changing the phases of the $|0\rangle$- and $|1\rangle$-states and

$$e^{4i\alpha} = \frac{1}{1 + (\delta/J)^2} \left[ (\delta/J)^2 + \cos (2\tilde{t}) \right] - 2i \left| \sin \tilde{t} \right| \sqrt{\cos^2 \tilde{t} + (\delta/J)^2}.$$

For $t = 0$ this gives the identity ($\alpha = 0$), as required. And $\alpha$ also tends to 0 for $\delta/J \to \infty$, i.e. we again find that the coupling term becomes negligible in a sense. This transformation provides another point of view and avenue to quantify this statement.
3 The Cross-Resonance Gate

The cross-resonance gate is a specific scheme to induce a CNOT gate between two fixed-frequency qubits. It relies on an always-on coupling, like the one explored in the previous chapter, between the two qubits. The gate itself is then turned on and off in principle only via a single microwave drive, not including single-qubit gates to be applied before/after the two-qubit gate. Optimisation likely includes tones on multiple qubits though [19, 8].

The drive is applied to the control qubit at the frequency of the target qubit (which is supposed to be sufficiently, though not by more than the anharmonicity, detuned from the control qubit’s frequency), thus the name of the gate. The following two-qubit Hamiltonian thus drives a CNOT gate with qubit 1 as control and qubit 2 as target

\[ H = -\frac{\omega_1}{2} Z_1 - \frac{\omega_2}{2} Z_2 + J \left( \sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+ \right) + \Omega(t) \cos(\omega_2 t) X_1. \] (3.1)

Using this cross-resonance effect to perform gates was proposed by Paraoanu in 2006 [16], Rigetti and Devoret in 2010 [18], and demonstrated by Chow et al. in 2011 coining the CR gate [4].

Notable advantages include the use of fixed-frequency qubits, here transmons, which are less susceptible to flux noise than tunable ones, because they can always be kept at their sweet spot where dephasing time is maximal, and apart from the bus resonators only require a single microwave drive line/readout resonator per qubit for driving single- and two-qubit gates and performing measurements.

A prime disadvantage is the long gate time.

3.1 Derivation

Rigetti and Devoret apply a series of frame transformations and time-independent unitaries, i.e. change of bases, to the system Hamiltonian to ultimately arrive at a Hamiltonian of rapidly oscillating, entirely nonlocal terms (i.e. no single-qubit terms). Some of these terms are identified to become static when the drive frequency is fixed by the cross-resonance condition. Applying a rotating wave approximation to keep only these stationary terms and reversing the previous transformations to go back to the original frame the resulting Hamiltonian is seen to produce a CNOT gate.

Another way to arrive at (almost) the same conclusion is taken by Chow et al. They go directly to the eigenbasis of the undriven Hamiltonian, where the drive Hamiltonian \((X_1)\) gets a second term proportional to \(Z_1X_2\), which on its own would
again drive a CNOT gate. Here the drive is applied at the shifted eigenfrequency of qubit 1 instead of the bare one. The idea is then to “echo out” the single-qubit Pauli-Z terms, i.e. applying $X$-gates halfway through and at the end of the gate evolution that reverse the sign of the $Z$-terms and thus undoing their part in the evolution while also changing the sign of the drive at this midway-point so that this part is not cancelled, and to neglect the remaining $X_1$ term as off-resonant drive. Implicitly Rigetti and Devoret also do that when they just drop the single-qubit terms. Though since $X_1$ does not commute with $Z_1X_2$, it is not obvious how good that approximation is.

Strictly speaking the two gates are not exactly the same as they are performed in slightly different bases and use slightly different drive frequencies. In the following it will become clearer that the perturbative techniques used become exact in the limit of $J \rightarrow 0$ which is also where the two gates just described coincide. So finding that there can be multiple (slightly) different schemes all sharing the same limit and thus justification is entirely plausible.

3.1.1 Local Equivalence: Makhlin Invariants

Turning the $ZX$ into a CNOT gate still requires applying single-qubit gates (a “simple” task compared to two-qubit gates)

$$\text{CNOT} = e^{\pm i \frac{\pi}{4}} \exp \left( \pm i \frac{\pi}{4} Z_1 X_2 \right) \exp \left( \mp i \frac{\pi}{4} Z_1 \right) \exp \left( \mp i \frac{\pi}{4} X_2 \right).$$  \hspace{1cm} (3.2)

We say that $\exp \left( \pm i \frac{\pi}{4} Z_1 X_2 \right)$ is locally equivalent to a CNOT gate.

In general two two-qubit unitaries $U$, $V$ are locally equivalent if and only if there exist single-qubit gates $S_i$, $i = 1, \ldots, 4$ such that

$$U = S_1 \otimes S_2 V S_3 \otimes S_4,$$

i.e. they are the same up to single-qubit gates. In other words two locally equivalent unitaries share the same nonlocal or entangling properties. This invariance can be captured in a set of invariants derived by Makhlin in 2002 [11]. Zhang et al. explored the concept geometrically in 2003 [22].

Following the notation in [11], the invariants are basically given by the spectrum of $U_B^T U_B$ as specified by

$$G_1 = \frac{\text{tr}^2 \left( U_B^T U_B \right)}{16 \det (U)}$$

$$G_2 = \frac{\text{tr}^2 \left( U_B^T U_B \right) - \text{tr} \left( \left( U_B^T U_B \right)^2 \right)}{4 \det (U)}.$$  \hspace{1cm} (3.3)
where $U_B$ is $U$ in the Bell basis

$$U_B = Q^† U Q, \quad Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{pmatrix}. $$

In this section I want to explore a new way to understand the CR gate with the help of the Makhlin invariants. One goal of this process is to make the derivation more transparent and thus better understand the approximations made along the way or equivalently the conditions for a high-fidelity CNOT gate.

Given Eq. (3.1) and (3.3) the derivation is very straightforward:

1. The time evolution operator $U(t)$ is a complete description of the gate dynamics. Evaluated at the gate time (i.e. the duration for which the drive is applied) it gives the unitary operator which is supposed to be (locally equivalent to) a CNOT gate.

2. For the simple case of a constant drive amplitude $\Omega(t) = \Omega$ the remaining time dependence can be removed by going to a frame rotating at the drive frequency (and thus the transition frequency of the target qubit) and neglecting fast rotating terms $\propto \exp(\pm 2i\omega_2 t)$. This is the only rotating wave approximation used. It assumes that $2\omega_2 \gg |\Omega|$. Note that this is a much faster rotation than the one at frequency $\omega_2 - \omega_1$ which would suppress the interaction term when going to a frame rotating each qubit at its respective transition frequency.

3. The time evolution can then be computed analytically by taking the matrix exponential $\exp(-iHt)$ of the (now time independent) Hamiltonian

$$H = \frac{\Delta}{2} Z_1 + \frac{\Omega}{2} X_1 + \frac{J}{2} (X_1 X_2 + Y_1 Y_2) \quad (3.4)$$

where $\Delta = \omega_2 - \omega_1$.

4. Finally we search for the smallest time $t = t_{\text{gate}}$ such that

$$G_i(U(t_{\text{gate}})) = G_i(\text{CNOT}) \text{ for } i = 1, 2 \quad (3.5)$$

where $G_{1,2}(\text{CNOT}) = (0, 1)$. Then $U(t_{\text{gate}})$ is locally equivalent to a CNOT gate and the necessary single-qubit gates to apply before and afterwards to get a CNOT can be calculated following [11].

Note that this does not necessarily involve a change of basis, but can just as well be done in the eigenbasis of the undriven Hamiltonian as you can see in Section 3.2.

It turns out that Eq. (3.5) can be solved exactly only in the limit $J \to 0$. But this also sends $t_{\text{gate}} \to \infty$. From Chapter 2 we already know to maintain $|J| \ll |\omega_1 - \omega_2|$.
So we expand the Makhlin invariants for small $J$, but with $t = O(1/J)$, to solve Eq. (3.5) perturbatively. The results are

$$t_{\text{gate}} = \frac{\pi \sqrt{\Delta^2 + \Omega^2}}{2 |J\Omega|}$$

(3.6)

and

$$G_1(U(t_{\text{gate}})) \approx \frac{\Delta^4 J^4 \left((4 - \pi) \Delta^2 + 4 \Omega^2 + 4 \Omega^2 \cos \left(\frac{\pi (\Delta^2 + \Omega^2)}{2|J\Omega|}\right)\right)^2}{16 \Omega^4 (\Delta^2 + \Omega^2)^4}$$

$$G_2(U(t_{\text{gate}})) \approx 1 - \frac{8 J^2}{\Delta^2 + \Omega^2} \sin^2 \left(\frac{\pi (\Delta^2 + \Omega^2)}{4 J \Omega}\right).$$

An important thing to note is that if the drive strength $\Omega$ was weaker than the coupling $|\Omega| \leq |J| \ll |\Delta|$, we would have to leading order $G_1 \propto (J/\Omega)^4 \gg 1$. Thus to get a good CNOT gate we need to require $|J| \ll |\Omega|, |\Delta|$. A plot of the Makhlin invariants (before series gate expansion) can be seen in Fig. 3.1. For realistic parameters the second, small amplitude, high frequency oscillation which is superposed on but entirely dominated by the slow oscillation from the identity to the CNOT invariants is completely invisible.

Figure 3.1: Example Makhlin invariants’ behaviour as a function of time, for $\Delta/2\pi = 0.2$ GHz, $J/2\pi = 3.8$ MHz, and $\Omega/2\pi = 175$ MHz (left).
3.1 Derivation

3.1.2 Single-Qubit Unitaries

Following the steps outlined in [11], the single-qubit unitaries $O$, $O'$ required to make $U (t_{\text{gate}})$ a CNOT gate can be determined analytically

$$O' U (t_{\text{gate}}) O = \text{CNOT}, \quad O^{(t)} = V^{(t)}_1 \otimes V^{(t)}_2.$$  \hspace{1cm} (3.7)

The calculation determining $O^{(t)}$ is performed in the Bell basis, as defined in [11]. Transforming them back to the computational basis, the actual $U (2)$ single-qubit gates $V^{(t)}_1/2$ can be read off by examining the action of $O^{(t)}$ on the basis states, or, for non-vanishing trace, by tracing out one system at a time.

Equation (3.7) by definition only holds if the Makhlin invariants of $U (t_{\text{gate}})$ and the CNOT match exactly. Otherwise $O'$ will not be a single-qubit unitary. However as we have seen above, for finite $J$ the Makhlin invariants will only match approximately. $O^{(t)}$ are then determined in the limit of $J \to 0$, although some factors of $\sin$ and $\cos$ of arguments $\propto 1/J$, as well as $\text{sgn} J$ have to be retained where the limit cannot be performed ($\text{sgn}$ is the sign function). In practice this can be accomplished by performing a zeroth order expansion in $|J|$. We thus modify Eq. (3.7) to define our single-qubit gates $O^{(t)}$ by

$$O' \lim_{J \to 0} [U (t_{\text{gate}})] O = \text{CNOT}.$$ \hspace{1cm} (3.8)

This definition is not unique, for an explanation see the end of this section. In the following we give one possible solution.

Carefully taking the limit of $J \to 0$ in $U (t_{\text{gate}})$ as described gives

$$U_{\text{ideal}} = \lim_{J \to 0} U (t_{\text{gate}}) = \begin{pmatrix} a_- & b_- & c & d \\ b_- & a_- & d & c \\ c & d & a_+ & b_+ \\ d & c & b_+ & a_+ \end{pmatrix}$$ \hspace{1cm} (3.9)

with entries

$$a_{\pm} = \cos \phi \pm i \sin \kappa \sin \phi \text{sgn} J \Delta \Omega$$

$$b_{\pm} = -\sin \phi \pm i \sin \kappa \cos \phi \text{sgn} J \Delta \Omega$$

$$c = -i \sin \phi \cos \kappa \text{sgn} J$$

$$d = -i \cos \phi \cos \kappa \text{sgn} J$$

where we have defined $\cos \kappa = |\Omega| / \sqrt{\Delta^2 + \Omega^2}$, $\sin \kappa = |\Delta| / \sqrt{\Delta^2 + \Omega^2}$, and $\phi = \pi (\Delta^2 + \Omega^2) / (4J\Omega)$.
\[
\cos \kappa = \frac{|\Omega|}{\sqrt{\Delta^2 + \Omega^2}} \quad \sin \kappa = \frac{|\Delta|}{\sqrt{\Delta^2 + \Omega^2}}
\]

These definitions ease calculations, since you do not have to reinvent the wheel but can instead make direct use of any trigonometric identities. Additionally, since for $\Omega, \Delta \neq 0$

\[0 < \kappa < \pi/2\]

it is $\cos (\kappa/2) > \sin (\kappa/2) > 0$, opening up some more small, useful identities, e.g.

\[
\cos \frac{\kappa}{2} \pm \sin \frac{\kappa}{2} = \sqrt{1 \pm \sin \kappa}
\]

and

\[
\sqrt{\frac{1 + \text{sgn } x \cos \kappa}{2}} = \begin{cases} 
\cos \frac{\kappa}{2} & x > 0 \\
\sin \frac{\kappa}{2} & x < 0
\end{cases}
\]

and other simplifications of all kinds become more obvious and/or easier to prove.

From here we move to the bell basis via

\[
Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & i \\
0 & i & 1 & 0 \\
0 & i & -1 & 0 \\
1 & 0 & 0 & -i \end{pmatrix}
\]

and proceed as described in [11], with one variation. Since $\det \text{CNOT} = -1 \neq 1 = \det U(t)$ we have to introduce a phase-factor of $\pm \exp (\pm i\pi/4)$ to match the spectrum of $U_B^\dagger U_B$, $\{-i, -i, i, i\}$, to that of $\text{CNOT}_B^\dagger \text{CNOT}_B$, $\{-1, -1, 1, 1\}$, where the subscript $B$ refers to the Bell basis, e.g. $U_B = Q^1 U_{\text{ideal}} Q$. Here we choose to do this by making the temporary replacement

\[U_B \rightarrow \exp (i\pi/4) U_B\]  \hspace{1cm} \text{(3.10)}

for the calculation of $O_B$ only. Undoing the replacement for the calculation of $O_B'$ will imply that $O_B' \notin SO(4, \mathbb{R})$, since $\det O_B' = -1$. Of course $O_B'$ is still prefectly unitary, just not real. So we only have to keep in mind to invert it by taking the adjoint $O_B'^\dagger O_B' = 1$ instead of the transpose $O_B^\dagger O_B' \neq 1$.

Computing the single-qubit unitaries in the Bell basis this way gives

\[
O_B = Q^\dagger O Q = \frac{1}{\sqrt{2}} \begin{pmatrix} -R_+ \text{sgn } J \Delta \Omega & 0 & R_- \text{sgn } \Delta \Omega & 0 \\
0 & -R_+ \text{sgn } J \Delta \Omega & 0 & R_- \text{sgn } \Delta \Omega \\
R_- \text{sgn } J & 0 & R_+ & 0 \\
0 & R_- \text{sgn } J & 0 & R_+ \end{pmatrix},
\]
3.1 Derivation

with \( R_\pm = \sqrt{1 \pm \sin \kappa} \) and

\[
O'_B = Q^\dagger O'Q = \frac{1 + i}{2} \begin{pmatrix}
- \text{sgn}(J\Delta\Omega) C_+ & - \text{sgn}(J\Delta\Omega) S_- & -S_+ & C_-\\
\text{sgn}(J\Delta\Omega) S_- & - \text{sgn}(J\Delta\Omega) C_+ & S_- & C_+\\
\text{sgn}(J\Delta\Omega) C_- & - \text{sgn}(J\Delta\Omega) S_+ & C_- & S_+\\
\text{sgn}(J\Delta\Omega) S_+ & - \text{sgn}(J\Delta\Omega) C_- & S_+ & C_-
\end{pmatrix}
\]

with

\[
C_\pm = \cos \left( \frac{\kappa}{2} \pm \Phi - \frac{1}{2}\pi \delta_{-1,\text{sgn} J} \right) \\
S_\pm = \sin \left( \frac{\kappa}{2} \pm \Phi + \frac{1}{2}\pi \delta_{-1,\text{sgn} J} \right)
\]

where \( \Phi = \phi \text{sgn} J = \pi \left( \Delta^2 + \Omega^2 \right) / (4 |J| |\Omega|) \), and

\[
\delta_{i,j} = \begin{cases} 
1 & i = j \\
0 & \text{else}
\end{cases}
\]

is the Kronecker delta. You can confirm that indeed \( O'U_{\text{ideal}}O = \text{CNOT} \).

Having left the Bell basis and simplified \( O^{(i)} \) as much as possible, the actual single-qubit unitaries \( (\in U(2)) \) can be determined with a simple Solve[] in Mathematica (or read off after a thorough look at the structure of \( O^{(i)} \)). Here we split the results up into the two cases \( J\Delta\Omega \geq 0 \) for simplicity.

For \( J\Delta\Omega > 0 \) we have

\[
O = \frac{1}{\sqrt{2}} \begin{pmatrix}
\text{sgn}(J)\sqrt{1 - \sin(\kappa)} & -\sqrt{1 + \sin(\kappa)} \\
-\sqrt{1 + \sin(\kappa)} & - \text{sgn}(J)\sqrt{1 - \sin(\kappa)}
\end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

\[
O' = \frac{1}{\sqrt{2}} \begin{pmatrix}
ie^{-i\phi}\text{sgn}(J)\sqrt{1 - \sin(\kappa)} & -ie^{-i\phi}\sqrt{1 + \sin(\kappa)} \\
e^{i\phi}\sqrt{1 + \sin(\kappa)} & e^{i\phi}\text{sgn}(J)\sqrt{1 - \sin(\kappa)}
\end{pmatrix} \otimes \frac{-1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}
\]

and for \( J\Delta\Omega < 0 \) it is

\[
O = \frac{1}{\sqrt{2}} \begin{pmatrix}
\sqrt{1 + \sin(\kappa)} & \text{sgn}(J)\sqrt{1 - \sin(\kappa)} \\
- \text{sgn}(J)\sqrt{1 - \sin(\kappa)} & \sqrt{1 + \sin(\kappa)}
\end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

\[
O' = \frac{1}{\sqrt{2}} \begin{pmatrix}
ie^{-i\phi}\text{sgn}(J)\sqrt{1 + \sin(\kappa)} & ie^{-i\phi}\sqrt{1 - \sin(\kappa)} \\
e^{i\phi}\sqrt{1 - \sin(\kappa)} & e^{i\phi}\text{sgn}(J)\sqrt{1 + \sin(\kappa)}
\end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & i \end{pmatrix}
\]

Note that there is some freedom in choosing the single-qubit unitaries. First of all in the above tensor-product decomposition the phases of the two SU(2)-matrices can be set at will, since obviously \( \exp(i\varphi)A \otimes \exp(-i\varphi)B = A \otimes B \).

Then in general, if there is a single-qubit unitary \( V \) that commutes with \( U_{\text{ideal}} \), it and its inverse can multiply the single-qubit gates freely \( O'U_{\text{ideal}}O = O'VU_{\text{ideal}}V^\dagger O = O'VU_{\text{ideal}}V^\dagger O \). It is not a given though that a nontrivial \( V \) exists.
In our algorithm as well the arbitrariness already starts in Eq. (3.10). Assume $O_U$ and $O_C$ are the orthogonal matrices

$$O_U^\top O_U = O_C^\top O_C = 1$$

that diagonalise $U_B^\top U_B$ and CNOT$_B^\top$CNOT$_B$ respectively

$$O_U U_B^\top U_B O_U^\top = \begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix} = O_C \text{CNOT}_B^\top \text{CNOT}_B O_C^\top.$$ 

Those are the matrices that define $O = QO_U^\top O_C Q^\dagger$ and $O' = Q\text{CNOT}_B O_C^\top O_U U_B^\dagger Q^\dagger$. These are arbitrary in so far as a) there are two doubly degenerate eigenvalues, and b) by choosing the phase in Eq. (3.10) we can change the order of the eigenvalues, or rather we then have to reorder the eigenvectors in $O_U$ to maintain the same order of the eigenvalues as set by $O_C$ for the CNOT.

Also note that we have defined the single-qubit unitaries such that they implement a CNOT gate in the frame where the time-evolution operator is easy to calculate, which is the frame that is rotating both qubits at the drive frequency. As long as a change of frame is of the form $\exp [-it(\alpha Z_1 + \beta Z_2)]$, $\alpha, \beta \in \mathbb{R}$, we can easily move the CNOT to that frame, by basically undoing the change of frame with the single-qubit gates (since the change of frame at the gate time is a single-qubit gate itself). That way we can have a CNOT gate e.g. in the lab frame, or the frame rotating all qubits at their own transition frequency.

### 3.1.3 Fidelity

The average gate fidelity is determined as

$$F = \frac{\left| \text{tr} (U_{\text{ideal}}^\dagger U) \right|^2}{d+1},$$

with $d = 4$, the dimension of the Hilbert space. This neat little formula is a special case of the formula given in [7] based on the derivation in [13] for comparing a general operation to an ideal unitary gate when the non-ideal operation is unitary as well.

$U_{\text{ideal}}$ is the CNOT gate and $U$ is $U(t_{\text{gate}})$ expanded in $|J\rangle$ and multiplied by the single-qubit gates $O^{(j)}$ determined in the previous section (for $|J\rangle \to 0$). We can replace the CNOT by the exact Eq. (3.8), such that the single-qubit gates cancel out (using the cyclic invariance of the trace). It is thus equivalent to directly take $U_{\text{ideal}}$ as $\lim_{J \to 0} U(t_{\text{gate}})$ and $U$ as $U(t_{\text{gate}})$.

For convenience, following the analysis of the Makhlin invariants, this trace can still be performed in the Bell basis. For $U = U_{\text{ideal}}$ (i.e. when $J = 0$), the fidelity

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3.2 Redefining the Qubit Basis

trivially is equal to unity because then $\text{tr} \left( U^\dagger_{\text{ideal}} U \right) = 4$. For non-vanishing $J$, corrections appear in second order

$$\text{tr} \left( U^\dagger_{\text{ideal}} U \right) \approx 4 + \frac{J^2}{32\Omega^2 (\Delta^2 + \Omega^2)^2} \left[ -4 \left( 8 + \pi^2 \right) \Delta^4 - 4 \left( 24 + \pi^2 \right) \Delta^2 \Omega^2 \\
+ 32\Omega^2 (\Delta^2 + \Omega^2) \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{2J\Omega} \right) - (32 + \pi^2) \Omega^4 \right]$$

and therefore

$$F \approx 1 - \frac{J^2}{80\Omega^2 (\Delta^2 + \Omega^2)^2} \left[ 4 \left( 8 + \pi^2 \right) \Delta^4 + 4 \left( 24 + \pi^2 \right) \Delta^2 \Omega^2 \\
- 32\Omega^2 (\Delta^2 + \Omega^2) \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{2J\Omega} \right) + (32 + \pi^2) \Omega^4 \right]. \quad (3.12)$$

### 3.2 Redefining the Qubit Basis

If we want to do a derivation closer to [4], we should move to the eigenbasis of the undriven system to redefine our qubits as was done in the reference. One advantage of this is that the eigenstates are by definition stationary under the undriven Hamiltonian, i.e. when no gate is applied. That way we circumvent all problems analysed in Chapter 2. The price to pay for this is that our qubit definitions become non-local. So we expect this to introduce small non-local errors to single-qubit gates and measurements if those are not tailored specifically to the redefined, or dressed, qubits.

The Hamiltonian of the undriven system of two coupled qubits

$$H_1 = -\frac{\omega_1}{2} Z_1 - \frac{\omega_2}{2} Z_2 + \frac{J}{2} \left( X_1 X_2 + Y_1 Y_2 \right)$$

is block diagonal in the standard computational basis

$$H_1 = \begin{pmatrix} \omega & J & -\delta \\ \delta & J & \delta \\ -J & -\delta & \omega \end{pmatrix}$$

where we have defined the average frequency $\omega = (\omega_1 + \omega_2) / 2$ and the deviation from it $\delta = (\omega_2 - \omega_1) / 2$. It can be diagonalised with a rotation $R$

$$RH_1 R^\top = -\frac{\tilde{\omega}_1}{2} \tilde{Z}_1 - \frac{\tilde{\omega}_2}{2} \tilde{Z}_2$$

where $\tilde{\omega}_1 / 2 = \omega \mp \lambda$, $\lambda = \delta \sqrt{1 + (J/\delta)^2}$, and

$$R = \begin{pmatrix} 1 & \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta & 0 \\ \cos \theta & -\sin \theta & \cos \theta \end{pmatrix} \quad (3.13)$$
with \( \cos \theta = \frac{1}{\sqrt{2}} \sqrt{1 + \delta/\lambda} \) and \( \sin \theta = \text{sgn} (J \delta) \frac{1}{\sqrt{2}} \sqrt{1 - \delta/\lambda} \), and \( \tilde{Z}_i \) is a Pauli-Z matrix in the new basis. For small \( J, \theta \approx J / (\omega_2 - \omega_1) \), so that in the limit of \( J \to 0 \) the new qubit basis coincides with the original basis, i.e. \( R \) becomes the identity, \( \tilde{Z}_1 \) becomes \( Z_1 \) etc.

After diagonalising, we can do the same analysis as before utilising the Makhlin invariants.

Transforming a drive on the original qubit 1 into this basis gives \( RX_1 R^\dagger = \cos \theta \hat{X}_1 + \sin \theta \tilde{Z}_1 \hat{X}_2 \). Assuming we drive at frequency \( \tilde{\omega}_2 \) with amplitude \( \Omega \) our total Hamiltonian at time \( t \) in the dressed basis becomes

\[
H_2(t) = -\frac{\tilde{\omega}_1}{2} \tilde{Z}_1 - \frac{\tilde{\omega}_2}{2} \tilde{Z}_2 + \Omega \cos(\tilde{\omega}_2 t) \left[ \cos \theta \hat{X}_1 + \sin \theta \tilde{Z}_1 \hat{X}_2 \right].
\]

Going to a frame rotating at \( \tilde{\omega}_2 \), i.e. w.r.t. \( V(t) = \exp \left( i \tilde{\omega}_2 t (\tilde{Z}_1 + \tilde{Z}_2)/2 \right) \) where \( H_3(t) = \left( V^\dagger H_2 V - i V^\dagger \frac{\partial V}{\partial t} \right) \) (t), gives

\[
H_3(t) = \lambda \tilde{Z}_1 + \frac{\Omega}{2} \left( e^{i \tilde{\omega}_2 t} + e^{-i \tilde{\omega}_2 t} \left[ \cos \theta (e^{i \tilde{\omega}_2 t} \tilde{\sigma}_1^+ + e^{-i \tilde{\omega}_2 t} \tilde{\sigma}_1^-) + \sin \theta \tilde{Z}_1 (e^{i \tilde{\omega}_2 t} \tilde{\sigma}_2^+ + e^{-i \tilde{\omega}_2 t} \tilde{\sigma}_2^-) \right] \right).
\]

Just as in the undressed case, this becomes time-independent after a RWA, dropping terms \( \propto \exp (\pm 2i \tilde{\omega}_2 t) \)

\[
H = \lambda \tilde{Z}_1 + \frac{\Omega}{2} \left( \cos \theta \hat{X}_1 + \sin \theta \tilde{Z}_1 \hat{X}_2 \right).
\]  

(3.14)

Calculating the Makhlin invariants of \( U(t) = \exp (-i Ht) \) for \( t \propto J^{-1} \) in the limit of small \( J \) gives (to zeroth order)

\[
G_1(t) \approx \cos^2 \left( \frac{Jt\Omega}{\sqrt{4\delta^2 + \Omega^2}} \right)
\]

\[
G_2(t) \approx 2 + \cos \left( \frac{2Jt\Omega}{\sqrt{4\delta^2 + \Omega^2}} \right)
\]

which coincides with \( (G_1, G_2) \) (CNOT) = (0, 1) at

\[
t = \frac{\pi \sqrt{4\delta^2 + \Omega^2}}{2 |J\Omega|} = \frac{\pi \sqrt{\Delta^2 + \Omega^2}}{2 |J\Omega|} = t_{\text{gate}}
\]

with \( \Delta = \delta/2 = \omega_2 - \omega_1 \), which is the same time as determined previously for the analogous scheme on the undressed qubits. Higher order expansions reveal corrections in fourth order (that are the same for \( G_1 \) and \( G_2 \) up to a factor)

\[
G_1(t_{\text{gate}}) \approx \frac{J^4}{256\delta^4 (4\delta^2 + \Omega^2)^4} \left[ \pi \left( 48\delta^4 + 4\delta^2\Omega^2 - \Omega^4 \right) + 4\Omega^4 \cos \left( \frac{\pi \left( 4\delta^2 + \Omega^2 \right)}{2J\Omega} \right) \right]^2
\]

\[
G_2(t_{\text{gate}}) \approx 1 + 2G_1(t_{\text{gate}}).
\]
We can also calculate an average fidelity again
\[
F = \frac{\text{tr} \left( U_{\text{ideal}}^\dagger U \right)^2}{d + 1} \approx 1 - \frac{J^2 \left( \pi^2 (16\delta^3 + 3\delta\Omega^2)^2 + 8\Omega^6 \right)}{80\delta^2\Omega^2 (4\delta^2 + \Omega^2)^2},
\]
where \( U_{\text{ideal}} = \lim_{J \to 0} U(t_{\text{gate}}) \), and \( d = 4 \) is the dimension. The decrease in the fidelity is again starting in second order in \( J \). Here the characteristic oscillations with frequency \( 1/J \) only appear in higher orders though.

Note that \( U_{\text{ideal}} \) is actually the same as the one given in Eq. (3.9), since in the limit of \( J \to 0 \) the dressed qubits coincide with the undressed ones. This means that Section 3.1.2 applies equally to the dressed qubits, giving the same single-qubit gates.

3.3 Echo and Simple Single-Qubit Gates

Given the Hamiltonian Eq. (3.14), the only nonlocal term is the \( Z_1X_2 \) which is responsible for driving the CR gate. If we could isolate this term we would get a perfect CNOT gate by applying the simple single-qubit gates given in Eq. (3.2). If the drive was sufficiently weak, so that the off-resonant drive term \( X_1 \) could be neglected, then the action of the remaining single-qubit term \( Z_1 \) which commutes with \( Z_1X_2 \) can be undone with a single-qubit gate or in the form of an echo.

\[
e^{i\Delta_1 (\lambda Z_1+\Omega'Z_1X_2)}X_1e^{i\Delta_1 (\lambda Z_1-\Omega'Z_1X_2)}X_1 = e^{i\Delta_1 \Omega Z_1X_2}
\]

By applying an \( X \) gate on the control qubit halfway through the gate time while changing the sign of the CR drive \( \Omega \to -\Omega \) and applying a second \( X_1 \) afterwards, we thus “echo out” the \( Z_1 \) contribution, where we have used the anticommutation relations of the Pauli operators \( XZX = -Z \).

To find out how well this approximation holds up we can repeat the above fidelity analysis for the echo unitary
\[
U(t) = \exp \left( i \frac{t}{2} H \right) X_1 \exp \left( i \frac{t}{2} H_{\Omega \to -\Omega} \right) X_1
\]
where the gate time remains unchanged \( t = t_{\text{gate}} \).

Inspired by the previous sections there are multiple obvious questions to ask here:

- Does the echo work equally well in both bases?
- How relevant is the basis in which the \( X_1 \) gates are applied (\( X_1 \) versus \( \tilde{X}_1 \))?  
- How well do the simple single-qubit gates from Eq. (3.2) work compared to those derived from taking the limit of \( J \to 0 \)?
We will try to answer them based on the average fidelity. To that end we go back to Eq. (3.11), where we insert Eq. (3.15) for $U$. We will vary $H$ and $X_1$ in Eq. (3.15) to account for implementations using different qubit bases. To compare different single-qubit gates, we compute two fidelities each, $F_1$ and $F_2$, that differ by which $U_{\text{ideal}}$ is used in Eq. (3.11).

$F_1$ takes

$$U_{\text{ideal}} = \lim_{J \to 0} U(t_{\text{gate}}),$$

i.e. the Makhlin invariants of $U_{\text{ideal}}$ will match those of the CNOT gate exactly and we could thus find the single-qubit gates that together with $U_{\text{ideal}}$ give a perfect CNOT gate. I say “could” because to compute the fidelity it is not necessary to know the exact form of the single-qubit gates. Since as long as $O$ exist such that

$$O^U_{\text{ideal}}O = \text{CNOT}$$

holds exactly (which is guaranteed by the equality of the Makhlin invariants), the single-qubit gates will cancel in the trace

$$\text{tr} \left( \text{CNOT}^\dagger O^U O \right) = \text{tr} \left[ \left( O^U_{\text{ideal}}O \right)^\dagger O^U O \right] = \text{tr} \left( U_{\text{ideal}}^\dagger U \right).$$

$F_1$ then only describes how close the unitary is to the zero coupling limit, implicitly assuming that we can apply the single-qubit gates with no error.

In practice simple rotations around the standard axes of the Bloch sphere can likely be applied faster and more accurately. $F_2$ therefore takes

$$U_{\text{ideal}}^{(2)} = \exp \left( - \text{sgn} (J\Omega \Delta) i \frac{\pi}{4} Z_1 X_2 \right),$$

assuming that we apply the “simple” single-qubit gates from Eq. (3.2) (again with no error), quantifying how close we are to the zero drive limit as well as the zero coupling limit.

### 3.3.1 Qubits in Bare Basis

The echo was motivated in the dressed basis, but we will establish a baseline for comparison by first analysing it in the bare basis to see how it would act on the physical qubits. That is we analyse Eq. (3.15) with

$$H = \frac{\Delta}{2} Z_1 + \frac{J}{2} (X_1 X_2 + Y_1 Y_2) + \frac{\Omega}{2} X_1$$

as Hamiltonian, where $\Delta = \omega_2 - \omega_1$ is again the qubit detuning. We confirm that in the limit $J \to 0$ indeed the Makhlin invariants reach 0 and 1 respectively (and find that for finite $J$, corrections appear in fourth order). We then compute the fidelities as explained above which gives

$$F_1 \approx 1 - \frac{2 J^2 \Delta^2 \left( \frac{\Delta^2}{2} + 2 \Omega^2 \left( 2 - \sqrt{2} \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{4 J \Omega} \right) \right) \right)}{5 \Omega^2 (\Delta^2 + \Omega^2)^2}.$$
and

\[ F_2 \approx 1 - \frac{2\Omega^2}{5\Delta^2} - \frac{4\sqrt{2}J\Omega \sin\left(\frac{\pi(\Delta^2+\Omega^2)}{4J\Omega}\right)}{5\Delta^2} - J^2 \left( \frac{2}{5\Omega^2} + \frac{4(\pi - 4)\sqrt{2}\cos\left(\frac{\pi(\Delta^2+\Omega^2)}{4J\Omega}\right) + \pi + 26}{20\Delta^2} \right). \]

Here \( F_1 \) and \( F_2 \) are expanded to second order in \( J \), and \( F_2 \) additionally to second order in \( \Omega \). We find that both have terms of the order of \( J^2/\Omega^2 \) so \( \Omega \) cannot be arbitrarily small. \( F_2 \) thus has a maximum for \( \Omega \ll \Omega \ll \Delta \), while \( F_1 \) increases for larger \( \Omega \) (see Fig. 3.2). Another advantage of strong drives is that the gate time becomes minimal for \( \Omega \to \infty \). At this point we should not forget the approximations that led us here though. Since we use a pure qubit Hamiltonian having neglected all higher transmon levels there is no downside to a strong drive. Whereas for an actual transmon, a strong drive can cause leakage into higher levels and should thus be avoided. Of course we could also take this as motivation to move away from transmons to something closer to a true two-level system which can be driven quite strongly.

### 3.3.2 Qubits in Dressed Basis

We now move to the eigenbasis of the undriven system, assuming that we can also apply the single-qubit \( X_1 \) gates in this dressed basis. So our unitary is given again

![Figure 3.2: Fidelity of echo in undressed qubit basis, with \( J/2\pi = 3.8 \text{ MHz} \) and \( \Delta/2\pi = 200 \text{ MHz} \), (not using expansion in \( \Omega \)).](image-url)
by Eq. (3.15), but now with the Hamiltonian

\[ H = \lambda Z_1 + \frac{\Omega}{2} (\cos \theta X_1 + \sin \theta Z_1 X_2) \]

with \( \lambda = \delta \sqrt{1 + (J/\delta)^2} \), \( \cos \theta = \frac{1}{\sqrt{2}} \sqrt{1 + \delta/\lambda} \), \( \sin \theta = \text{sgn} (J\delta) \frac{1}{\sqrt{2}} \sqrt{1 - \delta/\lambda} \), and \( \delta = \Delta/2 = (\omega_2 - \omega_1)/2 \) as defined in Section 3.2.

We proceed the same as before and now get

\[
F_1 \approx 1 - \frac{2J^2\Omega^4}{5\Delta^2 (\Delta^2 + \Omega^2)^2} \left[ 3 - 2\sqrt{2} \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J\Omega} \right) \right]
\]

\[
F_2 \approx 1 - \frac{2\Omega^2}{5\Delta^2} + \frac{J^2\Omega^2}{20\Delta^2} \left[ 40 + 3\pi + 8\pi \sqrt{2} \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J\Omega} \right) \right].
\]

This means that if we define our qubits in the eigenbasis and use the echo scheme,

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.3}
\caption{Echo in dressed basis, same parameters as in Fig. 3.2.}
\end{figure}

we can now get a very high fidelity for \( \Omega \ll J \) as well. For weak drives even the simple single-qubit gates perform quite well here. But for stronger drives \( F_2 \) decays quadratically (cf. also Fig. 3.3).

As an aside we note that the zeroth order (in \( J \)) term of \( F_2 \) is the same for both schemes analysed so far. This also holds if we do not expand in \( \Omega \) where the term is

\[
\frac{2}{5} \left( 1 + \frac{|\Delta|}{\sqrt{\Delta^2 + \Omega^2}} + \frac{\Delta^2}{2(\Delta^2 + \Omega^2)} \right).
\]

We can easily understand this by remembering that the two schemes coincide in the limit of \( J \to 0 \).
3.3.3 Qubits in Dressed, but Single-Qubit Gates in Bare Basis

In the previous section we assumed that we can perform the single-qubit parts of the echo (the $X_1$ gates) in the dressed basis. (So we should have actually written $\tilde{X}$ and $\tilde{Z}$ throughout.)

In practice a single-qubit gate is performed by applying a drive at the frequency of the qubit to that qubit’s readout resonator. And while the frequency may be the shifted frequency, i.e. the one of the dressed qubit, the drive is still applied to the physical qubit.

So the single-qubit unitaries will likely not be perfectly in the dressed basis, but there will be some (coherent) error on them. One reasonable worst-case model of that error is to assume that the single-qubit gates are applied in the undressed basis, i.e. to the physical qubits. To find out how that impacts fidelity we thus consider the echo

$$U(t) = \exp \left( i \frac{t}{2} \left[ \lambda \tilde{Z}_1 + \frac{\Omega}{2} \left( \cos \theta \tilde{X}_1 + \sin \theta \tilde{Z}_1 \tilde{X}_2 \right) \right] \right) X_1$$

$$\times \exp \left( i \frac{t}{2} \left[ \lambda \tilde{Z}_1 - \frac{\Omega}{2} \left( \cos \theta \tilde{X}_1 + \sin \theta \tilde{Z}_1 \tilde{X}_2 \right) \right] \right) X_1$$

where $\sim$ marks operators in the dressed basis. Matrix-wise we can transform between the two bases with the matrix $R$ as defined in Eq. (3.13), e.g. to get the representation of $X_1$ (on the physical qubit 1) in terms of the dressed qubits we do

$$X_1 = R \tilde{X}_1 R^T = \cos \theta \tilde{X}_1 + \sin \theta \tilde{Z}_1 \tilde{X}_2. \quad (3.19)$$

To make the computation with $U$ simpler we can move the $R^{(\dagger)}$s into the exponents

$$U(t) = \exp \left( i \frac{t}{2} H \right) R \tilde{X}_1 R^T \exp \left( i \frac{t}{2} H' \right) R \tilde{X}_1 R^T$$

$$= R \exp \left( i \frac{t}{2} R^T H R \right) \tilde{X}_1 \exp \left( i \frac{t}{2} R^T H' R \right) \tilde{X}_1 R^T$$

with

$$R^T H^{(\dagger)} R = R^T \left[ \lambda \tilde{Z}_1 \pm \frac{\Omega}{2} \left( \cos \theta \tilde{X}_1 + \sin \theta \tilde{Z}_1 \tilde{X}_2 \right) \right] R.$$ 

From Eq. (3.19) we already know how the second part transforms. The complete transformation is

$$R^T H^{(\dagger)} R = \frac{1}{2} (\lambda + \delta) \tilde{Z}_1 + \frac{1}{2} (\lambda - \delta) \tilde{Z}_2 + \frac{J}{2} (\tilde{X}_1 \tilde{X}_2 + \tilde{Y}_1 \tilde{Y}_2) \pm \frac{\Omega}{2} \tilde{X}_1.$$ 

This should look very familiar, since more or less all we did is undo the diagonalisation that led us here. The remaining difference to Eq. (3.18) is due to the driving frequency and thus frequency of the rotating frame we use being $\omega_2$ in one case and $\tilde{\omega}_2 = (\omega_1 + \omega_2)/2 + \lambda$ in the other (here).
At this point the analysis veers off compared to the two previous sections. If we apply the intermittent $X_1$ gates on the physical qubits, for consistency the same should go for the single-qubit gates before and after $U(t_{\text{gate}})$. Since this means that we introduce an error into the single-qubit gates, we can no longer use Eq. (3.17), which relied on the validity of Eq. (3.16). So we now need to compute the full matrix product in the trace including the single-qubit gates

$$\text{tr} \left[ \text{CNOT}^\dagger \left( ROR^\dagger \right) U \left( ROR^\dagger \right) \right].$$

This is simple enough for $F_2$, but to do this for $F_1$ we have to actually determine the corresponding single-qubit gates $O^{(0)}$ first.

Having done that though, we can continue basically as before. For simplicity we expand both $F_1$ and $F_2$ to second order in $J$ and $\Omega$ (see also Fig. 3.4)

$$F_1 \approx 1 - \frac{2J^2}{5\Delta^2} \left\{ 2\sqrt{2} \left[ 2\Omega^2 + \left( \Omega^2 - \Delta^2 \right) \text{sgn} \Omega - \Delta^2 \right] \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J\Omega} \right) - 5\Omega^2 
+ 2 \left( \Delta^2 - \Omega^2 \right) \text{sgn} \Omega - 2\sqrt{2} \left( \Omega^2 - \Delta^2 \right) \sin \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J |\Omega|} \right) + 11\Delta^2 \right\}$$

$$F_2 \approx 1 - \frac{2\Omega^2}{5\Delta^2} - \frac{2\Omega J}{5\Delta^2} \left\{ 2\sqrt{2} \sin \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J\Omega} \right) + 1 \right\} - \frac{J^2}{20\Delta^4} \left\{ -(121 + 3\pi)\Omega^2 
+ 48\Delta^2 + 2\sqrt{2} \left( 4\Delta^2 - 9\Omega^2 \right) \sin \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J\Omega} \right) + 4\Omega^2 \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{2J\Omega} \right) 
+ 2\sqrt{2} \left[ 4(\pi - 3)\Delta^2 + (23 - 8\pi)\Omega^2 \right] \cos \left( \frac{\pi (\Delta^2 + \Omega^2)}{4J\Omega} \right) \right\}. $$

![Figure 3.4: Echo in dressed basis, but with single-qubit gates acting on the physical qubits, same parameters as in Fig. 3.2.](image-url)
3.3 Echo and Simple Single-Qubit Gates

There are several things to note here. By the same reasoning as above the zeroth order in $J$ is no different from the previous sections. Taking $\Omega \ll J$ is allowed without negatively impacting fidelity; it is apparently a feature of the dressed qubits. But in contrast to the previous case where we applied the appropriate single-qubit gates in the dressed basis, here the fidelities do not automatically reach unity in the limit of $\Omega \to 0$. The limit of $J \to 0$ is still required to right the single-qubit gates.

We note that the behaviour around $\Omega = 0$ is slightly peculiar here, as can be seen in Fig. 3.5.

3.3.4 Comparison

Looking at Fig. 3.6, we have a clear winner in the dressed basis, where echo performance is concerned. On the other hand if our qubit basis is in fact the undressed
one, this kind of echo is not a good idea (not that we had reason to believe it was).

If we want to use the dressed qubit basis, but can only apply single-qubit gates in the undressed basis, for strong drives we might as well be working entirely in the undressed basis, as the fidelities behave similarly in this parameter regime. For weak drives though this mixture still performs quite well. In particular the simple single-qubit gate setup \( F_2 \) can hold its own here (see Fig. 3.7).

As was clear from the beginning, the simple single-qubit gates only work for weak drives, after which their fidelity generally falls off as \( \Omega^2 \).

For \( \Omega/2\pi \) below 10 MHz, fidelities above 99.9% can in principle be reached even with the simple single-qubit gates, especially when operating completely in the dressed basis.

### 3.4 Spectator Qubits: CR Gate as Three-Qubit Problem

An advantage of the CR gate is that it only uses fixed-frequency qubits and microwave control drives. This requires an always-on interaction between qubits though. And in a real quantum computer it is clearly not sufficient to be able to perform two-qubit gates between isolated pairs of qubits only. Instead we need a whole network of coupled qubits. Thus the realistic setup in which we want to perform a CR gate is never a pure two-qubit problem. Though the expectation remains that if the qubit frequencies involved are sufficiently different, so that the control drive is only (cross-)resonant with the one target qubit, the effect on far detuned qubits will be small and averages out.

In a way this is a similar problem to the one studied in Chapter 2. We examine the quality of supposed identity gates in the presence of qubit interactions. Thus we might wonder if it can be “solved” the same way by diagonalising the system Hamiltonian, and thus defining a new delocalised qubit basis. While in principle of course there exists an eigenbasis (even though we may not be able to determine it analytically), expressing a single (physical) qubit drive in it should lead to a multi qubit drive on all dressed qubits corresponding to physical qubits coupled to the driven one. Say there is a pairwise coupling between (physical) qubits 1, 2, and 3. Diagonalising it we define new qubits \( \tilde{1}, \tilde{2}, \text{ and } \tilde{3} \) that become identical to the physical qubits in the limit of vanishing interaction, e.g. \( \lim_{J \to 0} \tilde{Z}_i = Z_i \). Then if we drive qubit 1 at the frequency of qubit 2 in hopes of inducing a CR gate between qubits \( \tilde{1} \) and \( \tilde{2} \), in the new qubit basis the drive on qubit 1 should transform not
only to a drive on qubit 2 but also to a non-resonant one on qubit 3, which is an additional source of errors.

To quantify this, for a start, I consider only one additional qubit which is not supposed to be acted on, a so-called spectator qubit. Analogously to Eq. (3.4), the Hamiltonian in a frame rotating at the target-qubit frequency is now given by

\[ H = \frac{\Delta C}{2} Z_C + \frac{\Delta S}{2} Z_S + \frac{\Omega}{2} X_C + \frac{J_{CT}}{2} (X_C X_T + Y_C Y_T) + \frac{J_{CS}}{2} (X_C X_S + Y_C Y_S) + \frac{J_{TS}}{2} (X_T X_S + Y_T Y_S), \]

where \( \Delta_i = \omega_T - \omega_i \) are the detunings from the target qubit frequency \( \omega_T \) for the control and spectator qubit \( i = C, S \), and \( J_{ij} \) are the coupling strengths between qubits \( i \) and \( j \), with \( i, j \in \{C, T, S\} \).

In this case, while the Hamiltonian is still time-independent in this frame (under the same RWA as before), it cannot be exponentiated analytically any more. To still get an approximate analytical expression for the time-evolution operator, the couplings to the spectator qubit (terms proportional to \( J_{CS} \) and \( J_{TS} \)) are treated in time-dependent perturbation theory. That means we go to an interaction picture with respect to

\[ U_0(t) = \exp \left[ -it \left( \frac{\Delta C}{2} Z_C + \frac{\Delta S}{2} Z_S + \frac{\Omega}{2} X_C + \frac{J_{CT}}{2} (X_C X_T + Y_C Y_T) \right) \right], \]

and then compute the interaction picture time-evolution operator up to first order as

\[ U_I(t) = 1 - i \int_0^t U_0^\dagger(\tau) \left[ \frac{J_{CS}}{2} (X_C X_S + Y_C Y_S) + \frac{J_{TS}}{2} (X_T X_S + Y_T Y_S) \right] U_0(\tau) \, d\tau. \]

Performing the integral shows this only has an oscillatory dependence on \( t \) which bodes well for using this approximation even for the large gate time \( t \to t_{gate} \). It also supports the idea that the effect of the additional couplings may average out.

Leaving the interaction picture and applying the previously determined single-qubit gates \( O^{(0)} \) while setting the time to the previously determined gate time should give a unitary that is close to a CNOT gate between control and target qubit with a rotation of the spectator qubit at its transition frequency, at least for small couplings \( J_{ij} \),

\[ U = O' U_0(t_{gate}) U_I(t_{gate}) O, \quad U_{ideal} = \text{CNOT}_{CT} \exp \left( -\frac{i\Delta s t_{gate}}{2} Z_S \right). \]

Here \( U \) is expanded in the \( J_{ij} \) up to first order (specifically to first order in \( \lambda \) for \( J_{ij} \to \lambda J_{ij} \), \( ij = CT, CS, TS \), i.e. all couplings are treated as equally weak). The result is of the form

\[ V = U_{\text{ideal}}^\dagger U = 1 + i\lambda A + \mathcal{O}(\lambda^2) \]
with $A$ hermitian and traceless. This implies that within first order the average fidelity as defined by Eq. (3.11) is equal to 1. Nevertheless in this case there is actually a way to process the information contained in $A$ as a nontrivial fidelity. Extending the computation to second order will give

$$V = 1 + i\lambda A + \lambda^2 B + \mathcal{O} \left( \lambda^3 \right)$$

with some operator $B$. This result will then have to be unitary up to the same order

$$V^\dagger V = 1 + \mathcal{O} \left( \lambda^3 \right).$$

This yields a condition for the hermitian part of the second order, since

$$V^\dagger V = 1 + \lambda^2 \left( B + B^\dagger + A^2 \right) + \mathcal{O} \left( \lambda^3 \right) = 1 + \mathcal{O} \left( \lambda^3 \right),$$

i.e.

$$\frac{B + B^\dagger}{2} = -\frac{A^2}{2} \implies B = \frac{B + B^\dagger}{2} + \frac{B - B^\dagger}{2} = -\frac{A^2}{2} + \tilde{B}.$$

Thus there remains some antihermitian contribution $\tilde{B}^\dagger = -\tilde{B}$ that would have to be determined from the second order calculation. But it turns out that for this specific problem of computing the fidelity, it is not necessary to know more about $\tilde{B}$. For the average fidelity we are interested in $|\text{tr} V|^2$, which since $A$ is traceless is given by

$$|\text{tr} V|^2 = \left| \text{tr}1 - \frac{\lambda^2}{2} \text{tr} A^2 + \lambda^2 \text{tr} \tilde{B} + \mathcal{O} \left( \lambda^3 \right) \right|^2.$$

Since $A$ is hermitian, so is $A^2$ and its trace is real, while $\tilde{B}$ which is antihermitian has a purely imaginary trace. Representing $|\cdot|^2 = (\Re \cdot)^2 + (\Im \cdot)^2$, it is clear that within second order $\text{tr} \tilde{B}$ does not contribute, as it acquires a prefactor of $\lambda^4$

$$|\text{tr} V|^2 = 64 - 8\lambda^2 \text{tr} A^2 + \mathcal{O} \left( \lambda^3 \right).$$

Thus with Eq. (3.11) and $d = 8$ the fidelity is given by

$$F = 1 - \frac{\lambda^2}{9} \text{tr} A^2 + \mathcal{O} \left( \lambda^3 \right)$$

which after inserting the result for $A$ and simplifying gives the second order fidelity

$$F = 1 - \frac{J^2_{\text{CS}}}{72\Omega^2} \left[ 4 \left( 16 + \pi^2 \right) \Omega^2 \Delta_C^2 + 4 \left( 8 + \pi^2 \right) \Delta_C^4 + \pi^4 \Omega^4 \right] - \frac{4J^2_{\text{TS}}}{9\Delta_S^2}$$

$$- \frac{4J^2_{\text{CS}}}{9\Delta_S^2} \left[ \Omega^2 \left( \Delta_C + \Delta_S \right) \left( 3\Delta_C + \Delta_S \right) + 2\Delta_C^2 \left( \Delta_C + \Delta_S \right)^2 + \Omega^4 \right]$$

$$+ \left( \frac{4\Omega^2 J^2_{\text{CS}}}{9\Delta_S^2 \left( \Delta_C^2 + \Omega^2 \right)} + \frac{4J^2_{\text{TS}}}{9\Delta_S^2} \right) \cos \left( \frac{\pi \Delta_S \sqrt{\Delta_C^2 + \Omega^2}}{2\Omega J_{\text{CT}}} \right) - 1 \right]$$

$$+ \frac{4J^2_{\text{CT}}}{9 \left( \Delta_C^2 + \Omega^2 \right)} \left[ \cos \left( \frac{\pi \Delta_S \left( \Delta_C^2 + \Omega^2 \right)}{2\Omega J_{\text{CT}}} \right) - 1 \right] \right].$$

(3.20)
3.4 Spectator Qubits: CR Gate as Three-Qubit Problem

Figure 3.8: Fidelity, with minima at 0 and $\Delta_\pm = \pm \Delta C \sqrt{1 + (\Omega/\Delta C)^2}$.

A sketch can be seen in Fig. 3.8. The $J_{TS}$ contribution diverges for $\Delta_S \to 0$, i.e. when target and spectator qubit have the same frequency, so precisely when the (cross-)resonance condition is also satisfied by the spectator-qubit. Less obviously the $J_{CS}$ contribution has a divergence at $\Delta_S = \Delta C (\omega_S = \omega_C)$ at $\Delta_S = \text{sgn}(\Delta C) \sqrt{\Delta_C^2 + \Omega^2} = \Delta C \sqrt{1 + (\Omega/\Delta C)^2}$ is the broader one. There are oscillatory corrections whose amplitudes become larger for $\Delta_S \to 0$. Since the cosines come with positive prefactors the fidelity can be upper-bounded by setting the cosines to 1

$$ F \leq 1 - \frac{J_{CT}^2}{72\Omega^2 (\Delta_C^2 + \Omega^2)^2} \left[ 4(16 + \pi^2) \Omega^2 \Delta_C^2 + 4(8 + \pi^2) \Delta_C^4 + \pi^2 \Omega^4 \right] - \frac{4J_{TS}^2}{9\Delta_S^2} - \frac{4J_{CS}^2}{9 (\Delta_C^2 + \Omega^2)(\Delta_C^2 - \Delta_S^2 + \Omega^2)^2}$$.

We can also compare Eq. (3.20) to the previously obtained result Eq. (3.12) when setting $J_{CS}$ and $J_{TS}$ to 0. The functional dependencies are the same, there is only a difference in one prefactor owing to the dependence of Eq. (3.11) on dimension. A simple calculation shows that if we compare a fidelity $f_n$ in dimension $d = 2^n$ to the fidelity $f_{n+1}$ in dimension $d' = 2^{n+1}$, where the unitary operators to be compared are extended by the same single-qubit unitary on the additional qubit Hilbert space, the results obtained from Eq. (3.11) differ for finite $n$

$$ 1 - f_{n+1} = \frac{2^{n+1} + 2}{2^{n+1} + 1} (1 - f_n) \, . $$
or more generally going from a fidelity $f_d$ in $d$ dimensions to a fidelity $f_{d'}$ in $d' \geq d$ dimensions gives

$$1 - f_{d'} = \frac{(d + 1) d'}{(d' + 1) d} (1 - f_d).$$

Either way in this case ($d = 2^2$ to $d' = 2^3$) the prefactor differs by $10/9 = 80/72$. So the results are consistent with each other.
4 Measurement

We have seen that the cross-resonance gate works very similarly in two different bases. And while the difference between the two bases is small, a change of basis between them is still not entirely trivial, since it corresponds to a two-qubit gate. What then is the “correct” basis, if such a thing exists?

One way to try to answer this question is to look at the measurement process. At the end of the day we want to measure our qubits, e.g. to extract some results or do error correction. Then the basis our measurement projects on defines the qubit basis.

4.1 Measurement Model

A common measurement implementation is to have each qubit couple dispersively to its own readout resonator which is driven and then measured using homodyne or heterodyne detection. The basic difference between the two methods is that homodyne detection measures one quadrature and heterodyne detection measures two orthogonal quadratures while introducing noise. Both work by using a beam splitter to mix a strong coherent signal from a local oscillator (LO) with the output signal from the readout cavity. This way the output is mostly noise and information is gained slowly, and incrementally, inducing a continuous measurement in the limit of an infinitely strong LO. Implementation-wise the two methods differ in the frequency of the LO, it is the same frequency as the input drive for homodyne detection and a different frequency for heterodyne. Both are covered in [21].

For two possible measurement outcomes, as should be the case when measuring a qubit, all the information is contained in a single quadrature. If we chose to measure exactly this quadrature with homodyne detection, there should not be much of a difference between homo- and heterodyne. So for simplicity we will only use homodyne detection when we want to describe a realistic measurement in the following. But first we will review how the coupling between qubit and cavity enables us to measure the qubit by measuring the cavity.

We start from the Hamiltonian

\[
H = \omega_a a^\dagger a + \omega_b b^\dagger b + g \left( a^\dagger \sigma^- + a \sigma^+ \right) + \sum_{i=1}^{2} \left[ -\frac{\omega_i}{2} Z_i + g_i \left( b^\dagger \sigma^- i + b \sigma^+ i \right) \right]
\]
where qubits 1 and 2 with transition frequencies $\omega_1$ and $\omega_2$ are coupled via a bus resonator $b$ with resonance frequency $\omega_b$ via Jaynes-Cummings couplings of strength $g_1$ and $g_2$ respectively and qubit 1 is additionally coupled to a readout resonator $a$ with resonance frequency $\omega_a$ with coupling strength $g$ (see Fig. 4.1). We choose to study this model in the current section because it is the smallest setup that can still see non-trivial interaction of the single-qubit measurement with the two-qubit coupling.

In the dispersive regime (for all couplings) we can again use a Schrieffer-Wolff transformation to eliminate the resonator-qubit couplings in favour of effective qubit-qubit interactions. Since we now have two resonators coupled to the same qubit this will also induce an effective coupling between the resonators mediated by qubit 1. The transformation is of the familiar form

$$H_{\text{eff}} = H_0 + \frac{1}{2} [V, S], \quad \text{with } S = \frac{g}{\omega_1 - \omega_a} (a^\dagger \sigma^-_1 - a \sigma^+_1) + \sum_{i=1}^{2} \frac{g_i}{\omega_i - \omega_b} (b^\dagger \sigma^-_i - b \sigma^+_i)$$

where $V$ is the sum of all interaction terms in $H$, i.e. those proportional to some $g_{(i)}$, and $H_0 = H - V$. This gives

$$H_{\text{eff}} = \left(\omega_a + \frac{g^2}{\omega_a - \omega_1} Z_1\right) a^\dagger a + \left(\omega_b + \sum_{i=1}^{2} \frac{g^2_i}{\omega_i - \omega_b} Z_i\right) b^\dagger b - \frac{1}{2} \left(\omega_2 + \frac{g^2_2}{\omega_2 - \omega_b}\right) Z_2$$

$$- \frac{1}{2} \left(\omega_1 + \frac{g^2_1}{\omega_1 - \omega_b} + \frac{g^2}{\omega_1 - \omega_a}\right) Z_1 + \frac{g_1 g_2}{2} \left(\frac{1}{\omega_b - \omega_1} + \frac{1}{\omega_a - \omega_1}\right) (a^\dagger b + ab^\dagger)$$

$$+ \frac{g_1 g_2}{2} \left(\frac{1}{\omega_1 - \omega_b} + \frac{1}{\omega_2 - \omega_b}\right) (\sigma^+_1 \sigma^-_2 + \sigma^+_1 \sigma^+_2).$$

(4.1)

We want to neglect the occupation of the bus resonator, $b^\dagger b \to \langle b^\dagger b \rangle \to 0$, move the readout resonator to a frame rotating at its resonance frequency $\omega_a$, and neglect the resonator coupling term in a rotating wave approximation. The latter is justified because the readout resonator frequency is far detuned from all other frequencies. The Hamiltonian we are then left with is of the form

$$H = \chi Z_1 a^\dagger a - \frac{1}{2} \sum_{i=1}^{2} \omega_i Z_i + J \left(\sigma^+_1 \sigma^-_2 + \sigma^+_1 \sigma^+_2\right)$$

(4.2)

with (re-)definitions for the new parameters following from comparison to Eq. (4.1).

The standard procedure would then be to also move the two qubits to a frame rotating at their respective resonance frequencies, make a RWA to drop the interaction term and keep only the dispersive shift

$$H_{\text{meas}} = \chi Z_1 a^\dagger a.$$  

(4.3)
This describes a shift of the resonator frequency dependent on the state of qubit 1.

**Example**  A conceptionally simple example capturing the essence of a possible measurement scheme based on Eq. (4.3) is looking at the time evolution of an arbitrary state of qubit 1 when the resonator is initialised in a coherent state $|\alpha\rangle$

$$e^{-iH_{\text{meas}}t} \left( \psi_0 |0\rangle + \psi_1 |1\rangle \right) |\alpha\rangle = \psi_0 |0\rangle |\alpha e^{-i\chi t}\rangle + \psi_1 |1\rangle |\alpha e^{i\chi t}\rangle. \quad (4.4)$$

Initially in a product state, over time the qubit becomes more entangled with the resonator until a maximum is reached at time $t = \frac{\pi}{2|\alpha|}$ where for a large coherent state amplitude $|\alpha|$ the two resonator states $|\pm i\alpha\rangle$ are almost orthogonal

$$\langle -i\alpha | i\alpha \rangle = e^{-2|\alpha|^2}.$$  

Measuring the coherent state of the resonator then corresponds to a good approximation to a measurement of the qubit state in the $Z$-basis. This is assuming an instantaneous strong measurement of the resonator following unitary evolution in contrast to the continuous homodyne measurement discussed before, and serves only to illustrate the principle.

So the operator we want to measure in this scheme is $Z_1$. But from Eq. (4.2) it is apparent that this is not a quantum nondemolition (QND) measurement, i.e. the measurement operator $Z_1$ does not commute with the rest of the Hamiltonian, at least not with $\sigma_U^+ \sigma_U^- + \sigma_U^- \sigma_U^+$ that is. It is only approximately, in the sense of Eq. (4.3), QND. Being QND means that repeating the measurement yields the same result, so a quite desirable quality in a measurement.

It might thus be impossible to answer the question with which we opened this chapter should we find that the measurement is too non-QND to be described as a projection on any qubit basis. But some descriptions should still be better than others.

### 4.2 Four-Outcome Measurement Approximation

If we move Eq. (4.2) to the dressed basis the resonator will couple to both of the redefined qubits. This seems problematic, given that we want to implement a single-qubit measurement. The following sections will be devoted to examining this measurement problem more closely.

Going to the dressed basis via Eq. (3.13), $Z_{1/2}$ transform as

$$RZ_{1/2}R^\dagger = \cos^2 \theta \tilde{Z}_{1/2} + \sin^2 \theta \tilde{Z}_{2/1} \mp \sin 2\theta \left( \tilde{\sigma}_1^+ \tilde{\sigma}_2^- + \tilde{\sigma}_1^- \tilde{\sigma}_2^+ \right).$$

For now we want to neglect the interaction term $\left( \tilde{\sigma}_1^+ \tilde{\sigma}_2^- + \tilde{\sigma}_1^- \tilde{\sigma}_2^+ \right)$ in $Z_{1/2}$ in the spirit of a rotating wave approximation. Admittedly it is not entirely clear if this is a better approximation than neglecting the interaction term already in Eq. (4.2) by a RWA. Basically it comes with an extra factor of $\chi$ in front now which should make
the RWA better. This problem can also be explored with a Magnus expansion, a tool from the field of average Hamiltonian theory, which provides an algorithm to find an operator $\Omega$ such that the time evolution with respect to a time-dependent Hamiltonian can be written as $\exp(-i\Omega t)$. In this case we would explicitly go to the rotating frame and compute the Magnus expansion of the then time-dependent Hamiltonian. The result is not entirely conclusive either though, since we also have the scaling with the photon number, and not only $\chi$, which produces terms $\propto (a^\dagger a)^2$ in second order which potentially should not be neglected. We will return to this question later.

This approximation changes the spectrum of our “measurement operator” from two values, $\pm 1$ for $Z_1$, to four for $\cos^2 \theta \tilde{Z}_1 + \sin^2 \theta \tilde{Z}_2$ with the two additional eigenvalues slightly smaller in magnitude $\pm \cos 2\theta = \pm 1/\sqrt{1 + (J/\delta)^2} \approx \pm 1 \pm \frac{1}{2} (J/\delta)^2$.

Making this basis change with the given approximation in our measurement model Eq. (4.2) gives

$$RHR^\dagger = \chi \left(\cos^2 \theta \tilde{Z}_1 + \sin^2 \theta \tilde{Z}_2\right) a^\dagger a - \frac{1}{2} \sum_{i=1}^{2} \tilde{\omega}_i \tilde{Z}_i.$$ 

Simplifying notation let our model Hamiltonian be

$$H = \chi (Z_1 + \epsilon Z_2) a^\dagger a - \frac{1}{2} \sum_{i=1}^{2} \omega_i Z_i.$$  \hspace{1cm} (4.5)

Let us build a most simple, phenomenological measurement model that still captures the essential two-qubit dynamics. To this end we will follow the style of section II of reference [5].

We want to do a homodyne measurement of the readout cavity and see

1. how well this realises a $\tilde{Z}_1$ or $Z_1$ measurement, and
2. how it affects the coupled qubit ($\tilde{Z}_2$).

From Eq. (4.5) we expect a strong measurement, i.e. one with a high signal-to-noise ratio (SNR), to perform a two-qubit measurement. Thus we would want to keep the SNR below some threshold so as not to be able to resolve four different eigenvalues. We want to implement a single-qubit measurement after all, which does not disturb the state of any other qubit.

We assume that the signal we measure is proportional to the eigenvalue of the measured state $(Z_1 + \epsilon Z_2) |ij\rangle = (i + \epsilon j) |ij\rangle$, where as an exception we for once refer to states by their eigenvalue, so $Z = |+1\rangle \langle +1| - |-1\rangle \langle -1|$ instead of $|0\rangle \langle 0| - |1\rangle \langle 1|$. Given the two qubits are in state $|ij\rangle$, due to (photon shot) noise the probability for measuring a signal $s$, $p_{ij}(s) \, ds$, is given by a Gaussian distribution with variance $\sigma^2 = 1/(\tau_f \text{SNR})$ and mean $i + \epsilon j$, where $\tau_f$ is the measurement time.

$$p_{ij}(s) \, ds = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(s - i - \epsilon j)^2}{2\sigma^2}\right] \, ds.$$
4.2 Four-Outcome Measurement Approximation

Figure 4.2: Probability densities for measuring signal \( s \) given qubits are in state \( \{|11\}, |10\}, |01\}, |00\} \) (peaks from left). Variance \( \sigma \) should be chosen such that the overlap between the two left and the two right peaks is minimised, while the overlap between peaks on the same side of zero is maximised, corresponding to being able to distinguish the states of qubit 1 but not those of qubit 2. This obviously depends on the distance \( 2\epsilon \) between peaks.

A sketch can be seen in Fig. 4.2.

We put the threshold for discriminating between \( \pm 1 \) eigenvalues of qubit 1 at \( s = 0 \), i.e. upon measuring \( s \geq 0 \) we say we have measured qubit 1 in state \( |\pm 1\rangle \). Conversely if we know a measurement with the result say \( -1 \) has occurred, we conclude that an \( s \in (-\infty, 0) \) was measured.

The measurement operator associated with measuring \( s \) is

\[
M(s) = \sum_{i,j=\pm 1} \sqrt{p_{ij}(s)} \, ds \, |ij\rangle \langle ij|.
\] (4.6)

Now if we only know the outcome (“\( \pm 1 \)”), but not which \( s \) specifically was measured, the state after the measurement is described by a (potentially mixed) state \( \rho_f \) which sums all the possible final states given a pre-measurement state \( |\psi\rangle \)

\[
\rho_f = \int_{s \geq 0} M(s) \, |\psi\rangle \langle \psi| \, M(s)^\dagger \equiv \mathcal{E}^\pm (\langle \psi| \langle \psi|).
\]

More generally we could also replace \( |\psi\rangle \langle \psi| \) by a mixed state \( \rho \). For every component \( |ij\rangle \langle kl| \) we can compute the integrals over the two Gaussians (from \( s = 0 \) to \( \infty \) and
Chapter 4 Measurement

\( s = -\infty \) to 0 respectively) which gives error functions

\[
\mathcal{E}^\pm (\rho) = \frac{1}{2} \sum_{i,j,k,l=\pm 1} \langle ij | \rho | kl \rangle \left( 1 \pm \text{erf} \left( \frac{i + k + \epsilon (j + l)}{2\sqrt{2}\sigma} \right) \right) \\
\times \exp \left( -\frac{(i - k + \epsilon (j - l))^2}{8\sigma^2} \right) |ij \rangle \langle kl |.
\]

For \( \epsilon \ll 1 \), the \( 1 \pm \text{erf} \) term realises a projection on \(|\pm 1 \rangle \langle \pm 1|_1 \) in the limit of a perfect measurement \( \sigma \to 0 \), but the exponential then also suppresses off-diagonal terms of the second qubit; i.e. the measurement of the first qubit causes dephasing on the second qubit.

An alternative description of the measurement operation \( \mathcal{E}^\pm \) is possible in terms of Kraus operators

\[
\mathcal{E}^\pm (\rho) = \sum_i M_i^\pm \rho M_i^\pm \dagger.
\]

Taking \( \{E_{ij} = |ij \rangle \langle ij|\} \) as an operator basis of the subspace spanning \( \mathcal{E}^\pm \) we can define a \( \chi \)-matrix representation

\[
\mathcal{E}^\pm (\rho) = \sum_{i,j,k,l} E_{ij} \chi_{ijkl} E_{kl}^\dagger \\
\chi_{ijkl} \equiv \frac{1}{2} \left( 1 \pm \text{erf} \left( \frac{i + k + \epsilon (j + l)}{2\sqrt{2}\sigma} \right) \right) \exp \left( -\frac{(i - k + \epsilon (j - l))^2}{8\sigma^2} \right)
\]

and by diagonalising the \( \chi \)-matrix determine the Kraus operators [12]

\[
\chi_{ijkl} = \sum_{a,b} m_{ijab} d_{ab} m_{klab}^\dagger \\
\implies M_{ab}^\pm = \sqrt{d_{ab}} \sum_{i,j} m_{ijab}^\pm E_{ij}.
\]

In practice it is not that easy to diagonalise \( \chi \). Therefore we will do so perturbatively, expanding in \( \exp \left( -\frac{1}{2\sigma^2} \right) \), and then applying (non-/)degenerate perturbation theory to the leading order result. Apart from that we also assume that the ratio \( \epsilon/\sigma \ll 1 \). This is just expressing the condition that the measurement should not resolve differences of order \( \epsilon \) in the eigenvalues. But then there is still another scale appearing in the problem which is \( x = \epsilon/\sigma^2 \). We assume here that \( x \lesssim 1 \) and also expand in \( x \). Even though \( x \) could be slightly bigger than \( 1 \), the mistake we make in this series expansion is not overly big. What we can at least exclude as a somewhat trivial case is \( x \gg 1 \), because this would imply that

\[
\epsilon \ll \sigma \ll \frac{\epsilon}{\sigma} \ll 1
\]

so the coupling to the second qubit is absolutely negligible and we also have a near perfect measurement of the first qubit.
4.2 Four-Outcome Measurement Approximation

In leading order there are two Kraus operators; for outcome “+1” they are given by

\[
M_1^+ = |+1\rangle \langle +1|_1 \left\{ 1 - \frac{\epsilon^2}{8\sigma^2} - \frac{e^{-\frac{1}{2\pi \sigma^2}} (4 + \frac{\epsilon^2}{\sigma^2})}{8\sqrt{2\pi}} + \frac{e^{-\frac{1}{2\pi \sigma^2}} \epsilon}{2\sqrt{2\pi \sigma}} Z_2 \right\}
\]

\[
+ \langle -1|_1 \left\{ \frac{1}{16} e^{-\frac{1}{2\pi \sigma^2}} \left[ 8 - \frac{(\sigma^2 - 2) \epsilon^2}{\sigma^4} \right] + \frac{e^{-\frac{1}{2\pi \sigma^2}} (\sqrt{2\pi \sigma} + \pi) \epsilon}{4\pi \sigma^2} Z_2 \right\}
\]

\[
M_2^+ = |+1\rangle \langle +1|_1 \left\{ \frac{e^{-\frac{1}{2\pi \sigma^2}} \epsilon^2}{4\sqrt{2\pi \sigma^2}} + \left\{ \frac{e^{-\frac{1}{2\pi \sigma^2}} (3\sigma^2 + 1) \epsilon}{4\sqrt{2\pi \sigma^2}} - \frac{\epsilon}{2\sigma} \right\} Z_2 \right\}
\]

\[
+ \langle -1|_1 e^{-\frac{1}{2\pi \sigma^2}} \left\{ \frac{1}{12\pi \sigma} \left[ \pi \left( \frac{(1 - 3\sigma^2) \epsilon^2}{\sigma^4} + 6 \right) - 6\sqrt{2\pi \sigma} \right] - \frac{\epsilon}{48\sigma^3} \left[ -\frac{\epsilon^2}{\sigma^4} + 6\sigma^2 \left( \frac{\epsilon^2}{\sigma^4} + 2 \right) - 12 \right] Z_2 \right\}
\]

If we neglect all terms \( \propto e^{-\frac{1}{2\pi \sigma^2}} \), basically neglecting the possibility of a measurement error, the dominant Kraus operator is just the correct measurement operator (slightly reduced in norm)

\[
M_1^+ \approx |+1\rangle \langle +1|_1 \left( 1 - \frac{\epsilon^2}{8\sigma^2} \right)
\]

and the next-to-leading order Kraus operator is proportional to \( Z_2 \), describing the dephasing we already expected

\[
M_2^+ \approx |+1\rangle \langle +1|_1 \frac{\epsilon}{2\sigma} Z_2.
\]

For outcome “−1”, the Kraus operators \( M_{1/2}^- \) are the same as \( M_{1/2}^+ \) when switching \( |\pm 1\rangle \langle \pm 1| \) to \( |\mp 1\rangle \langle \mp 1| \) and \( Z_2 \) to \(-Z_2\).

The simple RWA-style approximation in the dispersive coupling term in the dressed basis creates a QND measurement model. This would explain four distinct measurement outcomes being observed in this two-qubit setup at high SNRs. It also predicts dephasing on the coupled qubit when treating it as a single-qubit (=two-outcome) measurement.

The model can also straightforwardly be expanded to multiple coupled qubits.

While this paints a neat little picture, it is still not clear how good the initial and essential approximation is. How much sense does it make to describe a non-QND single-qubit measurement in terms of a weak QND two-qubit measurement? Section 4.3 aims at supplementing this analysis with a numeric approach.
4.3 Stochastic Master Equation Evolution

“Certainly nothing fluctuates in the Schrödinger equation; indeed, the Schrödinger equation describes no realized happenings of any sort – no realized events; it governs the time evolution of probabilities of events. To actually realize events, the probabilities must be put into action, to play out as a stochastic process. But here is the sticking point: the playing out is not unique, not only in the trivial sense that the throwing of a die yields different answers on every throw, but because the very shape of the die is not uniquely defined from within the Schrödinger equation itself.” – Howard Carmichael, Auckland, January 2007, preface to Statistical Methods in Quantum Optics

To really capture the non-QND nature of the problem and its effects we have to analyse it in full. While this becomes difficult to do analytically, it is entirely possible numerically (with some precision).

The tool at hand to model a realistic measurement is stochastic calculus. The time-evolution according to the Schrödinger equation provides a complete description of the state of a closed system. To perform a measurement though we need to extract information from the system making it no longer closed. Now an open (Markovian) system is usually described by a (Lindblad) master equation. This is a differential equation for density matrices, since an open system in general does not stay in a pure state when interacting with and becoming entangled to an environment. But this describes the average evolution of the system. If it is in a superposition of eigenstates of our measurement operator, we want a measurement to randomly, with a set probability, select only one of these eigenstates (assuming they are non-degenerate) and project onto it.

This is where stochastic calculus comes in. It provides a description of the incremental evolution to what usually is an eigenstate of the measurement operator in the form of the stochastic master equation (SME). Like the (non-stochastic) master equation it acts on density matrices. But in the case of an ideal measurement where each channel carrying information out of the system is monitored with 100% efficiency, an initially pure state remains pure, and the SME can be translated into a stochastic Schrödinger equation (SSE) mapping pure states to pure states. A derivation and discussion of both can be found in Wiseman and Milburn [21] whose notation we will adopt for the most part.

4.3.1 Ideal Measurement

If we assume that the only loss channel of our coupled qubits plus readout resonator system is the cavity leaking photons into a transmission line which is monitored
with homodyne detection, the stochastic master equation is given by
\[
\frac{d\rho(t)}{dt} = -i[H, \rho(t)] + \kappa \left( \frac{1}{2} a^\dagger a \rho(t) - \frac{1}{4} \rho(t) a^\dagger a \right) dt + \sqrt{\kappa} \left[ \frac{1}{2} \rho(t) + \rho(t) a^\dagger - \langle a + a^\dagger \rangle \rho(t) \right] dW(t),
\]
where \( \kappa \) is the cavity linewidth and \( dW \) is the Wiener increment satisfying
\[
dW^2 = dt, \quad \langle dW \rangle = 0.
\]

If we neglect the qubit-qubit coupling and move to a rotating frame as in Eq. (4.3), we have a pure single-qubit measurement. For \( H_{\text{meas}} \) to have an informative, non-zero expectation value, we need to drive the resonator out of vacuum. A drive term \( \epsilon e^{i\omega t} a + \epsilon^* e^{-i\omega t} a^\dagger \) becomes time-independent in the rotating frame, such that
\[
H = \chi Z a^\dagger a + \epsilon a + \epsilon^* a^\dagger.
\]

If we just consider the master equation without the measurement term (\( \propto dW \)), it is clear that eigenstates of \( Z \) are stationary under this evolution. Thus we can replace \( Z \) by its eigenvalue \( \sigma \) and by solving the equation separately for the two eigenstates reduce the problem size to the resonator Hilbert space. We will search for a coherent state steady state solution \( \rho_{ss} = |\alpha\rangle\langle\alpha| \) with
\[
0 = \frac{d\rho_{ss}}{dt} = -i \left[ \chi \sigma a^\dagger a + \epsilon a + \epsilon^* a^\dagger, \rho_{ss} \right] + \kappa \left( \alpha \rho_{ss} a^\dagger - \frac{1}{2} a^\dagger a \rho_{ss} - \frac{1}{2} \rho_{ss} a^\dagger a \right).
\]
It can easily be confirmed that such a solution exists for
\[
\alpha = \alpha_\sigma = \frac{-ie^*}{\sigma + i\chi}. \quad \sigma = \frac{2|\epsilon\chi|}{\kappa^2 + \chi^2}
\]
This means there is a phase space separation between \( \pm 1 \) eigenstates of \( Z \) in steady state of
\[
|\alpha_+ - \alpha_-| = \frac{2|\epsilon\chi|}{\kappa^2 + \chi^2}
\]
which for a given \( \kappa \) is maximised by \( \chi^2 = \kappa^2/4 \). Setting \( \kappa \) to 2\( \chi \)
\[
\alpha_\sigma = -\frac{e^*}{\sqrt{2\chi}} \frac{\sigma + i}{\sqrt{2}},
\]
so we can have \( \epsilon \) be real and all the information about \( \sigma \) will be in the \( a + a^\dagger \) (\( x \)) quadrature. So from now on we will assume \( \epsilon \) to be real and set \( \kappa = 2\chi \). Defining
\[
x = \sqrt{\kappa} \left( a + a^\dagger \right)
\]
it is
\[
\langle \alpha_\sigma | x | \alpha_\sigma \rangle = 2\sqrt{\kappa} \Re \alpha_\sigma = -\frac{\sqrt{2}e\sigma}{\sqrt{\chi}}.
\]
From the SME we thus expect the measurement current

\[ J_{\text{hom}} = \langle x \rangle + \frac{dW}{dt} \]

to converge to \( \pm \epsilon \sqrt{2/\chi} \) on average indicating a measurement of \(|\pm 1\rangle\).

### 4.3.2 Quantum Process Tomography

In this section we will derive how to determine the operation corresponding to the evolution according to a stochastic master equation. The derivation uses ideas similar to those in [14, 6] to arrive at an operation and then applies quantum process tomography to it as described in [12].

The SME can be derived by applying the Kraus operators corresponding to the measurement outcomes, e.g. detection of a photon, and then renormalising. The latter necessarily introduces non-linearity into the equation. For example, if \( \rho_n = \rho(t = n\delta t) \) is the state of the system after \( n \) time steps \( \delta t \), it is completely determined by the measurement record or equivalently the corresponding Kraus operators

\[
\rho_n = \frac{M_n \rho_{n-1} M_n^\dagger}{\text{tr} \left( M_n \rho_{n-1} M_n^\dagger \right)} = \frac{M \rho_0 M^\dagger}{\text{tr} (M \rho_0 M^\dagger)}, \quad \text{with } M = M_n M_{n-1} \ldots M_1 = \prod_{i=1}^n M_i. \tag{4.8}
\]

Each trajectory can be described in the above form, potentially with different \( M \), where the denominator gives the probability for this trajectory. We then group different measurement records into a small number of outcomes, e.g. by whether the integrated signal

\[
\int \frac{dJ_{\text{hom}}}{dt} = \int (\langle x \rangle dt + dW)
\]

is positive or negative, \( \pm \). For every distinct outcome we can define an operation

\[
\mathcal{E}(\rho_0) = \frac{\sum_i M_i \rho_0 M_i^\dagger}{\text{tr} \left( \sum_i M_i^\dagger M_i \rho_0 \right)} \tag{4.9}
\]

where the sum is over all trajectories leading to that outcome, and the \( M_i \) here corresponds to \( M \) in Eq. (4.8). This potentially mixed state gives the action of the measurement on an initial state \( \rho_0 \) if we only know the (group of) outcome(s), e.g. \( \pm \) or \( \pm \), and not the specific trajectory that produced it. That is we average over all possible trajectories that could have produced that outcome weighted by their probabilities and then renormalise again by what is the probability to get this outcome.

To determine \( \mathcal{E} \) from a numeric simulation or an experiment we need to sample a very large number of trajectories. But we would also need to know the probability of each trajectory. In a numeric simulation we can substitute the normally distributed Wiener increment by a discrete version \( dW = \pm \sqrt{\delta t} \), the validity of which is based on the central limit theorem. This makes the calculation of the trajectory probability...
especially simple, since in this case every (possible) trajectory is equally likely. Then we only need to take an equal weight superposition

$$\mathcal{E}^\pm (\rho_0) = \frac{1}{|F^\pm (\rho_0)|} \sum_{\rho_f \in F^\pm (\rho_0)} \rho_f$$

$$F^\pm (\rho_0) = \{ \rho_f : \text{ integrating SME from } \rho_0 \text{ gives final state } \rho_f \text{ and } \int dJ_{\text{hom}} \geq 0 \}.$$  

We have already noted that $\mathcal{E}$ is not a linear operation. But if we would need to do the above for every possible initial state $\rho_0$ to fully determine $\mathcal{E}$, our simulation would never finish. There is a way around that though. We can define a trace-decreasing linear operation

$$\tilde{\mathcal{E}} (\rho_0) \equiv \text{tr} \left( \sum_i M_i^\dagger M_i \rho_0 \right) \mathcal{E} (\rho_0) = \sum_i M_i \rho_0 M_i^\dagger$$  \hspace{1cm} (4.10)

which in its trace encodes the probability to get this outcome. Practically, to do this for a simulation, we can approximate the probability for an outcome by its relative frequency

$$\text{tr} \left( \sum_i M_i^\dagger M_i \rho_0 \right) \approx \frac{\# \text{ of runs with outcome}}{\text{total } \# \text{ of runs}} \sum_i M_i^\dagger M_i. \hspace{1cm} (4.11)$$

Note that the way we have derived Eq. (4.10) it is not a Kraus representation or at least not a minimal one, but once we have determined $\tilde{\mathcal{E}}$ we can easily find that one as well.

To fully determine a linear superoperator $\mathcal{L}$ it is sufficient to know its action on a basis of operators. Given a state Hilbert space basis $\{ |n \rangle : n = 1, ... d \}$ a possible choice for an operator basis is $|n \rangle \langle m|$ with $n, m = 1, ... d$. For any $n$ we can determine $\mathcal{L} (|n \rangle \langle n|)$ by choosing $|n \rangle$ as initial state. We cannot prepare $|n \rangle \langle m|$ since it is not a state, but it can be written as a superposition of states \[12\]

$$|n \rangle \langle m| = |+ \rangle \langle +|_{nm} + i |- \rangle \langle -|_{nm} - \frac{1+i}{2} |n \rangle \langle n| - \frac{1+i}{2} |m \rangle \langle m|$$

where $n \neq m$ and

$$|+\rangle_{nm} = \frac{|n \rangle + |m \rangle}{\sqrt{2}}, \quad |-\rangle_{nm} = \frac{|n \rangle + i |m \rangle}{\sqrt{2}}.$$  

Thus for a linear operator $\mathcal{L}$ it is

$$\mathcal{L} (|n \rangle \langle m|) = \mathcal{L} (|+ \rangle \langle +|_{nm}) + i \mathcal{L} (|- \rangle \langle -|_{nm}) - \frac{1+i}{2} \mathcal{L} (|n \rangle \langle n|) - \frac{1+i}{2} \mathcal{L} (|m \rangle \langle m|),$$  \hspace{1cm} (4.12)

i.e. for two qubits $(n, m = 1, 2, 3, 4)$ by preparing the four states $|n \rangle$, the six states $|+ \rangle_{n \neq m}$, and the twelve states $|- \rangle_{n \neq m}$, and applying $\mathcal{L}$ we can fully characterise $\mathcal{L}$. Here we have introduced some redundancy. Since

$$|- \rangle \langle -|_{nm} + |- \rangle \langle -|_{mn} = |n \rangle \langle n| + |m \rangle \langle m|$$
we need only consider six of the \(|-\rangle_{n \neq m}\) and get the other half for free. Or in other words, a basis for operators on two qubits contains exactly \((2^2)^2 = 16\) elements. Equivalently we could say we make use of

\[ \mathcal{L} (|n \rangle \langle m|) = \mathcal{L} (|m \rangle \langle n|) \dagger. \]

The linearity of the simulated \(\hat{E}\) depends on the quality of the approximation Eq. (4.11). To confirm the expected emergent linearity we can use the redundancy mentioned above to check if indeed

\[ \hat{E} (|-\rangle \langle -|_{nm}) + \hat{E} (|-\rangle \langle -|_{nm}) = \hat{E} (|n \rangle \langle n|) + \hat{E} (|m \rangle \langle m|). \]

Apart from that we also expect the non-selective operation, i.e. averaging over all different measurement outcomes, to be trace-preserving, and all operations to be positive, which are all things the simulation can be tested against.

### 4.3.3 Simulation Prescriptions

We specifically want to examine the effect of the qubit coupling on the measurement while keeping everything else as ideal as possible. Thus we can use the SME (4.7), with the Hamiltonian

\[ H = \chi Z_1 a^\dagger a - \frac{1}{2} \sum_{i=1}^{2} \omega_i Z_i + J \left( \sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+ \right) + \epsilon (t) \left( a + a^\dagger \right). \]

In this case though the SME is equivalent to a stochastic Schrödinger equation (SSE) [21]

\[ \frac{d}{dt} |\psi (t)\rangle = \left\{ -iH dt - \frac{\kappa}{2} \left[ a^\dagger a - \langle a + a^\dagger \rangle (t) a + \frac{1}{4} \langle a + a^\dagger \rangle^2 (t) \right] dt \right. \\
+ \left. \sqrt{\kappa} \left[ a - \frac{1}{2} \langle a + a^\dagger \rangle (t) \right] dW (t) \right\} |\psi (t)\rangle \]

implementing which saves resources compared to the SME.

Of course theoretically this is still a vector in an infinite Hilbert space, so some choice has to be made on how many and which states to keep for the resonator Hilbert space. One obvious choice for a basis are the Fock states which are also eigenstates of the resonator part of the bare Hamiltonian Eq. (4.2). For this basis, it is also clear how to cut off part of the Hilbert space, as you can chose to only keep states up to a maximum photon number that is very unlikely to ever be exceeded as long as the drive is weak enough.

The quantum process tomography is performed as explained in the previous section. Projectors on the qubit initial states form a basis for two-qubit operators while vacuum is chosen as initial state for the resonator. The resonator is driven for some time \(\tau\), after which the drive is turned off again, and we allow the resonator to relax back to vacuum, i.e. we wait for a time of several \(1/\kappa\). While the turning
4.3 Stochastic Master Equation Evolution

on and off of the drive can be made smooth, for this problem an instant toggling
\( \epsilon(t) \propto \theta(t) \theta(\tau - t) \) may also be possible without causing much harm.

In this case there are only two different Hamiltonians (drive turned on or off), so
the Hamiltonian part of the evolution can be performed at a higher precision at only
a constant time cost by once calculating \( U(t) = \exp(-iH(t)dt/2) \) for both versions
of \( H(t) \) and then for advancing the simulation by one time step, calculating

\[
|\psi(t + dt)\rangle = U^2(t)|\psi(t)\rangle + U(t) \left\{ -\frac{\kappa}{2} \left[ a^\dagger a - \langle a + a^\dagger \rangle(t) a + \frac{1}{4} \langle a + a^\dagger \rangle^2(t) \right] dt \\
+ \sqrt{\kappa} \left[ a - \frac{1}{2} \langle a + a^\dagger \rangle(t) \right] dW(t) \right\} U(t)|\psi(t)\rangle.
\]

Once the operation is determined and sufficiently tested for linearity, positivity
and so on, subsequent analysis of the operation should include finding the measure-
ment basis and basically testing how well the measurement does what it claims to
do, i.e. projecting onto the measurement basis (with high fidelity).
5 Conclusion and Outlook

The Makhlin invariants were demonstrated to be a valuable and educational tool in analysing two-qubit gates. They can act as a measure of the quality of (the nonlocal action of) a gate. Makhlin’s theory also allows us to calculate the single-qubit gates necessary to reach the desired two-qubit gates, which in turn can be compared to alternative single-qubit gates in terms of e.g. fidelity. This partly splits the analysis of a two-qubit gate implementation into nonlocal and local properties, which can be optimised separately (though not independently).

Using these tools we have gained new insights into the cross-resonance gate. We are now able to better understand the approximations involved and the limits in which they become exact. These limits potentially differ depending on the details of the implementation. Then it becomes important to remember the details not included in our simple models to decide which is appropriate.

In Chapter 4 we derived how to determine by simulation the operation corresponding to a measurement, thus gaining much deeper insight into its quality and errors. This simulation still remains to be performed (and thereby the reasoning behind its derivation put to a test). We already did some analytic modeling in the same chapter which may yet be verified by the numerics.

It may also be interesting to have a look at other measurement paradigms in this context. For example a simple, small change would be doing heterodyne instead of homodyne detection. Something more fundamentally different could be a fast, strong measurement model as proposed in [15].

When discussing the question of the qubit basis, we here settled on analysing whether the measurement favours one choice over another. Another aspect to consider is the compatibility of single-qubit gates with the choice of qubit basis. Derivations and discussions of single-qubit gates usually focus on the single-qubit problem for obvious reasons, in which case they are naturally applied to the physical qubits (lacking an alternative). How the fidelity of single-qubit gates is impacted by a small rotation of the qubit basis is another possible topic for future research.
Epilogue

Let us for a second dwell on one of the main assumptions that carried us through this thesis. We always assumed that $J$ had to be small, so that single-qubit operations still do what they are supposed to. Also the limit of $|J| \ll |\Omega|, |\Delta|$ was the only limit in which we found a good CNOT gate being implemented in the bare basis (via the Makhlin invariant analysis). Apart from that, we derived the $J$-coupling from a dispersive approximation which implies that $J$ has to be small.

All in all, there were many valid reasons to consider small $J$, and they still hold. And yet, from the point of view of just implementing a CNOT gate on two qubits, merit may be found in looking at the bigger picture. It may be there is more to the dressed basis than we thought.

In turns out that in the dressed basis we can find very good CNOT gates even in wildly different parameter regimes. Let us have a look at some examples.

Note: This is supposed to be purely a mathematical exercise at this point. We therefore use dimensionless quantities, but you can choose some arbitrary units. If you like, you can imagine frequencies to be given in GHz and times in ns, or whatever pair of (frequency) unit and its inverse you prefer.

As a reference point, we define our predicted gate time from the main text $t_0 = \frac{\pi \sqrt{\Delta^2 + \Omega^2}}{|2\Omega J|}$, and some metric for how well the Makhlin invariants match those of a CNOT gate $g = |G_1|^2 + |G_2 - 1|^2$. Quoted gate times $t$ are determined by numerical minimisation of $g$.

![Figure E.1: Makhlin invariants for $J = \Delta = \Omega = 0.1$ in bare (left) and dressed basis (right). Note the different time scales.](image-url)
Figure E.2: Makhlin invariants for $J = \Delta = 0.1$, at different drive strengths $\Omega = 1$ (left) and $\Omega = 10$ (right). Vertical lines mark CNOT gates in dressed basis at $t = 13.8$ with $g = 2.0 \times 10^{-19}$, and in bare basis at $t = 17.1$ with $g = 3.0 \times 10^{-4}$ for $\Omega = 1$. And for $\Omega = 10$ the gates are at $t = 13.3$ ($g = 3.2 \times 10^{-18}$) in the dressed basis and $t = 15.7 \approx t_0$ ($g = 1.9 \times 10^{-16}$) in the bare basis.

We start at $J = \Delta = \Omega = 0.1$ (pictured in Fig. E.1). In the bare basis we see a fairly complex oscillation, with a good CNOT gate at $t = 46.1$ ($g = 8.0 \times 10^{-10}$), and no good CNOT gate at $t_0 = 22.2$ ($g = 0.05$). In the dressed basis on the other hand the Makhlin invariants reach a great CNOT ($g = 1.6 \times 10^{-24}$) at $t = 32.1$ without additional oscillations.

We can create oscillations in the dressed basis too though by turning up the drive strength, as can be witnessed in Fig. E.2. But in the dressed basis this does not seem to impact the quality of the CNOTs.

If we now turn the coupling all the way up to $J = 10$ (or turn the detuning and drive strength down if you prefer to see it that way, $\Delta = 0.2$, $\Omega = 0.6$), there is no good CNOT gate in sight in the bare basis (see Fig. E.3). While $G_1$ is pretty small at $t_0 = 0.17$, $G_2$ is all wrong. The smallest $g = 0.06$ is found at $t = 0.08$. In the dressed basis on the other hand there is still a perfectly good CNOT ($g = 2.5 \times 10^{-27}$), even if it takes some more time $t = 3.7$.

One characteristic all plots of the Makhlin invariants in the dressed basis share so far, is that $G_1$ and $G_2$ seem to behave absolutely identically; more precisely, it looks as if

$$G_2 = 1 + 2G_1.$$ 

And indeed we can confirm that this is an exact equality. This increases the likelihood of finding an exact CNOT gate, since it is sufficient to solve only one equation,
As long as the ratio of the \( \tan \)-arguments is not a rational number, this equation should always have a solution (albeit not an analytic one).

So it seems like it is almost always possible to get an in principle perfect CNOT gate in the dressed basis. Keep in mind that so far this is only a property of the two-qubit model, and does not necessarily imply anything at all about the behaviour of two or more actual transmons. It shines a different light on the preceeding analysis though.

If it is true that we can always generate a perfect CNOT gate in the dressed basis at some time, then perhaps we should consider the CNOT in the bare basis possible only because in the limit of \( J \to 0 \) the bare basis is close to the dressed basis (and not the other way around!) and we can thus access the appropriate basis for the CNOT gate (approximately).

The possibility prompts some interesting question that warrant further analysis. Some immediate ones include:

- Does this work in any way for more than two qubits?
- Does this have any practical use, i.e. does it ever make sense to leave the small \( J \) limit?
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Bibliography


