Strong Coupling of Qubits to Spectrally Structured Media using Superconducting Circuits

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Abstract

The advent of superconducting quantum circuits as a robust scientific platform and contender for quantum computing applications is the result of decades of research in light-matter interaction, low-temperature physics, and microwave engineering. There is growing interest to use this advancing technology to study domains of light-matter interaction that were previously thought to be beyond experimental reach. Our work is part of an initiative to explore non-equilibrium condensed matter physics using photons instead of atoms. Open questions in this area currently pose significant challenges theoretically due to analytical complexity and system sizes which prohibit complete numerical simulations, thus experiment-based research has the potential to lead to significant advancements in this field. Here we examine phenomena that arise when moving beyond standard single-mode strong coupling towards the realm of many-body physics with light in two distinct directions.

First we study multimode strong coupling, where a single artificial atom or qubit is simultaneously strongly coupled to a large, but discrete number of non-degenerate photonic modes of a cavity with coupling strengths comparable to the free spectral range. This domain, which falls in between small, discrete and continuum Hilbert spaces, is experimentally realized by coupling a qubit to a low fundamental frequency coplanar waveguide cavity. In this system we report on resonance fluorescence and narrow linewidth emission directly resulting from complex qubit mediated mode-mode interactions.

In the second part we explore qubits strongly coupled to photonic crystals, which give rise to exotic physical scenarios, beginning with single and multi-excitation qubit-photon dressed bound states comprising induced, spatially localized photonic modes, centered around the qubits, and the qubits themselves. The localization of these states changes with qubit detuning from the band-edge, offering an avenue of in situ control of bound state interaction. Due to their localization-dependent interaction,
these states offer the ability to create one-dimensional chains of bound states with tunable interactions that preserve the qubits’ spatial organization, a key criterion for realization of certain quantum many-body models.

The unique domains of light-matter interaction discussed here are a subset of exciting research initiatives growing our general understanding of complex, strongly coupled quantum systems.
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To my family
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Chapter 1

Introduction

Interacting light and matter has been an area of prolific research - contributing to the advancement of fundamental quantum theory and leading to many groundbreaking applications, including sensors and lasers. The advent of precision quantum experiments and demonstration of strong coupling between a single photon and single atom has led to a rapid resurgence of the field, particularly in the direction of quantum information and computation [1, 2, 3].

In the broader context, this atom-light coupling gives rise to effective light-light interaction, enabling us to leverage the quantum building blocks of Circuit Quantum Electrodynamics (cQED), superconducting microwave cavities and quantum bits (qubits), to study non-equilibrium condensed matter physics with photons. Open questions in this area share ties with ongoing research of strongly correlated systems and currently pose significant challenges theoretically due to the many degrees of freedom, general analytical complexity, and lack of data from observations. The work presented in this dissertation is part of the growing effort to investigate this domain with targeted experiments and use observations to guide ongoing and future theoretical work. Here we examine interactions that arise when moving beyond the single-mode strong coupling limit towards the realm of many-body physics with light.
In Chapter 3, we explore a new domain of cQED where the qubit is simultaneously strongly coupled to many modes of a single harmonic cavity. The physics of multimode strong coupling bridges the gap between small, discrete and continuum Hilbert spaces, where complex many-body phenomena begin to emerge. We access this domain by strongly coupling a single qubit to a coplanar waveguide cavity that is two orders of magnitude longer than typical (∼70 cm vs. 7 mm). In this device, the coupling strengths between the qubit and the cavity modes are comparable to the free spectral range, which means that the rate at which a qubit can absorb a photon from the cavity is comparable to the round trip transit rate of a photon in the cavity. We study the response of the system to a continuous microwave drive and discover remarkably ultranarrow linewidth multimode emission, a signature of correlated spontaneous emission arising from strong mode-mode interactions mediated by the qubit. We push the boundary further by exploring the emission characteristics manifested in a system with even longer waveguide cavity (∼2 m), where the coupling surpasses the mode spacing, for comparison.

In the limit of an infinitely long cavity, the discrete set of modes can be described by a continuum, corresponding to an environment with a uniform density of states. One can tailor the density of states in such a way to move beyond a uniform distribution to that of a band-gap medium. We do this in Chapter 4 by coupling a qubit to a periodic, stepped impedance transmission line, analogous to one-dimensional optical photonic band-gap crystals. In the weak coupling limit, perturbation theory accurately predicts Purcell modification of qubit radiative decay due to the variable local density of states. However, in the strong coupling domain, a non-perturbative approach must be taken to capture system behavior. In this strong coupling condition, there is a new photonic mode that is exponentially localized around the qubit, which due to coupling with the qubit results in qubit-photon dressed bound states. These bound states introduce a new form of tunable and spatially localized inter-
action between qubits, which we experimentally and theoretically explore in a two qubit-crystal device.

These two distinct, yet related domains of light-matter interaction are a subset of ongoing research seeking to improve our general understanding of complex, strongly coupled quantum systems. In such explorations, theoretical modeling must go hand in hand with experiment for each to improve and offer insight relevant to the other. In this dissertation we rely on this ideology: using theory to inspire system design and experimental observations to motivate and support theoretical insights. While we successfully employ this strategy in many instances in this dissertation, these explorations mark early steps in long research endeavor that encompasses the field of light-matter interaction today.
Chapter 2

Circuit QED background

2.1 Superconducting qubits

The superconducting circuit implementation of a qubit that will be used throughout this thesis is the transmon [4, 5]. After reviewing fundamental principles of Josephson Junctions to orient the reader, we will examine key characteristics of the transmon. While there are a variety of superconducting qubits (e.g., fluxonium, tunable coupling qubit, flux qubit [6, 7, 8]) the transmon is the simplest to implement and its properties have been well-studied and understood. We note that while all of these are called ”qubits,” they are not the two-level systems quintessential to quantum optics. Rather, due to the inherent anharmonic energy levels, these circuits can be approximated as two or few-level systems in the appropriate parameter regimes. Thus at times it is essential to take into account higher transmon levels when looking to understand certain experimental observations.

The goal here is to design a circuit which, in certain parameter space or domain of operation, mimics the behavior of a two or few-level system. One can realize such a system by creating an anharmonic oscillator such that transition levels can be addressed individually and excitations of different energy are required to ”climb the
Figure 2.1: **a** Illustration of a Josephson junction, characterized by two superconducting electrodes separated by a thin insulating layer. **b** In the DC-SQUID configuration of Josephson junctions (symbolized as a square with ×), the total Josephson energy depends on magnetic flux Φ through the loop. **c** Transmon qubits feature a Josephson element (e.g., DC-SQUID loop) shunted by a large capacitance (Island 1 and Island 2), the latter enabling capacitive coupling between transmon and CPW. See main text for calculation of relevant capacitance terms. **d** A half-wave CPW cavity has voltage antinodes near the input and output capacitors (gaps in the center pin), optimal locations for the qubit to maximize coupling. Diagrams in this figure are not to scale.

ladder.” This is in contrast to a harmonic oscillator which features equally spaced energy levels and is made of linear elements (e.g., an LC oscillator).

Thus for an anharmonic oscillator we must include a nonlinear circuit element. Unsurprisingly, it is important that there is minimal intrinsic loss for a qubit circuit as these will limit qubit lifetime and function. In superconducting circuits the nonlinear element that is the building block for most qubits is the Josephson junction, an ideally dissipation-less element that we can use as a nonlinear inductor.

### 2.1.1 Josephson junctions

A Josephson junction (see Fig. 2.1a) comprises two superconducting electrodes separated by a thin insulating barrier and is also known as an SIS junction. In our devices, we fabricate the junctions using a three-step, double angle aluminum evaporation technique - where the second step is a careful oxidation of the aluminum to form the aluminum oxide insulating barrier (see Appendix C).
Electrons can travel between electrodes by quantum mechanically tunneling through the junction. We motivate use of these junctions as nonlinear inductors by studying the I-V relations. We define the electron current across the junction \( I_J \)

\[
I_J = I_0 \sin \delta
\]  

(2.1)

where \( I_0 \) is the critical current of the junction (below which these relations hold) and depends on properties such as area, and barrier thickness. \( \delta \) is the phase difference between the two superconducting electrodes. The voltage across the junction is then

\[
V = \frac{\Phi_0}{2\pi} \frac{d\delta}{dt}
\]  

(2.2)

where \( \Phi_0 = \frac{h}{2e} \) is the flux quantum.

\[
\frac{dI_J}{dt} = I_0 \cos(\delta) \frac{2\pi}{\Phi_0} V
\]  

(2.3)

This is the standard I-V relation of an inductor, \( V = L \frac{dI}{dt} \). (For comparison, \( I = C \frac{dV}{dt} \) for a capacitor.) Rewriting this formula reveals the nonlinearity of the inductance \( L_J \) resulting from the \( \cos(\delta) \) term.

\[
L_J = \frac{V}{\frac{dI_J}{dt}} = \frac{\Phi_0}{2\pi I_0 \cos(\delta)}
\]  

(2.4)

Thus the nonlinearity of the junction will impart nonlinearity to the qubit energy levels. For the purpose of qubit calculations, we define Josephson energy \( E_J = I_0 \Phi_0 / 2\pi \).

**2.1.2 DC-SQUID configuration**

While a single junction, constant \( E_J \), may be sufficient for some applications, at times we would like in situ control over the Josephson energy. A simple configuration
affording such control is the DC-SQUID loop (see Fig. 2.1b), featuring two junctions in parallel in a superconducting loop. Due to flux quantization in the loop, \( E_J \propto (E_{J1} + E_{J2})\cos(\pi\Phi/\Phi_0) \), where \( \Phi \) is the (applied) magnetic flux through the loop [4]. This sensitive dependence on magnetic field motivated the use of SQUID loops for magnetic field sensing for many decades.

In practice, we will never have perfectly identical junctions. We may also choose to intentionally vary the junctions for various reasons - i.e., reducing sensitivity to flux noise [9, 10] by limiting range of Ej tunability, or ensuring that frequencies of various components in a system will not collide regardless of magnetic field [11]. This leads to a modification of transmon questions as explained in [4, 5].

This parallel junction configuration is not the only method for introducing magnetic field tunability. In addition to another common design, the RF-SQUID which features a single junction in a loop, many other qubit circuits employ a variety of junction-loop designs [12, 13, 14] to engineer desired energy levels, interactions, and magnetic field dependences.

### 2.1.3 The transmon qubit

The transmon qubit is a Josephson junction(s) shunted by a large capacitance with the criteria that \( E_J \) is significantly larger than the charging energy \( E_C \). This criteria marks the critical evolution of the Cooper pair box charge qubit [15] to the transmon, which features significantly improved dephasing times due to decreased charge noise sensitivity and ease of use.

Colloquially, the two paddles of the capacitor are called superconducting “islands” and the junction(s) define the link through which Cooper pairs can tunnel between the islands. Intuitively, it is easy to visualize the transmon as a large dipole, foreshadowing that the qubit can be readily electrically coupled to the microwave environment via the large electric field between the capacitor islands. The exact geometry of the
islands and qubit – environment coupling play a central role in determining qubit behavior.

The charging energy $E_C = \frac{e^2}{2C \Sigma}$, where the total capacitance $C \Sigma$ can be well-estimated knowing the capacitance matrix (which includes the capacitance contributions of the qubit islands, CPW center pin, and CPW ground planes, but neglects the significantly smaller junction capacitance). We can obtain the capacitance matrix through numerical, DC finite-element simulation (e.g., Maxwell Ansys) of these elements (see labeled elements in Fig. 2.1c).

From this capacitance matrix (i.e., $C_{I1,I2} =$ capacitance between elements I1 and I2) we can calculate,

$$C_{I1:Env} = C_{I1:G1} + C_{I1:G2} + C_{I1:CP}$$  \hspace{1cm} (2.5)  \\
$$C_{I2:Env} = C_{I2:G1} + C_{I2:G2} + C_{I2:CP}$$  \hspace{1cm} (2.6)  \\
$$C_{I:Env} = \left( \frac{1}{C_{I1:Env}} + \frac{1}{C_{I2:Env}} \right)^{-1}$$  \hspace{1cm} (2.7)  \\
$$C \Sigma = C_{I1:I2} + C_{I:Env}$$  \hspace{1cm} (2.8)

where $C_{I1:Env}$ ($C_{I2:Env}$) is the capacitance of qubit island I1 (I2) to the environment and is used to calculate the total capacitance of the islands to the environment $C_{I:Env}$. The capacitance ratio $\beta = \frac{C_{I:Env}}{C \Sigma}$ is a key metric [4] for determining the strength of qubit – waveguide coupling.

As mentioned, the critical condition for the transmon is $E_J/E_C >> 1$. This criterion is a direct consequence of balancing anharmonicity and charge dispersion dependences on $E_J/E_C$, which decreases algebraically and exponentially in $E_J/E_C$ respectively (see [4] for details). From a usage perspective, we typically target a 300-400 MHz anharmonicity which allows for fast qubit manipulation pulses while retaining sufficient insensitivity to charge noise.
We can estimate the anharmonicity from the approximate transmon energy levels [4]

\[ E_m \simeq -E_J + \sqrt{8E_CE_J}(m + \frac{1}{2}) - \frac{E_C}{12}(6m^2 + 6m + 3). \]  

Comparing the transition energies \( E_{ij} = E_j - E_i \), anharmonicity is \( \alpha = E_{12} - E_{01} \simeq -E_C \). This assumes fixed Josephson energy; we can incorporate tunability via a SQUID loop by replacing \( E_J \) with

\[ E_J \propto \left| E_{J1} + E_{J2} \right| \cos(\frac{\pi \Phi}{\Phi_0}) \sqrt{1 + \left( \frac{E_{J1} - E_{J2}}{E_{J1} + E_{J2}} \right)^2 \tan^2(\frac{\pi \Phi}{\Phi_0})} \]  

however we note that this is not significant to the calculation of anharmonicity from qubit geometry.

From an experimental point of view - we want to reduce intrinsic loss and decay by choosing good qubit design. The limit to which this matters depends on the system that qubit will interact with or is coupled to. Thus in the scope of this thesis, we will not realize long qubit coherence times precisely due to the complex and strong coupling to structured environments. We refer the interested reader to other resources for optimization for long lifetimes.

### 2.2 Coupling qubits to microwave elements

We interact with and manipulate the qubit by coupling it to microwave circuit elements. In turn, these linear microwave circuit elements inherit ”qubit-like” properties from this coupling.

The prototypical coupling, central to quantum computing, is that between a qubit and a single microwave cavity mode. Such a cavity, that can be coupled to superconducting qubits, can be realized experimentally in a number of ways, e.g., a coplanar
waveguide (CPW) resonator (full, half or quarter-wave depending on boundary conditions), a lumped element resonator, a 3D cavity, a photonic crystal cavity, etc., [16, 17, 18].

In this work, we focus solely on circuits constructed from CPWs (see Sec. 4.1.1 for more details). In Fig. 2.1d, we illustrate the method in which a transmon qubit can be coupled to a half-wave CPW cavity. As will be discussed for each project, the physical orientation and placement of a qubit inside the larger microwave circuit is critical to device function and must be designed carefully. While some attributes can be simulated through finite-element solvers, for larger, more complex devices it is not computationally practical to simulate the entire circuit. Therefore, we limit simulation to key subsections of the circuit (e.g., coupling capacitances) and use iterative device fabrication and testing to improve device design as needed.

2.3 Light-matter interaction

The quintessential example of a system exhibiting light-matter interaction is a two-level system dipole coupled to a harmonic oscillator. The coherent, closed system is described by \((\hbar = 1)\),

\[
H = \frac{\sigma_z \omega_q}{2} + \Sigma_m \omega_m (a_m^\dagger a_m + \frac{1}{2}) + \Sigma_m g_m (\sigma^+ a_m + a_m^\dagger \sigma^-) \tag{2.11}
\]

where the first term captures qubit excitation, the second the bosonic modes of the cavity, and the third the dipole interaction between the two. The interaction term in this Jaynes-Cummings Hamiltonian is the result of performing the rotating wave approximation to eliminate excitation non-conserving terms such as \(\sigma^+ a_m^\dagger\), valid for systems where \(g_m \ll \omega_q, \omega_m\).
We can further simplify this Hamiltonian with the single-mode approximation provided that the coherent behavior of the system is determined predominantly by interaction with one mode.

\[
H_{JC,SM} = \frac{\sigma_z \omega_q}{2} + \omega_r(a^\dagger a + \frac{1}{2}) + g(\sigma^+ a + a^\dagger \sigma^-) \tag{2.12}
\]

Experimentally, this is most often due to either reduced coupling to other modes due to system design or large energy separation between the two-level system transition energy and the other modes. In circuit QED, the common design choice is to ensure the qubit interacts predominantly with the fundamental mode \((\omega_r = \omega_1)\) of the cavity, valid when \(g_1 \ll \omega_q < \omega_1\). Although we will rely on these two approximations in this chapter for the purpose of understanding the behavior of this simple system, they are not always desired or valid. Research in the regime of ultra-strong coupling \([19, 20, 21, 22, 23]\) specifically explores the Hamiltonian where the rotating wave approximation is not valid and the interaction term is instead \((a + a^\dagger)(\sigma^+ + \sigma^-)\).

In Chapter 3 we explore a system where the multimode nature of the cavity, and coupling between qubit and multiple modes must be retained.

The simplicity of the \(H_{JC,SM}\) is more readily revealed in matrix form, which is block diagonal

\[
\begin{pmatrix}
0 & 0 & \cdots & 0 \\
0 & \begin{pmatrix} \omega_r & g \\ g & \omega_r + \Delta \end{pmatrix} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \begin{pmatrix} n\omega_r & g\sqrt{n} \\ g\sqrt{n} & n\omega_r + \Delta \end{pmatrix}
\end{pmatrix}
\]

where the qubit frequency is given as \(\omega_r + \Delta\) and each 2x2 matrix along the block diagonal connects elements of the same excitation number, \(n\). From this form, one
could derive the dressed state eigenstates of the system in each excitation manifold (see David Schuster thesis for details).

Of course, in experiment there are always sources of incoherent behavior such as photon decay from the cavity to the input/output waveguides, $\kappa$, and non-radiative qubit decay, $\gamma_\perp$. Though often collectively called "non-radiative," this term includes qubit decay into any channel other than that of the cavity mode (or desired channel). With these two decay terms, we can define the strong coupling regime as $g > \kappa, \gamma_\perp$ which is readily accessible with superconducting circuits. To understand the implications of strong coupling, we will consider the standard resonant and dispersive limits.

### 2.3.1 Resonant Jaynes-Cummings

The energy level diagram in the resonant condition, $|\omega_r - \omega_q| << g$, is shown in Fig. 2.2a. In this parameter condition, the eigenstates of the system have both photonic and qubit-like contributions. Exactly on resonance the eigenstates are

$$|\pm\rangle = \frac{|g\rangle|n\rangle \pm |e\rangle|n-1\rangle}{\sqrt{2}}. \quad (2.13)$$
2.3.2 Dispersive Jaynes-Cummings

The energy level diagram in the dispersive limit, $|\omega_r - \omega_q| = \Delta >> g$, is shown in Fig. 2.2b. Rewriting the interaction term as a perturbative effect, to second order in $g/\Delta$

$$H \approx \frac{\sigma_z \omega_q}{2} + \omega_r (a^\dagger a + \frac{1}{2}) + \frac{g^2}{\Delta} \sigma_z a^\dagger a + \frac{g^2}{2\Delta} \sigma_z$$

(2.14)

where the third term can be intuitively understood as a qubit state dependent shift of the cavity frequency (useful for quantum non-demolition measurement of qubit state) or a cavity photon number induced shift of the qubit frequency. And the last term is a finite vacuum noise induced shift in qubit frequency.

2.3.3 Purcell effect

Modification of qubit radiative decay (spontaneous emission) $\gamma_\kappa$ into the cavity mode due to qubit-cavity coupling is captured by the Purcell-factor. This factor reflects the changing photonic and qubit-like contributions in the eigenstates of the system.

For comparison, at resonance the $|\pm\rangle$ single-excitation eigenstates decay at $\kappa + \gamma_\perp 2$, where typically $\kappa >> \gamma_\perp$ such $\gamma_\kappa \approx \kappa/2$. In the dispersive limit, $\gamma_\kappa \approx (\frac{\kappa}{\Delta})^2 \kappa$. There is similarly a change in cavity decay due to the finite non-radiative qubit decay.

In comparison, in Chapter 3 and 4 we will consider qubits coupled to vastly different photonic environments and thus will have significantly different Purcell modifications.

2.3.4 Free-space resonance fluorescence

In this final section we take a slight tangent to review resonance fluorescence of a qubit in free-space (as opposed to in a cavity [25, 26]). Resonance fluorescence is the emission response of the qubit to monochromatic, resonant drive. While we leave the
Figure 2.3: Transitions between high excitation manifolds (n and n+1 large such that \(\sqrt{n} \approx \sqrt{n + 1}\) so that energy level splitting within each manifold is approximately equal) in the dressed atom-drive picture reveals origin of triplet emission structure.

full derivation of resonance fluorescence and the various properties to be found in any quantum optics textbook [27], we note that one can gain valuable insight by simply considering the dressed-state picture which arises from a familiar Hamiltonian

\[
H_{RF} = \frac{\sigma_z \omega_q}{2} + \omega_d a^\dagger a + g(\sigma^+ a + a^\dagger \sigma^-)
\]  

(2.15)

where now \(\omega_d\) is the quantized drive field-mode. Fig. 2.3 depicts the origin of the Mollow triplet [28, 29, 30, 31] structure from transitions between energy levels of adjacent excitation manifolds. Resonance fluorescence beyond the simple case of a qubit in free-space requires adding additional terms to Eq. 2.15 e.g., a cavity field mode, mode-qubit, and mode-drive interaction terms. In Chapters 3 and 4 we explore resonance fluorescence when the qubit is coupled to a multimode cavity and photonic crystal instead of free-space.
Chapter 3

Multimode Strong Coupling

As discussed, single-mode single-qubit interaction is one of the most fundamental systems in circuit QED and quantum optics. Now well understood due to rigorous experimental and theoretical study, this interaction is a building block for engineering larger, more complex systems. However, moving beyond the single-mode strong-coupling approximation we quickly reach regimes of light-matter interaction that are unknown, both theoretically and experimentally.

Some interest in going beyond strong coupling has focused on the ultrastrong coupling limit, where the breakdown of the rotating-wave approximation results in excitation non-conserving terms [20, 19, 21, 22]. In contrast, the direction which we pursue is the simultaneous strong coupling of the qubit to numerous modes [32, 33, 34], leading to qubit mediated mode-mode interactions and many-body physics not present in the single mode problem. Unlike the spin-boson problem, where the continuum bosonic modes are treated as a bath for the qubit, in multimode strong coupling (MMSC) the dynamics of individual modes and finite time correlations between modes are essential. Furthermore, the study of MMSC cannot rely on the integrability present in the single mode and continuum problems [35], thus requiring new theoretical ideas for its study.
In this chapter, we will discuss our experimental realization of MMSC, in which a single artificial atom is simultaneously strongly coupled to a large, but discrete, number of non-degenerate photonic modes of a cavity with coupling strengths comparable to the free spectral range. Portions of this chapter appear in Phys. Rev. X 5, 021035 (2015), where we presented these results.

The closed system is described by the Hamiltonian:

\[ H = \frac{\hbar}{2} \omega_a \sigma_z + \sum_m [\hbar \omega_m a_m^\dagger a_m + \hbar g_m (\sigma^+ + \sigma^-)(a_m^\dagger + a_m)] \] (3.1)

where \( \omega_a \) is the qubit frequency, \( \sigma_{x,y,z} \) are Pauli pseudo-spin operators, and \( m \) represents cavity mode number. The modes of the cavity are equally spaced, \( \omega_m = m\omega_1 = m(FSR) \), where \( FSR \) is the free spectral range. Here, \( a_m^\dagger (\sigma^+) \) and \( a_m (\sigma^-) \) are mode (qubit) raising and lowering operators. The coupling strength of the qubit to the \( m \)th harmonic is \( g_m = g_1 \sqrt{m} \), where \( g_1 \) is the coupling constant to the fundamental cavity mode [5].

As there are many modes simultaneously interacting with the qubit, many modes can be coupled to each other during the typical lifetime of an excitation in the system, with the effective qubit mediated interaction rate between a pair of modes being \( \frac{g_m g_n}{(n-m)FSR} \), leading to a delocalization of the excitation across many modes.

To achieve MMSC, the coupling between qubit and cavity must be comparable to the free spectral range, which is made possible through use of a long cavity due to the scaling of \( g_n/FSR \) with cavity length, \( L \). Previously, long cavities have been used for novel comb generation, with a Kerr nonlinearity provided by the bulk medium [36]. Other unique multimode platforms have also been studied, including systems where a quasi-degenerate set of transverse modes of a cavity are coupled to ensembles of atoms in cavity QED [37, 38, 39], and degenerate lumped LC resonators are coupled to qubits in circuit QED [18]. In contrast, here the nonlinearity is provided by
a single qubit that is coupled strongly to a large set of longitudinal modes (the transverse dimension does not support modes in the microwave regime) of a long coplanar waveguide cavity.

3.1 Designing the long cavity device

To successfully realize the MMSC Hamiltonian in a device and to be able to meaningfully isolate and study the resulting interactions and dynamics, we must simplify the experimental realization and eliminate extraneous potential sources of complexity. This desire for simplification directly motivates our device design. To reiterate, for MMSC we require coupling between the qubit and the modes of the cavity near the qubit frequency to be comparable to the uniform mode spacing. The well-studied transmon qubit and established microwave cryogenic measurement chain are designed for operating in the several GHz range (3-8 GHz). Typically, the transmon is coupled to the fundamental mode of a cavity, which is in the same frequency range. However this choice is unsuitable for MMSC as not only would it be challenging to increase coupling between qubit and mode to the several GHz range, but also the higher modes of the cavity would fall outside the measurement bandwidth. Therefore, reducing the cavity mode spacing will simultaneously address both issues: matching readily feasible qubit-mode coupling strengths and populating the measurement window with many modes.

Thus the first task is to design an effectively one-dimensional cavity with low fundamental frequency, as close to an ideal harmonic oscillator as possible. As the frequency of a CPW cavity is inversely proportional to cavity length, increasing the length of the cavity will meet the low-frequency requirement. The harmonics of this cavity will be nearly uniformly separated due to the essentially constant dielectric constant of sapphire in the microwave frequency range, thus meeting the requirement
that the fundamental mode frequency and mode spacing (free spectral range, FSR) are equivalent such that \( \omega_m = m\omega_1 \).

The fundamental frequency of our cavity must be sufficiently small in order to be comparable to the coupling between the qubit and modes nearest in frequency to the qubit. This distinction of which modes must meet the coupling requirement is important due to the scaling of coupling with mode number and reduction of overall coupling strength with cavity size. Transmon qubits are dipoles whose coupling to a cavity mode is proportional to the strength of the mode’s electric field at the qubit location. Qubit coupling to the \( m^{th} \) mode of a \( \lambda/2 \) cavity is

\[
g_m = \frac{P_{12}E_m}{\hbar} \cos(k_m x_q) \tag{3.2}
\]

where \( P_{12} \) is the dipole matrix element and \( E_m \cos(k_m x_q) \) is the electric field of the mode at the qubit location. As all relevant mode wavelengths are at least two orders of magnitude longer than the qubit footprint, it is valid to approximate the qubit as a point dipole at \( x_q \).

The electric field of a photon in the fundamental mode of a cavity is

\[
E_1 = \sqrt{\frac{\hbar \omega_1}{\varepsilon_0 V_{mode}}} \tag{3.3}
\]

where, for a one-dimensional cavity of length \( L \), the mode volume \( V_{mode} \sim L \) and \( \omega_0 = FSR \sim \frac{1}{L} \). Thus the field of a photon in the \( m \)th mode at frequency \( \omega_m \) is \( E_m = E_1 \sqrt{m} \) and qubit-mode coupling \( g_m = g_1 \sqrt{m} \) [40]. However, while coupling increases with mode number, coupling to the fundamental mode decreases with cavity length, \( g_1 \sim \frac{1}{L} \).

We are able to balance the two competing rates and reach coupling strengths comparable to mode spacing with the reminder that we are concerned with the modes near the qubit frequency, not of a particular mode number. Therefore for an arbitrary
mode number $n$ near the qubit frequency, $g_n \sim \frac{1}{\sqrt{L}}$ and $\omega_1 \sim \frac{1}{L}$ yielding $\frac{g_n}{\omega_1} \sim \sqrt{L}$, thus making the long cavity approach feasible.

As an example, let us consider a 7 GHz fundamental cavity mode coupled to a qubit at a strength of 300 MHz. The 7 GHz mode has wavelength of about 9 mm in our devices. If we increase the cavity from 9 mm to 900 mm, the fundamental mode frequency drops to 70 MHz and coupling strength drops to 3 MHz. The mode at 7 GHz is the 100th mode and the coupling to the 100th mode is $3\sqrt{100}M\text{Hz} = 30M\text{Hz}$. As 30 MHz is indeed comparable to 70 MHz (in contrast to 300 MHz and 7 GHz) these parameters would realize MMSC.

From the perspective of balancing fabrication challenges and $\frac{g_n}{\omega_1}$, we chose to limit our substrate size to 1 inch x 1 inch. As the meandering cavity divided the ground plane on the device, the cavity design had to be made amenable to significant on-chip wire-bonds to connect the ground planes together and suppress slot-line modes. Additionally, to increase device yield, the CPW dimensions (center pin width and distance between center pin and ground planes) were intentionally increased. Incorporating these design parameters, the final device (see Fig. 3.1.1) comprised a 68 cm long CPW cavity, yielding a fundamental mode frequency of $\sim 90$ MHz. With this cavity length, we anticipated that the qubit coupling to the first mode would be $\sim 4$ MHz and to the 75th mode would be $\sim 35$ MHz.

The final considerations for the design were the coupling capacitances defining the ends of the cavity, which set the mode decay rates into the input and output waveguides. As mode voltage at the capacitors decreases with cavity length, for fixed capacitance the mode linewidths $\kappa$ decrease with increasing cavity length. Therefore to accommodate the significantly longer cavity, we increased the cavity coupling capacitances to retain a moderate $\kappa_n \sim \text{MHz}$. From the perspective of our experimental goals, the linewidth of the modes needed to be sufficiently narrow such that modes could be selectively addressed with a drive tone (without also driving neigh-
boring modes) while not being internal loss dominated. Using the Ansys Maxwell finite-element electromagnetic field simulator, we designed an interdigitated coupling capacitor to realize the desired mode decay rates and, for simplicity and symmetry, chose to use identical capacitors on the input and output.

We coupled a transmon qubit, flux tunable via a SQUID loop, near one end of the resonator - an anti-node for all the cavity modes [4]. Qubit design prioritized strengthening coupling to the cavity, possibly at the expense of a reduced intrinsic qubit lifetime. However the latter consequence was not significant in this device as the qubit spontaneous decay rate was limited to 1-2 MHz due to a strong multimode Purcell effect - the dominant source of qubit decay [5].

The qubit frequency could be tuned via a local flux bias line and/or a large external superconducting magnet. While both were used in this experiment, the local flux bias line had a limited tuning range (beyond which there was significant heating of the device and fridge), so the magnet was predominantly used.

While the cavity itself was symmetric, input and output were defined such that the qubit was positioned near the output capacitor (see Fig. 3.1.1). Coherent RF drive, at frequency $\omega_d$, was introduced only via the input port, while radiative decay of cavity photons occurred via both input and output ports - with only the output port connected to the amplification chain.

### 3.1.1 Chip modes

In addition to the desired cavity modes, the spectrum of our actual device will inevitably include spurious modes. Common sources of undesired modes include chip modes set by the substrate dielectric and dimensions, sample packaging or box modes, and unintentional modes set by lithography such as slot-line modes due to insufficient grounding. Of these three classes, we can minimize the emergence of the latter two with careful sample preparation.
The decrease in chip mode frequencies with increasing chip area is taken as an unavoidable fact as this decrease can only be resolved by complex fabrication techniques (e.g., superconducting vias through the dielectric substrate) beyond the scope of our fabrication facilities.

Our sapphire substrate, approximately $25 \text{ mm} \times 25 \text{ mm} \times 0.5 \text{ mm}$ with an index of refraction $n \sim 1.77$, has its lowest frequency chip mode around 4.8 GHz. While this may be detrimental for other experiments, for MMSC a chip mode falling within the measurement window is not a critical defect precisely due to the abundance of cavity modes which are closer to resonance with and more strongly coupled to the qubit. In Sec. 3.2.1 transmission measurements are to qualitatively identify spurious modes.

3.2 Transmission characterization

3.2.1 Bare cavity mode characterization

Prior to investigating the multimode effects arising due to coupling with the qubit, it is helpful to characterize the bare modes of the cavity with a high power transmission measurement. *High power* is determined empirically by increasing input power until no further shifts in mode frequency or amplitude are detected - indicating that photon powers at the device are high enough to reveal the classical or bare cavity characteristics. Thus, while the cavity is always coupled to the qubit due to the physical device design, we can still easily gain intuition on the cavity and learn of any possible defects or qualities that are unrelated to the qubit or coupling. In practice, these defects typically arise from box modes (device packaging), chip modes (substrate size), slot line modes (insufficient ground plane-ground plane wire bonds), or other error in device fabrication.
Figure 3.1: **Device for achieving MMSC.**  

- **a** A low fundamental frequency, $\omega_0/2\pi \sim 92$ MHz, is realized by fabricating a meandering 0.68 m coplanar waveguide resonator on a 25 mm x 25 mm sapphire substrate. The capacitive coupling at the input and output ports allows coupling of radiation into and out of the resonator, at rates $\kappa_m/2\pi \sim 0.5$-4 MHz. Red rectangles show coupling capacitors. Blue rectangle encloses qubit. 
- **b** Symmetric interdigitated capacitors define the cavity boundaries and couple radiation to the transmission lines. 
- **c** A transmon qubit is capacitively coupled to the center pin near the output capacitor, an antinode for all modes. SQUID geometry allows for tuning qubit frequency, $\omega_a$, via the flux bias line (shown) or the external magnet [4]. The grid-like pattern in ground plane pins flux vortices. Scale bars denote **a** 10 mm, **b** 100 $\mu$m, and **c** 100 $\mu$m.

In Fig. 3.2.1a we plot $S_{21}$ over a 5 GHz frequency range. There is variation in $S_{21}$ amplitude - but we attribute the slow variation to the fixed, frequency-dependent measurement chain (amplifiers, isolators, etc.) that was not calibrated out of the measurement or otherwise optimized. Taking a closer look at the mode frequencies (see Figs. 3.2.1b-c), we extract a fundamental mode frequency of approximately 92.5 MHz and note that there is minimal disorder in mode spacing across this wide frequency range. The modes are well-resolved with minimal frequency-overlap as set by the large capacitors on either end of the CPW cavity. The linewidths fall within the
Figure 3.2: **High power transmission measurement for mode characterization**

**a** High power $S_{21}$ transmission measurement shows bare cavity modes by saturating out qubit effects. The fixed, frequency-dependent measurement chain (amplifiers, isolators, etc.) contribute to the variation in $S_{21}$ background over the 5 GHz frequency range. The lowest frequency chip mode for the $\sim 24.89 \times 24.89 \times 0.5$ mm sapphire substrate should be approximately 5 GHz and would likely disrupt the mode spectrum. However, this is not a critical defect due to the abundance of modes which are closer to resonance with and more strongly coupled to the qubit. **b-c** Harmonics of the $\sim 92.5$ MHz cavity show minimal deviation from the ideal case. There are two small pockets of disorder but the mode spacing is predominantly consistent. **d** Mode linewidths span from $\sim 0.5$ to 3 MHz, with moderate disorder. Linewidth is expected to scale with the square-root of the mode number. For the purposes of this experiment, the modes are sufficiently well separated such that each mode can be easily, individually resolved.
range of 0.3 to 5 MHz, which is only a few percent of the mode spacing. Ideally, it
should scale with square root of the mode number [5].

From the overall uniformity of the spectrum, we can conclude that most of the
possible box, slot-line, and other spurious modes were successfully suppressed by
extensive ground-plane wire-bonding and radiation shielding. We still see evidence
of unwanted modes via the distorted mode spectra near 5 and 7 GHz. We attribute
these interferences to modes coupling to unavoidable chip modes, the lowest of which
is approximated to be $\sim 4.8$ GHz for this size sapphire substrate (see Sec. 3.1.1). As
our experiments were conducted sufficiently far from these modes, we consider them
to have negligible impact on the results presented here.

3.2.2 MMSC - low power transmission measurement

Now, we turn to transmission measurements at the single photon power level such that
the effects of the qubit are no longer saturated. Measuring transmission while tuning
the qubit frequency reveals that the qubit strongly couples to a vast number of modes
(Fig. 3.3a). In fact, we are able to follow the trail of avoided crossings for several
GHz as the qubit energy tunes through the uniformly dense mode structure that was
characterized in the previous section (Sec. 3.2.1). The smooth transitions between
subsequent avoided crossings show that the qubit is perpetually near resonance with
some mode and as such the dispersive approximation is never valid. In Figs. 3.3b-c,
the marked difference in the magnitude of the avoided crossings, and thus coupling
strength, is apparent.

For this experiment, we extract the couplings, $g_m$, in the multimode Jaynes-
Cummings (MMJC) Hamiltonian,

$$H = \frac{\hbar}{2}\omega_a\sigma_z + \sum_m \hbar\omega_m a_m^\dagger a_m + \sum_m \hbar g_m (\sigma^+ a_m + a_m^\dagger \sigma^-) \quad (3.4)$$
Figure 3.3: **Demonstrating multimode strong coupling**  

A Low power cavity transmission as qubit frequency is tuned with an applied flux bias. Vacuum Rabi avoided crossings are visible as the qubit is tuned into resonance with each mode (bright vertical lines spaced by $\sim 92$ MHz). It is apparent that the Vacuum Rabi splitting is comparable with the free spectral range (mode spacing), thus indicating that MMSC has been achieved. White rectangles are shown in b, c. The coupling $g_m$ grows with $m$: $g_1 \sqrt{m}$.  

A single mode fit of the splittings (white dashed line) is not accurate, as evidenced by the strongly shifted states near the central avoided crossing. A fit to the first manifold of the multimode Jaynes-Cummings incorporates all nearby polariton states, yielding $g_1 \sim 3.75$ MHz.

by fitting the avoided crossings to the first excitation manifold. In this Hamiltonian, $\omega_a$ is the qubit frequency, $\sigma_x$, $\sigma_y$, $\sigma_z$ are Pauli pseudo-spin operators, and $m$ represents cavity mode number. Here, $a_m^\dagger (\sigma^+)$ and $a_m (\sigma^-)$ are mode (qubit) raising and lowering operators. The coupling strength of the qubit to the $m$th harmonic is $g_m = g_1 \sqrt{m}$ where $g_1$ is the coupling constant to the fundamental cavity mode.

$$H = \begin{pmatrix}
\omega_a & g_1 & g_1 \sqrt{2} & \cdots & g_1 \sqrt{n} \\
g_1 & \omega_1 & g_1 \sqrt{2} & \cdots & 2\omega_1 \\
g_1 \sqrt{2} & \omega_1 & \ddots & \ddots & \vdots \\
g_1 \sqrt{n} & \cdots & \ddots & \ddots & \ddots \\
g_1 \sqrt{n} & \cdots & \cdots & \ddots & n\omega_1
\end{pmatrix}$$
Figure 3.4: **Dressed mode frequencies** Frequency difference between bare and dressed mode frequencies when qubit is fixed $\sim 6.38$ GHz for experiment (blue circles) and MMJC simulation (red star) shows agreement. Experimentally, bare and dressed mode frequency are found through high and low power transmission measurements, respectively.

Therefore, in this method the free parameters we vary to determine the fit are $g_1$, $\omega_1$, $\omega_{a,min}$, and $\omega_{a,max}$. Our fit yields $g_1/2\pi \sim 3.75$ MHz, giving rise to $g_{75}/2\pi \sim 32$ MHz. To reiterate, while the coupling to the fundamental mode is small, coupling to the modes near the qubit frequency (i.e. the 75th mode is near 7 GHz) is a significant fraction (over one-third) of the mode spacing, thus placing this system in the MMSC domain.

The single mode approximation visibly fails to model the data, as seen in Fig. 3.3c. Attempting to fit the central avoided crossing using a single-mode single-qubit model (dashed white line) understandably cannot capture the significant shifts to nearby modes nor the suppression of the avoided crossing (reduced from $2g_m$) due to the mode-mode proximity. Based on the close correspondence between the data and the MMJC fit, we determine that the MMJC Hamiltonian is a good representation of this system as desired.

A maximum qubit frequency around 6.9 GHz was measured at the onset of the experiment, but due to degradation this shifted to $\sim 6.7$ and $\sim 6.4$ GHz on subsequent cool downs. The device was operated near the maximum qubit frequency, for minimum flux noise, for most of the results reported in this chapter.
Looking at a single, fixed qubit frequency, we can take both high and low power transmission measurements to determine the frequency difference between the bare and dressed mode frequencies (see Fig. 3.4). We compare the experimentally observed mode shifts with simulation to confirm that the shifts are in agreement with the MMJC model. It is important to note that the number of total modes included in the simulation is a crucial parameter for obtaining comparable mode shifts. A mode cutoff that is too high predicts vastly larger, diverging shifts, while too low a mode cutoff is unable to capture the measured mode shifts above the qubit frequency. From the sensitivity of mode cutoff in the simulation, it seems that in experiment there also could be a fundamental limit to the number of modes that the qubit is coupled to. Recent theoretical work by Malekakhlagh et. al., presents a relevant discussion on a cutoff-free approach for cQED calculations [41].

3.2.3 Two tone spectroscopy

Two-tone spectroscopy or dispersive readout is a standard measurement technique which uses the dispersive shift of a mode to precisely determine the frequency of the qubit [42]. In our multimode strong coupling experiment, such spectroscopy shows that the mode frequency is affected not only by the qubit state, but also by population of the modes nearby to the qubit. This is yet another manifestation of mode-mode interactions mediated via the qubit. The magnitude of transmission, a proxy for the dispersive shift, is indicated by the colorbar in Fig. 3.5. As the qubit frequency approaches a mode, the strength of interaction between that mode and the measurement mode steadily increases.

This interaction was so strong that the measurement mode shifted substantially even when the qubit was over 200 MHz away. Thus the frequency of the measurement mode needed to be recalibrated for each flux voltage (y-axis) in Fig. 3.5. Furthermore, to track the qubit in this frequency range with sufficient contrast, the designated
Figure 3.5: Mode-mode interaction in dispersive readout. Tracking the change in dispersive shift for measurement mode, at $\omega_M$, with varying probe frequency, $\omega_p$, shows the impact of populating nearby modes. The magnitude of the dispersive shift is related to the detuning of a mode from the qubit (at 7.08GHz for $\phi_b = 0.6$). The qubit frequency is tuned using the on-chip flux bias line. Fainter curves are attributed to higher order processes. Horizontal black lines indicate a change of $\omega_M$ (6.469, 6.653, and 6.747 GHz from top to bottom), chosen to maintain sufficient distance from the qubit.

measurement mode needed to be changed such that it was sufficiently far away from the qubit. For each change of measurement mode, there is a horizontal black line in Fig. 3.5.

### 3.3 Resonance fluorescence

Having verified that our experimental realization indeed meets the requirements for MMSC, we continue towards our objective of better understanding the consequence of dominant qubit - multimode interactions. Given the system complexity, we choose to first focus our attention on resonance fluorescence: the quintessential quantum optics problem studying the response of a qubit to coherent resonant drive. While the emission spectrum is straightforward to observe experimentally, understanding
the spectrum and how it differs from the spectrum of a free space qubit has the potential to illuminate fundamental physics unique to MMSC.

To begin, let us review the drive power dependent emission response of a qubit to resonant drive in free-space. Experimentally, in cQED this was precisely achieved with a qubit coupled to an open 1D transmission line with linear dispersion [29, 43].

Strong resonant driving of a qubit in free space results in emission forming a three peaked structure known as the Mollow triplet, composed of a center peak and two symmetric sidebands [28]. The sidebands are displaced linearly from the central peak by the Rabi amplitude $\Omega$ and their widths are proportional to the system dissipation [25]. This phenomenon is commonly explained using the intuitive dressed state picture approach [31], where resonant drive dresses qubit levels to produce a drive power dependent energy level splitting. When the qubit is coupled to another environment other than free space, changes in emission behavior offer insight into the impact of the new coupling. For example, coupling of a qubit to a single mode cavity has been proven to strongly modify the Mollow triplet [30, 44, 45]. For weak coupling, the cavity passively filters the fluorescence, while for strong coupling, the sideband width is proportional to the coupling rather than the system dissipation [25, 26].

Similarly for our multimode cavity, if the cavity mode is weakly coupled to the qubit we might expect the mode to passively filter emitted photons, while the strongly coupled modes should significantly alter emission spectrum and characteristics. With this fundamental intuition we turn to the experiment.

Here the qubit frequency is maintained on resonance with the 74th mode of the cavity, circa 6.38 GHz (near the maximum qubit frequency for minimal charge noise). The coherent, continuous, drive tone is resonant with the qubit (and mode), and fluorescence is measured across a range of drive powers. Unlike the transmission measurements in the previous section which detect $\langle a(\omega) \rangle$, here we seek $\langle a^\dagger a(\omega) \rangle$, power spectrum measurement. Experimentally this can be done using a spectrum
Figure 3.6: **Multimode resonance fluorescence.**

a Power spectrum for varying drive power, $P_d$, when $\omega_d = \omega_a = \omega_{74}$, measured at more than 50 modes. Mode index $n$ is the relative detuning from the drive mode, $n = m - 74$. Power is measured in a 10 MHz window around each mode, excluding the driven mode ($n = 0$). Increasing drive power unveils fluorescence at farther detuned modes, strong emission from multiphoton processes, and complex multi-lobed fluorescence spectra. b The drive power corresponding to peak fluorescence for each far detuned mode shows a quadratic dependence on detuning, suggesting this fluorescence is due to cavity enhanced sideband fluorescence [26]. Modes near the drive frequency (see inset) do not follow the quadratic fit due to strong multimode interaction. c Detailed plot of $n = -30$ from a shows a multi-lobed structure in fluorescence spectrum. Bare mode frequency is denoted with a vertical white line. For d-g, $\omega_d = \omega_a = \omega_{68}$. d We explore the difference between the two lobes seen in c for several modes ($n = -36, -34, -32, -30, -28$, from bottom to top with individual curves vertically displaced for clarity) by measuring the total fluorescence power in a 6 MHz window while varying drive power. The drive powers corresponding to peak fluorescence move oppositely with mode number for the two lobes. e-g For modes near the drive ($n = -1, 1, 2$), strong multimode interaction further yields a more complex multi-lobed structure. Bare cavity mode frequencies are denoted with vertical white lines.
analyzer or a high speed digitizer with proper digital signal processing. We measure the power spectrum in 10 MHz windows around each mode, excluding the driven mode (relative mode index \( n = 0 \)), and, ignoring the unmeasured frequency ranges, compress the spectrum in Fig. 3.3a with drive power varied along the vertical axis.

For weak drive, there is no incoherent scattering to the other modes. At a stronger drive power, fluorescence appears simultaneously at multiple nearby modes (three of which are displayed in Figs. 3.3e-g). In addition to detecting bright fluorescence at these nearby modes (three on either side of the center mode) we also observe incoherent scattering at the center mode itself. As drive power is further increased, the simultaneous fluorescence at the nearby modes fades away while fluorescence begins to spread to more detuned modes. At an even higher power, the emission at the nearby modes reappears, but at the bare cavity mode frequencies. The change in emission frequency at each of these modes, approaching the bare cavity mode from higher frequencies with increasing drive power, is qualitatively the same for modes on either side of the drive and cannot be attributed to a simple AC Stark shift.

To analyze the power dependent spread of fluorescence towards increasingly detuned modes, we extract the drive power corresponding to brightest emission at each mode and plot this in Fig. 3.3b on a linear power scale. Strongest fluorescence is observed at mode \( m \) when it is resonant with the Rabi sideband. As the displacement of Mollow sidebands is proportional to drive amplitude \( \Omega \), this occurs [26] when detuning from the \( m \)th mode \( \Delta_m \equiv \omega_m - \omega_d \approx \Omega \). For far detuned modes the drive power needed to reach the peak fluorescence at these modes \( P^{\text{peak}}_d \approx \Omega^2 \), and hence \( P^{\text{peak}}_d \approx \Delta_m^2 \) (Fig. 3.3b). Thus the clear quadratic dependence is well captured by the Mollow triplet from free space resonance fluorescence. However, the model does not capture the high intensity of emitted light far beyond single photon levels. It also cannot explain the simultaneous onset of fluorescence at the six modes nearest the drive

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(Fig. 3.3b inset), a dramatic deviation from the quadratic sideband displacement with drive power.

In the process of studying fluorescence dependence in the far detuned modes, we additionally observe a multi-lobed fluorescence structure (see Fig. 3.3c for example) for each mode. From Fig. 3.3d, the drive power which results in the peak of the secondary lobe approaches twice that of the first lobe for increasing detuning $\Delta_m$, indicating the second lobe originates from two photon interactions. These two photon enhancements, resulting from higher order interaction vertices $\sigma^+ a_m^2$, are of strength $g_m^2/\Delta_m$, which in MMSC exceed the decay rates.

Two photon processes in single mode cavities, where $\Omega = 2\Delta_m$, have previously been observed [46, 47]. For MMSC, the multiphoton processes can progress via combinations of many different modes. The resonance condition for single and multiphoton processes is thus shifted away from $\Omega = p \Delta_m$, for $p \in \mathbb{Z}$. (See Sec. 3.5 for fluorescence theory).

In total we recorded fluorescence across more than 50 modes, where this limit was imposed by our measurement chain bandwidth and thus not indicative of device operation. At fixed drive power, emission is spread over many modes, with the simultaneous enhancement at many nearby modes, differentiating the multimode fluorescence from the single mode case.

The impact of dominant multimode effects become increasingly apparent as we approach modes closer to the qubit, with the appearance of an intricate multi-lobed structure (see Fig. 3.3e-g) and deviation of drive powers for brightest fluorescence deviating from the quadratic fit (see Fig. 3.3b inset). These effects arise when qubit-induced interactions between modes, $\frac{g_m g_n}{(n-m)FSR}$, for $n$ and $m$ near the drive, are comparable to the direct qubit-mode interaction, $g_m$ (See Sec. 3.5 for fluorescence theory). Competition between these coherent processes leads to the rich phenomena we see in the experiment.
3.4 Narrow emission linewidth

Beyond the multimode resonance fluorescence discussed in the previous section, we observe a dramatic reduction in emission linewidth. The fluorescence at far detuned modes, example in Fig. 3.3c, have linewidths that are roughly equal to that of the bare modes. For modes nearest the qubit the fluorescence linewidth is smaller than $\kappa_m$, e.g. for the nearest mode above being respectively 650 kHz vs. 1.1 MHz. Detuning the drive from the center mode unveils a linewidth narrowing by over an order of magnitude.
magnitude to 65 kHz (Fig. 3.7). The significance of this narrow linewidth is underlined when directly compared to the bare cavity mode linewidths (∼ MHz) and Purcell-limited qubit relaxation rate (∼ 2 MHz), which are the fastest decay rates in the system. The narrowest fluorescence occurs when the drive is detuned by 2 MHz from the center mode, with a steady reduction in linewidth as the drive approaches this frequency.

In the region where narrowing is observed, the linewidth and steady state photon number are observed to be inversely proportional, as has been previously suggested for the case of a single mode [48]. For our multimode cavity, the narrowing is in fact observed simultaneously for multiple modes at the same drive frequency, as depicted in Figs. 3.7c-d for the two modes nearest the drive. While the modes directly neighboring the center mode exhibit the sharpest linewidths of 65 kHz, the next nearest modes also display a narrowed fluorescence, ∼ 300 kHz. The multi-lobed power dependent structure of fluorescence also appears at the optimal detuned drive frequency, however, the linewidth of the second lobe is of order κₘ, for the nearby modes. For more distant modes, while fluorescence follows a similar ∆m² dependence, there is no narrowing apparent.

The drive dependent narrowing is not unique to these described experimental parameters. When we translate the drive and qubit to another set of modes, we observe equally narrow linewidth fluorescence which indicates that the process behind the simultaneous narrowing is generic in this system.

Furthermore while the qubit is essential for establishing the coherence, the effective Rabi rate is very insensitive to qubit frequency and thus the narrowing is as well; the narrowed fluorescence produced with the detuned drive remains even as the qubit frequency is tuned over 150 MHz away from the center mode (see Fig. 3.8). This observed robustness will be discussed in the following theoretical analysis (Sec. 3.5).
Figure 3.8: Measured linewidth and emitted power versus flux bias. Spectral narrowing appears over a wide range of flux bias, corresponding to over 150 MHz of the qubit frequency. The other parameters are the same as in Fig. 3.7. We note that the fluorescence power and the linewidth are inversely related.

Finally it is important to distinguish the narrow linewidth emission from a coherent lasing. Experimentally, we confirm that the emission is incoherent (as is expected from resonance fluorescence) via an autocorrelation measurement on the emitted light from one mode, calculated at the drive parameters that produced the brightest and narrowest emission in Fig. 3.7. Specifically, $g_1(\tau)$ and $g_2(\tau)$ were not equal to 1 for all $\tau$ as is expected for coherent emission at a single frequency (see Appendix A for details on autocorrelation measurement). Though the simple theoretical model with few modes predicts mode-mode entanglement, two-mode correlation measurement did not reveal entanglement. It is our understanding that two-mode correlation measurement critically neglects the simultaneous emission that is occurring at other modes. This leads to a measurement of classical correlation, which we detect, but falls short of entanglement. We predict that while entanglement may exist between modes in this device, it likely involves more than two modes and thus is beyond the scope of our measurement capabilities.
3.5 Multimode theory

To gain intuition on the processes underlying multimode resonance fluorescence we turn to simplified analytical modeling and numerical simulation. In this section we summarize some of the key theoretical findings, and refer interested readers to [49, 50] for more details.

3.5.1 Effective Hamiltonian and master equation

The driven dissipative system can be described by the following master equation \((\hbar = 1)\)

\[
\frac{\partial \rho}{\partial t} = -i [H, \rho] + \frac{\gamma}{2} L_a \rho + \sum_m \frac{\kappa_m}{2} L_m \rho, \quad (3.5)
\]

where

\[
H = H_0 + H_D \quad (3.6)
\]

\[
H_0 = \sum_m \left[ \Delta_m a_m^\dagger a_m + g_m (a_m^\dagger + a_m) \sigma^x \right], \quad (3.7)
\]

\[
H_D = i \eta (a_r^\dagger - a_r) \quad (3.8)
\]

\[
L_a \rho = 2 \rho \sigma^– \sigma^+ - \sigma^+ \sigma^– \rho - \rho \sigma^+ \sigma^–, \quad (3.9)
\]

\[
L_m \rho = 2 a_m \rho a_m^\dagger - a_m^\dagger a_m \rho - \rho a_m^\dagger a_m. \quad (3.10)
\]

with \(\kappa_m\) the photon loss rate for mode \(m\), and \(\gamma\) is the qubit decay rate. As a reminder, MMSC corresponds to \(\Delta_m \sim g_m > \gamma, \kappa\). The above Hamiltonian is written in the rotating frame of the drive, where \(\eta\) is the amplitude of the external drive and the drive is assumed to be resonant with the \(r\)th mode and the qubit, \(\omega_d = \omega_r = \omega_q\).
(See Fig. 3.8 and Sec. 3.5.3 for experimental and theoretical justification for the resonant drive assumption).

The basis for the approximation that the input drive only couples to the resonant mode is apparent when we consider the uncoupled system \( g_m = 0 \). In an empty cavity, steady state photon numbers of other modes due to an off-resonant drive tone would scale as multiples of \( (\kappa/\omega_1)^2 \) and are significantly suppressed relative to the resonant term.

Applying a drive and dissipation dependent unitary displacement to the state of the system \( \tilde{\rho} = D^\dagger \rho D \), with

\[
D = \exp \left( \xi (a_r^\dagger - a_r) \right), \quad \xi = \frac{2\eta}{\kappa_r},
\]

(3.11)

translates the drive from the mode to the qubit. The Hamiltonian for the drive appearing in the master equation is now

\[
H_D = \frac{\Omega}{2} \sigma^x
\]

(3.12)

where \( \Omega = 8g_r \eta / \kappa_r \) is the effective Rabi frequency.

As the goal of this analysis is to determine some interaction terms that arise coupling the various modes, we will simplify this model (see [50, 49] for details). First, we define the modes to lie symmetrically around the drive \( \Delta_m = m \Delta, m = \pm 1, \pm 2, \pm 3... \) and ignore the center mode \( m = 0 \).

Then, after introducing a new basis for the qubit,

\[
| \tilde{0} \rangle = \frac{1}{\sqrt{2}} (|0 \rangle - |1 \rangle), | \tilde{1} \rangle = \frac{1}{\sqrt{2}} (|0 \rangle + |1 \rangle),
\]

(3.13)

and applying an atomic-state-dependent mode displacement operator,
\[ U = \prod_m \exp \left( \frac{g_i}{2\Delta_i} (a_i - a_i^\dagger) \hat{\sigma}^z \right) \]  

(3.14)

we arrive at the simplified, effective Hamiltonian

\[ H = \frac{\Omega}{2} \hat{\sigma}^z + \sum_m \left[ \Delta_m a_m^\dagger a_m + \frac{g_m}{2} (\hat{\sigma}^+ \prod_i V_i - \hat{\sigma}^- \prod_i V_i^\dagger)(a_m - a_m^\dagger) \right] , \]

(3.15)

where \( V_i = e^{\left( \frac{g_i}{\Delta_i} (a_i^\dagger - a_i) \right)} \).

We truncate the Taylor expansion of \( V_i \) and keep only secular terms, valid for \( g_i/\Delta_i \ll 1 \) and certain resonance conditions. Therefore from this truncation, while we hope to gain insight into interactions underlying some of the observed multimode fluorescence, we do not expect to capture spectral narrowing or other features that appear in experiment at the most strongly coupled modes directly neighboring the drive.

While ideally we would like to consider as many modes in theory as exist in experiment, this complexity is beyond our abilities (both in analytical and numerical study). Here, we look at a four-mode model and assume \( \Delta_{\pm 1} = \Delta_{\pm 2}/2 = \pm \Delta \), \( g_{\pm 1, \pm 2} = g, \kappa_{\pm 1, \pm 2} = \kappa \). In this case, the resonance conditions are \( \Omega \approx n\Delta \), for \( n = 1, 2, ... \). The effective Hamiltonian for the resonance condition \( \Omega = \Delta \) and \( \Omega = 2\Delta \) is then

\[ H_{\Omega=\Delta}^{\text{eff}} = \frac{\Delta}{2} \hat{\sigma}^z + \sum_{i=\pm 1, \pm 2} \Delta_i a_i^\dagger a_i + \left[ \frac{g}{\Delta} \hat{\sigma}^+ (a_1 - a_{-1}^\dagger) + \frac{g^2}{\Delta} \hat{\sigma}^+ \left( \frac{3}{4} a_1^\dagger a_2 - \frac{3}{4} a_{-1}^\dagger a_{-2} + \frac{1}{4} a_{-1} a_2 - \frac{1}{4} a_1^\dagger a_{-2} \right) + \text{h.c.} \right] \]

(3.16)

\[ H_{\Omega=2\Delta}^{\text{eff}} = \frac{\Delta}{2} \hat{\sigma}^z + \sum_{i=\pm 1, \pm 2} \Delta_i a_i^\dagger a_i + \frac{g^2}{2\Delta} \left[ \hat{\sigma}^+ (-a_1^2 + (a_{-1}^\dagger)^2) + \text{h.c.} \right] + \frac{g}{2} \left[ \hat{\sigma}^+ (a_2 - a_{-2}^\dagger) + \text{h.c.} \right] \]

(3.17)
Figure 3.9: Dressed state diagrams (dressing provided by the drive) illustrating various interaction vertices. Each excitation manifold (n) is separated by the drive frequency \( \omega_d \). **Sideband enhancement:** Due to the symmetric modes, both qubit excitation and relaxation (\( \sigma^+ \) and \( \sigma^- \)) are linked to radiative emission. **Wave-mixing:** Mode-mixing processes that generate photons in mode +2. **Two Photon Emission:** An example multiphoton emission process that arises when harmonic or sub-harmonic resonance conditions are met.

These effective Hamiltonians reveal various interaction terms that are a direct result of the symmetric mode structure. Terms such as \( \tilde{\sigma}^+ a_{-1}^\dagger \) appear as the negative index modes carry negative frequency in the rotating frame. Two photon processes (\( \tilde{\sigma}^+ a_2^\dagger \)) in Eq. 3.17 are suppressed relative to the single photon ones in Eq. 3.16 by \( g/\Delta \). Interaction vertices, \( \sigma^+ a_1^\dagger a_2 \), depict a qubit-mediated two-wave mixing process (see Fig. 3.9 for illustration). In MMSC, these mode-mode interaction terms become relevant as the corresponding interaction strengths \( \sim g^2/\Delta \) are larger than dissipation rates (\( \gamma, \kappa \)). For modes further away from the drive, the strength of the effective interaction \( \tilde{\sigma}^+ a_m a_{m+1}^\dagger \) will decrease (\( \sim 1/m \)) as the detuning increases. In comparison, the strength of higher order interaction \( \tilde{\sigma}^+ a_n^2 a_m^\dagger \) will drop as the exponential of \( g/\Delta \). The same analysis can be applied to \( \Omega = 2\Delta \) when two-photon interactions \( \tilde{\sigma}^+ a_1^2 \) and single photon interactions \( \tilde{\sigma}^+ a_2 \) all reach resonance and emission at all \( \pm 1, \pm 2 \) modes will be enhanced. In general, when the Rabi rate \( \Omega \) is commensurate with FSR, qubit mediated mode-mode scattering and multiphoton effects will be resonantly enhanced. As a result, resonance fluorescence in such a multimode system will strongly deviate from the free-space Mollow triplet, with different peak heights, widths and additional
sidebands. Correspondingly, photonic modes around the drive will simultaneously reach high occupation.

To better understand steady state photon occupation, one can use the full reduced master equation (derived in Liu’s thesis in detail) to obtain closed equations for correlators including \(\langle a_i^{\dagger} a_i \rangle\) and \(\langle a_i a_{-i} \rangle\). This reveals dipole interaction \(\tilde{\sigma}^- a_i^{\dagger}\) and wave-mixing \(\tilde{\sigma}^- a_1 a_2^{\dagger}\) to have rates \(g^2/\gamma\) and \(g^4/\Delta^2\gamma\) respectively, leading to

\[
\langle a_{\pm 1}^{\dagger} a_{\pm 1} \rangle = \langle n_{\pm 1} \rangle \propto g^2/(\gamma \kappa) \\
\langle a_{\pm 2}^{\dagger} a_{\pm 2} \rangle = \langle n_{\pm 2} \rangle \propto g^4/\langle n_{\pm 1} \rangle/\gamma \kappa \Delta^2 
\]

(3.18)

(3.19)

For comparison, steady state photon occupation considering only direct scattering to mode \(\pm 2\) \(\sigma^- a_{\pm 2}^{\dagger}\) leads to a reduced \(\langle n_{\pm 2} \rangle \propto g^2/\gamma \kappa \gamma /\Delta^2\) in the strong coupling limit. With mode-mode interactions, we see increased population in \(\pm 2\) modes directly resulting from \(\pm 1\) mode occupation. Due to this cascaded wave-mixing process, further sideband modes can be enhanced.

Comparing these results with those from single mode strong-coupling [25, 51], where \(\langle n \rangle \approx \gamma / (8 \kappa)\), we immediately see that qubit dissipation plays a very different role in determining steady state properties of the two systems. In the single mode case, fast qubit dissipation (large \(\gamma\)) is needed to increase photon emission into the mode \((\tilde{\sigma}^- a_1^{\dagger} + \tilde{\sigma}^+ a_1)\). However, in this multimode case, the symmetric mode configuration allows both qubit state flips to create photons into the modes \((\tilde{\sigma}^- a_{-1}^{\dagger} + \tilde{\sigma}^+ a_1^{\dagger})\). Thus a direct consequence of the longitudinal multimode configuration is significantly brighter fluorescence than is possible with a single mode. These results are also confirmed by numerical simulations (see Sec. 3.5.2 and Fig. 3.12a for details).
Figure 3.10: Numerical simulation of four-mode model fluorescence spectrum. \( \text{a} \) The parameters are \( |Δ_{\pm 2}|/4π = |Δ_{\pm 1}|/2π = 30\text{MHz}, κ_{\pm 1,\pm 2}/2π = 4\text{MHz}, γ/2π = 4\text{MHz} \) and \( g_{\pm 1,\pm 2}/2π = 5\text{MHz} \). White dashed lines indicate the bare photonic modes. \( \text{b} \) Normalized incoherent spectrum for \( Ω = 30\text{MHz} = Δ \). Comparison of relative peak amplitudes shows stronger sideband emission in multimode than in free-space. There is additional emission at \( \pm 2 \) modes, attributed to wave-mixing.

### 3.5.2 Numerical simulations

We use the Monte Carlo Wavefunction approach to numerically simulate the dynamics of a driven dissipative multimode system. In our simulation, the size of the Hilbert space needed grows as \( 2\prod_m N_m \), with \( N_m \) the photon cutoff for mode \( m \). The rapid growth of the dimension of the Hilbert space limits the number of modes that can be incorporated into the simulation. Expectation values of relevant operators are followed and steady state values for the driven system are presented below. To compute two time correlation functions such as the power spectrum, \( \int_{-∞}^{∞} e^{-iωτ} \langle a(τ) a(0) \rangle dτ \), using this method, we have to employ a two step procedure [52], equivalent to the quantum regression theorem, but at the expense of requiring large numbers of walks to produce reliable results. Simulations in this section will include either one, two, or four modes, with exact parameters specified accordingly.

In Fig. 3.10, the emission spectrum of a symmetric four mode system reveals a multiplet structure that deviates from Mollow triplet. At \( Ω ≈ Δ \), the central peak is suppressed and broadened and extra sidebands appear near \( m = \pm 2 \) modes (Fig. 3.10b). In fact, as sidebands become stronger, the central component will eventually vanish as the corresponding dipole moments will be comparably small. The
Figure 3.11: Simulated steady state photon number, qubit inversion and polarization.

a Parameters of the two mode system are $\Delta_1/2\pi = -\Delta_2/2\pi = 100$ MHz, $\kappa_1/2\pi = \kappa_2/2\pi = 1$ MHz, $\gamma/2\pi = 15$ MHz, $g_1/2\pi = g_2/2\pi = 15$ MHz. Parameters of the single mode system are $\Delta/2\pi = 100$ MHz, $\kappa/2\pi = 1$ MHz, $\gamma/2\pi = 15$ MHz, $g/2\pi = 15$ MHz.

b Parameters of the two mode system are $2\Delta_1/2\pi = \Delta_2/2\pi = 160$ MHz, $\kappa_1/2\pi = \kappa_2/2\pi = 1$ MHz, $\gamma/2\pi = 15$ MHz, $g_1/2\pi = g_2/2\pi = 25$ MHz. These plots include 24 different Rabi frequencies $\Omega$ with 1,000 quantum walks per Rabi frequency in the numerical simulations.

mechanism can also be understood perturbatively in the dressed picture subject to a drive [31] as shown in Fig. 3.9a.

To capture the lobe structure, experimentally observed in the far detuned modes (Fig. 3.3c), we next analyze two cases of a two mode model and recall $g/\Delta \ll 1$ is a good approximation at these detunings. These models reveal resonant enhancement by multiphoton processes in a single mode $i$ (via the interaction $\tilde{\sigma}^+ a_i^m + h.c.$), while tuning the qubit drive $\Omega$, leads to peaks in the steady state photon number near subharmonics of the Rabi frequency $|\Delta_i| = \Omega/m, m \in \mathbb{Z}$. Fig. 3.11a-c presents numerical results for the case where the two modes are symmetric around the qubit (and the drive which is resonant with the qubit). Fluorescence at these two modes'
Figure 3.12: Comparison of photon number dependence in one mode on a qubit decay and b interaction strength, between single mode and symmetric two mode models. General parameters of the two mode system are $\Delta_1/2\pi = -\Delta_2/2\pi = 100$ MHz, $\kappa_1/2\pi = \kappa_2/2\pi = 1$ MHz, and $\Omega/2\pi = 100$ MHz. For the single mode system, $\Delta_1/2\pi = 100$ MHz, $\kappa_1/2\pi = 1$ MHz, and $\Omega/2\pi = 100$ MHz. a $g_1/2\pi = g_2/2\pi = 15$ MHz. The symmetric two mode configuration yields higher photon numbers that decrease with increasing qubit decay, unlike the single mode case. b $\gamma/2\pi = 15$ MHz The two mode system reveals a distinct enhancement of photon number, with increasing interaction strength, over the single mode case [53].

frequencies are equally and simultaneously enhanced. Moreover, the two peaks in photon number (Fig. 3.11a) and qubit polarization $\sigma^+$ (Fig. 3.11c) deviate from the bare resonance conditions $\Omega = m|\Delta|$, $m = 1, 2$. Most notably, the qubit inversion $\sigma^z$ can be positive (Fig. 3.11b). The results for a single mode model are also shown for comparison. While multiphoton resonances are apparent in both cases, the two mode system reaches much larger photon numbers in the steady state as expected. We find that the strength qubit-mode coupling plays a more important role in determining steady-state photon number in the two mode system (see Fig. 3.12b).

Besides the two photon interaction in a single mode ($\sigma^-a_i^\dagger a_i^\dagger$), the interaction vertex coupling two different modes ($\sigma^-a_i a_j^\dagger$, $i \neq j$) will result in resonant enhancement in modes near harmonics of the Rabi frequency $|\Delta| = m\Omega$. This is demonstrated in Figs. 3.11d-e where another two mode case ($\Delta_2 = 2\Delta_1$) is investigated. Similarly to the previous case, this effect leads to co-enhancement of fluorescence at two modes, as evidenced by the brightening of the second mode at $\Delta \sim 80$ MHz. As this is
a second-order effect induced by the first mode, \( N_2 \) is much smaller than \( N_1 \). For stronger coupling, we would expect the difference to be smaller.

### 3.5.3 Multimode spectral narrowing

While the analytical modeling thus far has satisfactorily reproduced many experimentally observed fluorescence properties (two photon emission, wave-mixing, simultaneous emission at many modes, large steady state photon occupation etc.), the approximations used do not apply for the most strongly coupled modes nearer to the drive (larger \( g/\Delta_i \)). Therefore we attempt a new approach to understand the origin of ultranarrow linewidth emission observed at these modes (see Sec. 3.4 for experimental observation).

For intuition, let us consider a toy model consisting of two identical atoms that are dipole-dipole coupled to each other via vacuum. Dynamics of the system are described by the master equation,

\[
\frac{d\rho}{dt} = \frac{\gamma}{2} \sum_{i=1,2} \left( 2\sigma_i^- \rho \sigma_i^+ - \sigma_i^+ \sigma_i^- \rho - \rho \sigma_i^+ \sigma_i^- \right) \\
+ \frac{\gamma_c}{2} \left( (2\sigma_1^+ \rho \sigma_1^- - \sigma_1^+ \sigma_1^- \rho - \rho \sigma_1^+ \sigma_1^-) + h.c. \right)
\]

written in the rotating frame of the atomic frequency. For simplicity, we ignore the level shift caused by the dipole-dipole coupling and keep only the radiative component. Restricting the dissipation dynamics to the single excitation manifold, the equations of motion are

\[
\frac{d}{dt} \begin{bmatrix} \langle S|\rho|S \rangle \\ \langle A|\rho|A \rangle \end{bmatrix} = \begin{bmatrix} \gamma + \gamma_c & 0 \\ 0 & \gamma - \gamma_c \end{bmatrix} \begin{bmatrix} \langle S|\rho|S \rangle \\ \langle A|\rho|A \rangle \end{bmatrix}
\]

(3.21)
where $|S\rangle = \frac{|1,0\rangle + |0,1\rangle}{\sqrt{2}}$, $|A\rangle = \frac{|1,0\rangle - |0,1\rangle}{\sqrt{2}}$. The additional dissipative coupling $\gamma_c$ thus results in a modified lifetime of the two atoms $\gamma \pm \gamma_c$. In the case of $\gamma = \gamma_c$, the system can be exactly trapped in the pure antisymmetric state $|A\rangle$. As $\gamma$ approaches $\gamma_c$, we see lengthening lifetimes, spectrally appearing as narrowing resonances. We believe the narrowing emission in the multimode system descends from a similar origin.

Ultrannarrow resonance fluorescence has been predicted for the single mode cavity [48], where coherence between dressed states of the driven system arises from coupling to common vacuum fluctuations. The resultant spectrum linewidth of the mode could thus be much smaller than the natural linewidth of the bare system, with the linewidth of the sideband proportional to the inverse of the steady state photon number $1/\langle n \rangle$.

In our system, unlike the single mode case, the number of states in a single excitation manifold is not a constant but grows as $\binom{N+M-1}{M-1} + \binom{N+M-2}{M-1}$, where $M$ is the number of modes and $N$ is the excitation manifold. The rapid growth of the number of states per manifold hinders a simplified analysis via the dressed state picture, but makes possible the near resonance of many level spacings (Bohr frequencies), leading to a collective enhancement of the coherences from their mutual couplings. An external coherent drive allows us to dynamically access regions of the dressed states with large generated coherences, as evident in the drive dependence of the narrowing in Fig. 3.7. This dissipation-induced coupling ultimately leads to a constructive interference effect in the emission spectrum, i.e. the narrowing of the linewidth. Similar behavior has been predicted and observed in atoms with multiple closely spaced bare atomic levels coupled to vacuum or a single mode of a cavity [54, 55, 56], where the theoretical analysis is aided by the simpler dressed state structure.

In Figs. 3.13a-b, for the symmetric two mode system, spectral narrowing occurs for a range of Rabi frequency $\Omega$. In this simulation, linewidth is inversely proportional to the photon number such that the linewidth reaches its minimum as the photon
Figure 3.13: Properties of fluorescence spectrum of the right mode in a two mode system. Parameters of the two mode system are $\Delta_1/2\pi = -\Delta_2/2\pi = 100$ MHz, $\kappa_1/2\pi = \kappa_2/2\pi = 1$ MHz, $g_1/2\pi = g_2/2\pi = 15$ MHz. In a-b, $\gamma/2\pi = 15$ MHz. a Photon number reaches its peak at $\Omega/2\pi = 106$ MHz. This figure includes 12,000 quantum walks in the numerical simulation. The spectrum is generated by Fourier transforming the two time correlation function of the mode operator. The fluorescence linewidth is more than 3 times narrower than the natural mode linewidth. b Fluorescence linewidth versus Rabi frequency. c Photon number and d linewidth for varying drive amplitude when $\gamma = 5$ MHz. Though the sharpest line does not correspond to the brightest fluorescence, the linewidth is still a factor of 2 narrower than the natural linewidth of the bare system. The black dashed lines indicate the natural linewidth of the mode (1 MHz). The left mode also shows the same amount of spectral narrowing (data not shown).

number reaches its maximum at $\Omega = 106$ MHz (see photon number in Fig. 3.11a for same simulation parameters). The spectral narrowing in this simplified model doesn’t reach that of our experiments (a factor of $\sim 3.3$ in the simulation vs. $\sim 17$ in the experiment), yet it displays qualitatively similar features [50]. Moreover, the relation $\kappa_{\text{fluo}} \sim 1/\langle n \rangle$ suggests that the linewidth could be made much narrower than that of the current simplified model, when reaching larger steady state photon numbers. However, simulations including more modes (which in turn require higher photon number cutoff due to rise in steady state occupation) demand significantly more computational resources due to the growth of the Hilbert space.

Spectral narrowing is generally insensitive to the qubit frequency (observed experimentally in Fig. 3.8). For finite drive-qubit detuning $\Delta_a$, the effective Rabi frequency is $\Omega = (\Omega_0^2 + \Delta_a^2)^{1/2}$, with $\Omega_0$ the amplitude of the drive. Spectral narrowing occurs
when $\Omega$ is within the range $\Delta \pm \delta(\Omega_0)$, where $\Delta$ is again the mode frequency measured with respect to the drive (i.e., its detuning), and $\delta(\Omega_0)$ is generally determined by the number of modes, the coupling strength and the dissipation. For relatively small detuning $\Delta_a$ and large Rabi frequency $\Omega_0$, this gives a large effective range of qubit frequency $\delta(\Delta_a) \sim \frac{\Omega}{\Delta_a} \delta(\Omega_0)$ over which narrowing occurs. We find that even if the drive is not resonant with the qubit and the two modes are not symmetric around the drive, spectral narrowing still exists in our simulation.

For a single mode system, it was argued that spectral narrowing required the qubit decay rate $\gamma$ to be comparable to the coupling strength $g$ (i.e., the moderate coupling regime [48]). In Fig. 3.13c-d we study the effect of qubit decay rate $\gamma$ on steady state properties of the two mode system. Fig. 3.13c presents photon number $N_1$ versus Rabi frequency for a smaller $\gamma$. From this result, we conclude that spectral narrowing survives when going from moderate coupling to the strong coupling regime, which we attribute to the fact that the eigenstates of the multimode system in high excitation manifolds are more densely spaced than in the single mode system. Dynamically generated coherence between these closely spaced states then results in spectral narrowing of many modes simultaneously.

Despite surface level similarities, this phenomenon fundamentally differs from semiclassical multimode lasing [57], where linewidth is proportional to a sum of inverse powers of all lasing modes and cavity decay rates. Here $\langle a_i \rangle \approx 0$ excluding typical operator decoupling and mean field approximation. Furthermore, linewidths of different modes in this system will be correlated. Thus instead of the collective lasing response of many atoms, the multimode line narrowing comes from the collective interference of many excited dressed states.
Low Power
High Power
S21 (mW)
Frequency (GHz)

Figure 3.14: Ultra-long cavity a The 2m cavity created to reach $g_m > \omega_1$ fits on a $\sim 36 \times 36 \times 0.5$ mm sapphire substrate. This cavity has a mode spacing of $\sim 30.8$ MHz. Symmetric coupling capacitors of approximately 32 fF lead to mode linewidths varying between $< 1$ to $\sim 4$ MHz over a several GHz range. A flux-tunable transmon qubit is coupled at one end of the cavity, an voltage antinode. Aluminum wirebonds are used to connect sections of ground plane (diagonal across the device and along the chip border) b Comparison of transmission measurements taken using low and high drive powers for a fixed qubit frequency $\sim 8.7$ GHz. Shift in mode frequency and suppression of mode amplitudes are immediately visible, and indicative of the multi-mode qubit coupling.

3.6 Deep MMSC

Motivated by these experimental results, we sought to push deeper into MMSC by realizing qubit-mode couplings strengths that match and possibly even exceed the mode spacing. In addition to answering whether the long cavity method had any fundamental limits, we hoped to learn whether system function changed dramatically with increased $g/\omega_1$ by comparing multimode fluorescence and simultaneous linewidth narrowing.

Based on the measurement of $\sim 30$ MHz qubit coupling strength to the 75th mode in the first device, we anticipated that extending the cavity to 2 m would allow us to realize this new goal. We designed this longer cavity on a 36 mm $\times$ 36 mm sapphire substrate (our largest readily available PCB at the time) in a similar meandering pattern. The larger pattern area and decreased CPW dimensions proved exceptionally difficult to realize with conventional photolithography (with manual sample prepa-
ration and development) as defects larger than a few microns rendered a sample
unusable. Furthermore, to properly package the larger sample, many more wirebonds
were needed to connect the ground planes. This was technically challenging due to
the sheer number of bonds required and the small error margin (human and machine)
available when placing the bonds themselves. Nevertheless we successfully made the
device shown in Fig. 3.6a. We note that while newer methods and technology, such as
a direct-write laser writer (as used in later experiments) and aluminum air-bridges,
would significantly improve yield, simply lengthening the cavity further to reach even
larger $g/\omega_1$ is not a realistic strategy.

A comparison of high and low (single photon) power transmission measurements
in shown in Fig. 3.6b when the qubit frequency is around 8.7 GHz. High power
measurement reveals the uniformity of the bare modes, spaced by 30.8 MHz, while
low power captures the impact of coupling to the qubit. In addition to shifts in cavity
mode frequencies, we see a near-monotonic drop in peak mode transmission as the
modes approach the qubit frequency. Qualitatively, we know that the qubit is most
strongly hybridized with the modes nearest in frequency, which in turn inherit qubit
and qubit-mediated multi-mode decay pathways.

Using low power transmission, we similarly measure the trail of avoided crossings
(Fig. 3.6) as the qubit is tuned through resonance with a forest of modes (see Fig. 3.3
for comparable measurement with 92 MHz cavity). Fitting these to the MMJC
Hamiltonian yields $\omega_1 = 30.8$ MHz and $g_1 \sim 2$ MHz, translating to $g_{m=275} = g_{8.5GHz} =
33.25$ MHz which successfully exceeds the mode spacing.

Now deeper in MMSC, we repeated measurements of resonance fluorescence to
find qualitatively similar behavior to those observed in the first system with a few no-
table differences. Multi-photon, multi-lobed emission structure at far detuned modes
resembled that shown in Fig. 3.3c. Simultaneous onset of fluorescence at low drive
power occurred across more of the neighboring modes in this system, consistent with
Figure 3.15: **Characterization of the 2m cavity device**

a Low power transmission is measured as qubit frequency is tuned using an externally applied flux bias. In addition to almost 100 cavity modes measured in 3 GHz frequency range, there are several defects in the spectrum. These are attributed to chip modes (expected circa 3.4, 5.3, 6.7, 7.5, 8.6 GHz) and slot-line modes due to insufficient ground-plane wire-bonding.

b Zooming into a 500 MHz frequency range shows a uniform mode spectra that is free of defect modes. Thus despite the existence of defect modes in the larger frequency range, there are frequency windows in which the qubit will predominantly "see" only clean cavity modes. Fitting to the first excitation manifold of the MMJC Hamiltonian, we extract $g_1 \sim 2$ MHz. This yields $g_{m=275} = g_{8.5GHz} \sim 33.25$ MHz $> \omega_1 = 30.8$ MHz.
the increased multi-mode coupling. This similarly transferred to narrowing of emission linewidth with a detuned drive tone. In this system we observe a larger minimum linewidth of 110 kHz (vs. 65 kHz for the 92 MHz cavity) in the two modes nearest to the qubit, however the bare mode linewidth in this was also 50% larger at 1.5 MHz. We also see the simultaneous reduction in linewidth at more pairs of neighboring modes. This additional observation of narrowing highlights the non-trivial yet apparent relation between multimode coupling and emission linewidth. Finally, after initial onset of fluorescence at the nearest modes, we do not observe a subsequent reduction and then reappearance of emission at these modes (i.e., no multi-lobed structure). This last observation is relevant as, at this time, we do not have an understanding regarding this emission which is inconsistent with power-dependent Mollow triplet-like sidebands.

In summary, fabricating this 2m cavity demonstrated that reaching larger $g/\omega_1$ is possible. However future realizations would greatly benefit from stronger qubit coupling than attainable with the standard transmon qubit and CPW cavity such that cavity length can be held less than 1m. Others working in this area are seeking alternate approaches to reaching MMSC, including vacuum gap transmons coupled to high-impedance resonators [58, 23] and junction arrays.

### 3.7 Outlook

In this chapter we explored the MMSC regime and reported remarkably widespread and highly structured resonance fluorescence. The observed drive-dependence of the width, height and position of the fluorescence peaks cannot be explained by cavity enhancement of sidebands observed in the single-mode regime [26]. As expounded above, our observations reveal a generation of coherence across multiple frequencies mediated by a single qubit and necessitate a multimode analysis. Beyond the novel
phenomena presented here, the access to the MMSC regime opens up a new direction of exploration that is of interest both theoretically and experimentally.

The results presented here all relied on continuous drive tones. Preliminary experiments with time-dependent (e.g. pulsed) drive revealed even more complex behavior and a pressing need for more rigorous theoretical understanding. For example, the mode-mode coupling disallowed simple Rabi oscillations between one mode and the qubit. Attempts at observing Rabi oscillations through emission measurements showed the involvement of multiple frequencies. The downside of this additional complication is that we were not able to perform any experiment that required qubit state initialization, such as that described in Ref. [34]. However, this does not mean it is impossible to initialize a qubit in MMSC. One proposal involves simultaneously driving at multiple mode frequencies, where parameters for each drive pulse are calculated from measured mode-qubit couplings. Such a drive sequence, combined with parametric amplification for improved SNR, could provide insight into how the qubit excitation decays, and is exchanged between the many modes of the system.

Another potential area of interest is to modify the coupling between the qubit and modes with alternate qubit geometries. Reaching stronger coupling is being explored actively by others, one method involving a vacuum-gap transmon [58, 23]. In the work presented in this chapter, changing qubit frequency was the only mechanism through which we could access different ”levels” of coupling (considering that the modes nearest to qubit frequency are the ones that dominate system behavior). Another option for future experiments would be to replace the transmon with a tunable coupling qubit [7], with which one can in situ modify qubit-mode coupling while maintaining qubit frequency. This would allow for a more systematic study into the impact of relative coupling strengths (and thus the number of strongly coupled modes) on system behavior.
When we introduced the Hamiltonian (Eq. 3.1) to motivate MMSC, we assumed a harmonic cavity such that mode frequencies fall at multiples of the fundamental mode frequencies. While we chose this configuration for its elegant simplicity, it is not the only method to realize multimode-qubit interactions. For example, rather than one long cavity we could consider a one-dimensional chain of coupled (identical) cavities. The eigenmodes of the circuit would present as a discrete "band" of modes centered at the frequency of the individual cavity with eigenmode spacing determined by the hopping or tunneling rate between cavity sites. Spatially these eigenmodes would have different weighting at each site in the chain, thus placing a qubit in a single site would result in a distribution of eigenmode-qubit couplings.

In Phys. Rev. X 7, 011016 (2017), we realized a one-dimensional, 72-site chain of coupled cavities and observed such a mode spectrum [11]. In that work, rather than a single qubit we dispersively coupled one qubit to each site so as to explore the many-mode many-qubit limit where individual couplings and qubit frequencies are not relevant to overall system dynamics. In this system we recorded strong mode-mode interactions originating from the qubit nonlinearities and observed a dissipative phase transition. In future work one can explore the domain between the long cavity and coupled-cavity systems, as each revealed unique but correlated system dynamics originating from mode-mode interaction.

While we did not measure a coupled cavity array coupled to a small number of qubits, in the next chapter we consider a related system - two qubits strongly coupled to a microwave photonic crystal, akin to a coupled cavity array. As we will see in this system, the coupling regime reveals the emergence of photonic bound states - a novel interaction pathway for spatially separated qubits.
Chapter 4

Strong Coupling Qubits to a 1D Photonic Bandgap Crystal

Light-matter interaction between qubits (or atoms) and slow-light structures, ones with vanishing or significantly reduced group velocity such as photonic band edges in photonic crystals, has been an area of ongoing interest both in theory and recent experiment. Central to these studies is the localized bound photonic state that forms around the qubit in the strong coupling domain [59, 60, 61, 62, 63, 64]. This spatially-localized, single-photon state together with the qubit forms a qubit-photon dressed bound state. As we will see in this chapter, the frequency of the bound state changes with qubit frequency, though always falls within the band-gap. Furthermore, the state localization length tunes with qubit frequency, becoming less localized as the bare qubit frequency is tuned closer to the band edge (see Figs. 4.1a-b). In a finite-size system, these localized states overlap with the ends of the crystal, thus facilitating single-photon transport across the crystal at the bound-state frequency and providing an avenue to probe these states.

This tunable photonic interaction mechanism provides a platform for simulation of many-body quantum optics in one-dimensional systems, distinct from cavity or
Figure 4.1: Visualizing bound states - A qubit (pink circle) is coupled to one site of a 1D photonic crystal (gray line of alternating width). Coupling a qubit and band edge produces a photonic envelope (blue/purple) that is spatially centered at the qubit location. a and b The localization of the photonic component is determined by the detuning of the qubit from the band edge. a is more localized than b as the detuning is larger in the former. The overlap of the photonic wavefunction with the ends of the crystal (not shown) determines the linewidth of the bound state measured in transmission. The strength of the interaction between the bound states, when qubits are resonant with one another, can be understood in c and d as depending on the localization of the bound states. e In a larger system, this localization length dependent interaction of the bound states would preserve the importance of the spatial organization of qubits in determining the many-body interaction.
waveguide QED (see Figs. 4.1c-d). Unlike many qubits coupled to a common cavity mode but similar to the case of some optical multimode cavities [65, 66], coupling to a band edge creates bound states that intrinsically preserve the spatial organization of qubits; this offers the ability to create one-dimensional chains of bound states with tunable and potentially long-range interactions [67, 63, 64, 68, 69, 70, 71, 64]. The promise of engineering interaction profiles beyond the intrinsic flip-flop with additional microwave drive tones further opens the possibility of simulating quantum spin models in future devices [69].

The potentially long-range interaction possible between atoms due to these photonic bound states is a motivation for many projects coupling ultracold atoms to nanophotonic crystals [72, 73, 74, 75]. In such systems, super-radiance and other atom-atom interactions involving spatially separated atoms have been demonstrated [73, 75]. While ultracold atom experiments have shown remarkable progress in this regard, investigating dressed qubit-photon bound states in circuit QED offers an alternative approach to exploring this phenomena, with distinct advantages and disadvantages. Foremost, the strong coupling regime at the single-qubit single-photon level is readily accessible via crystal and qubit design, including both static (set in fabrication) and in situ tunability of key parameters. Due to low intrinsic loss (decay of qubit or bound state excitation into channels other than the waveguide), detection of the bound state in transmission is possible [76]. While we cannot study self-organization of qubits due to bound state interaction because qubit location is fixed by circuit design, we can design simple chains or configurations of qubits within a crystal to explore more complex interactions. Finally, control over the frequency of each qubit, not available in ultracold atoms, provides the means to dial up and down interaction in situ and thus opens up an important parameter space as bound state characteristics strongly depend on detuning of the qubit from the band-edge frequency.
In this chapter we will discuss a realization of qubit-photon dressed bound states using qubits coupled to a stepped impedance, coplanar waveguide, microwave crystal, building upon work from a previous group member Yanbing Liu (see [50, 76]). We explore tunable on-site and inter-bound state interactions in a two-qubit device, expanding our understanding of this platform with rigorous theoretical modeling. Portions of this chapter appear in [77], where we presented these results.

4.1 Photonic crystals

To realize a dressed bound state between a qubit and a band edge, we must couple a qubit to a photonic band edge, where a band edge consists of photonic states corresponding to the transition between a stopband and a passband that are “slow-light” due to reduced group velocity. Bandgaps and passbands are not unique to photonic crystals - we come across them in numerous other structures such as waveguides (near cutoff frequency) or aperiodic filters.

To motivate the benefit of photonic crystals, let us consider using an aperiodic filter instead. Filters are ubiquitous in the microwave domain with many established design methods that trade off optimizing various parameters such as roll-off or passband ripple. Stepped impedance filters are a standard model for implementing filters, where each impedance step is chosen precisely to meet filter design constraints with no periodicity requirement [78]. Due to this, aperiodic filters may also be more sensitive to fabrication errors than periodic filters.

The next requirement is to couple a qubit. However the lack of periodicity transfers also to the electric field distribution (no Bloch modes), and so we must numerically calculate the optimal location to place the qubit and recalculate for every modification of filter design. While this seems feasible for a single qubit, the lack of Bloch modes is highly problematic from a scalability standpoint as it is not guaranteed that we
can couple multiple qubits (or even just two), with near identical coupling strengths, to that band edge.

Furthermore, from a theoretical perspective, periodic crystals are simpler, cleaner structures that are described in the infinite limit by dispersion relations in momentum space, providing useful insight for predicting system behavior. Therefore, while it may be possible to realize dressed bound states with a qubit in an aperiodic structure, the benefits from using a periodic structure far outweigh the likely larger device footprint.

A photonic crystal is an electromagnetic structure formed by periodic modulation of the dielectric constant. This results in dispersion relations characterized by energy bands - alternating bandgaps ("forbidden energies") and passbands (continuous density of states). The electric field distribution is characterized by Bloch modes, allowing for the position of qubits at locations that optimize coupling to the band edge [79]. Engineering band edges via finite-size photonic crystals has been demonstrated in many systems, including nanophotonic structures [80, 81] and superconducting microwave coplanar waveguides [82, 76], and tremendous progress towards integration with ultracold atoms and superconducting qubits, respectively, has been reported [76, 75]. There are other ways to create superconducting microwave crystals, including using Josephson junction arrays or lumped element circuits.

In other quantum experiments, periodic structures and periodic structures with intentional defects (to seed high quality factor harmonic cavities) have been employed and demonstrated as promising mediums for engineering interaction. An ongoing series of experiments couple ultra-cold atoms to the band-edge of alligator nanophotonic crystal waveguides, demonstrating superradiance and long-range atom-atom interaction with the goal of simulating quantum many-body models [72, 81, 73, 75, 69]. Nanophotonic crystal cavities have also been employed to couple a single atom to a single optical cavity mode [83]. In optomechanics, phononic bandgap crystals and crystal cavities have been used to suppress bands of phononic excitations and create
defect cavities with which to couple phononic excitations [84]. Thus finite-size, periodic structures are a robust and versatile tool in a wide array of quantum experiments.

Our approach to create effective one-dimensional, superconducting, microwave crystals is to periodically alternate sections of high and low impedance coplanar waveguides (CPWs). To better understand design constraints, let us first briefly review underlying CPW properties.

### 4.1.1 Coplanar waveguide fundamentals

While there are many online CPW calculators available, it is helpful to have an intuitive understanding of the relationships between design choices and CPW properties. "Coplanar Waveguide Circuits, Components, and Systems" by Rainee N. Simons [85] is an invaluable reference for CPW circuit design, and Chapter 2 contains a detailed section on relevant properties and expressions describing CPWs derived from conformal mapping techniques.

For our purposes, we will consider a CPW on a finite thickness dielectric with no metal boundaries. Although in experiment we do have a variety of metal boundaries formed by the copper sample holder and printed circuit board, from our design perspective these can be safely neglected as we are more concerned with consistency throughout the crystal rather than achieving a single parameter with highest accuracy. To incorporate the effect of these boundaries, one could add in the contribution via partial capacitance [85]. Illustrated in Fig. 4.2 are two perspectives of a coplanar waveguide which highlight the relevant dimensions - all of which we have control over in experiment.

One’s choice of substrate, most commonly silicon or sapphire, determines the relative permittivity $\epsilon_r$ of the dielectric, where relative permittivity is absolute permittivity expressed as a ratio relative to the permittivity of vacuum, $\epsilon_0$. While the thickness (h) of the substrate is important, choosing a thickness that is large com-
Figure 4.2: Coplanar Waveguides a Top-down and b cross-sectional views of an example coplanar waveguide section. Approximate values: \( h = 500\mu m, t = 200nm, S = 10\mu m, W = 4\mu m \). To good approximation, we can neglect the metal boundaries provided by the PCB and sample holder when calculating CPW properties. (Not drawn to scale)

pared to the slot width results in only minor deviation of properties when compared to an infinitely thick dielectric substrate. Similarly, provided the conductor thickness (t) is small, it can be neglected from the approximate calculations that are shown below. For example, we choose to use a c-plane sapphire substrate that is \( \sim 430\mu m \) thick with a 200nm Niobium layer that we have sputtered on top.

The remaining parameters, S and W, are free to be modified as needed to achieve the desired impedances. We define two dimensionless quantities,

\[
k_0 = \frac{S}{S + 2W}
\]  

(4.1)
\[ k_1 = \frac{\sinh(\pi S/4h)}{\sinh(\pi(S + 2W)/4h)} \]  

(4.2)

and variants of these quantities,

\[ k'_{0,1} = \sqrt{1 - k^2_{0,1}} \]  

(4.3)

with which we compute complete elliptic integrals, \( K \).

The partial capacitance accounting for the lower dielectric substrate is,

\[ C_1 = 2\varepsilon_0(\varepsilon_r - 1) \frac{K(k_1)}{K(k'_1)} \]  

(4.4)

and the partial capacitance of the CPW in absence of all dielectric (replacing with vacuum) is,

\[ C_{\text{air}} = 4\varepsilon_0 \frac{K(k_0)}{K(k'_0)} \]  

(4.5)

As mentioned previously, to good approximation \( C_1 \) and \( C_{\text{air}} \) are the dominant contributions to the total capacitance.

\[ C_{\text{CPW}} = C_1 + C_{\text{air}} = 2\varepsilon_0(\varepsilon_r - 1) \frac{K(k_1)}{K(k'_1)} + 4\varepsilon_0 \frac{K(k_0)}{K(k'_0)} \]  

(4.6)

We can then compute the effective dielectric constant,

\[ \varepsilon_{\text{eff}} = \frac{C_{\text{CPW}}}{C_{\text{air}}} = 1 + \frac{(\varepsilon_r - 1)}{2} \frac{K(k_1)K(k'_0)}{K(k'_1)K(k_0)} \]  

(4.7)

characteristic impedance,

\[ Z_0 = \frac{1}{cC_{\text{air}}\sqrt{\varepsilon_{\text{eff}}}} = \frac{30\pi}{\sqrt{\varepsilon_{\text{eff}}} K(k'_0)} \]  

(4.8)

and phase velocity.
Figure 4.3: Illustration of a unit cell (not drawn to scale). We define a unit cell as having three parts: low impedance section \(Z_{lo}, \text{length } L_{lo}/2\), high impedance section \(Z_{hi}, \text{length } L_{hi}\), low impedance section \(Z_{lo}, \text{length } L_{lo}/2\). This is not the only possible choice for unit cell, however symmetry is helpful to avoid mistakes when defining direction and wavevectors.

\[ \nu_{ph} = \frac{c}{\sqrt{\epsilon_{eff}}} \quad (4.9) \]

Our photonic crystals are patterned using a direct-write laser writer, followed by a dry \(SF_6\) RIE (reactive ion etch) step to transfer the pattern. To ensure our waveguides are reasonably sized and can be reliably fabricated using photo-lithography, we are thus limited to impedances between approximately 25 Ω to 125 Ω.

### 4.1.2 Unit cell

We choose to define a unit cell (see Fig. 4.3) as a high impedance section of length \(L_{hi}\) sandwiched between two sections of low impedance of lengths \(L_{lo}/2\) for symmetry purposes. As with nearly any periodic modulation, there are naturally many gaps in the band-structure. While strong coupling to band-edge will allow us to realize bound states, we chose to strongly couple the qubit to the second band-edge, rather than the first, due to experimental, finite-size effects.

We use two methods for simulating crystals, infinite limit and finite limit, each providing valuable information when navigating the trade-offs to select unit cell parameters.
4.1.3 Crystal simulation - dispersion relation

We can use the unit cell to calculate the band structure or dispersion relation for an infinite crystal. While we can never make an infinite crystal, calculating the dispersion relation is a very useful starting point and gives us insight into crystal parameters such as band curvature. To a good approximation, the phase velocities in the high and low impedance CPW sections are effectively equal ($v_{p,\text{high}} \sim v_{p,\text{low}} \sim v_p \approx 1.248 \times 10^8$ m/s). This yields

$$\cos\left(\omega k L_{\text{lo}} \frac{L_{\text{hi}}}{v_p}\right) \cos\left(\omega k L_{\text{hi}} \frac{L_{\text{lo}}}{v_p}\right) - \frac{1}{2} \left(\frac{Z_{\text{hi}}}{Z_{\text{lo}}} + \frac{Z_{\text{lo}}}{Z_{\text{hi}}}\right) \sin\left(\omega k L_{\text{lo}} \frac{L_{\text{hi}}}{v_p}\right) \sin\left(\omega k L_{\text{hi}} \frac{L_{\text{lo}}}{v_p}\right) = \cos(k(L_{\text{lo}} + L_{\text{hi}})), $$

(4.10)

where $k$ is the momentum and $\omega_k$ is the dispersion.

We determine the band structure dependence on $L_{\text{lo}}$ and $L_{\text{hi}}$ for $Z_{\text{lo}} \approx 25\,\Omega$ and $Z_{\text{hi}} \approx 125\,\Omega$. We look to optimize trade-offs of four properties: the frequency of the band-edge, the width of the band-gap, the width of the pass-band, and the curvature of the band. From these simulations we see that small changes in the unit cell impedances do not significantly change the band dispersion - a promising quality that accommodates uncertainty in device fabrication.

For comparison, Figs. 4.4 a and b show the simulated dispersion for unit cell parameters in Liu et al. [76] and this work, respectively. The unit cell for this work was chosen to have a flatter band dispersion near the band-edge (analogous to effective mass), $\alpha$, so as to realize more spatially localized bound states and a larger range of interaction between bound states in a single device realization.

Finally, from Eq. 4.10 we see that we could obtain identical band structure by inverting the unit cell – swapping $L_{\text{lo}}$ with $L_{\text{hi}}$ and $Z_{\text{lo}}$ with $Z_{\text{hi}}$. We choose not to consider this configuration due to the additional fabrication challenge; creating long sections of narrow center pins with large gaps (high impedance) is easier than creating
Figure 4.4: First two bands of simulated dispersion for $Z_{lo} = 25\Omega$, $Z_{hi} = 124\Omega$ and a $L_{lo} = 0.45$ mm, $L_{hi} = 8$ mm (parameters from [76]), and b $L_{lo} = 1.2$ mm, $L_{hi} = 7.8$ mm (parameters from present paper). c Overlay of simulated $S_{21}$ from the transfer matrix method (blue; same parameters as b) and measured high-power $S_{21}$ (black) shows good agreement in bare crystal characteristics. d Overlay of simulated $S_{21}$ from the transfer matrix method (blue; same parameters as b) and from the hopping model (red; with $\kappa = 1$ GHz and $\kappa_0 = 4$ MHz) and measured high-power $S_{21}$ (black) near the band edge. Drop in transmission circa 8.3 GHz is due to TWPA dispersion, not device defect.

long sections of narrow gaps (low impedance) when considering hand-development of photo-resist and the effect of particles in the air and in the photo-resist itself. Furthermore, as we wish to capacitively couple a transmon to the crystal, we are better served by coupling it to a high impedance section (increased voltage) so that we can reach stronger coupling. We will discuss choosing qubit position in Sec. 4.1.6.

4.1.4 Crystal simulation - ABCD matrix simulation

While the dispersion relation assumes an infinite system, crystals of small, finite length have been shown to realize well-resolved gaps in dispersion where transmission is suppressed and bands where transmission is unimpeded. From an experimental
perspective, we use transmission-based measurements to probe the states. In the investigation of bound states, the finite size of the crystal is a practical advantage: the overlaps of bound states with ends of the crystal lead to only quasi-bound states, allowing for detection through transmission measurements. Direct detection of such a state in this way was first demonstrated in Liu et al. [76].

ABCD matrices are a convenient and accurate method for bare crystal simulation that incorporates both the exact number of cells and boundary conditions. In this simple method, we build up the response of the system by concatenating each element - in this case, by multiplication with the ABCD matrix of each subsequent element [78]. For our purposes the ABCD matrix for a section of coplanar waveguide with characteristic impedance $Z$ is

$$M_{CPW}(L, Z) = \begin{bmatrix}
\cos(\omega L/j\nu) & jZ\sin(\omega L/j\nu) \\
j\sin(\omega L/j\nu)/Z & \cos(\omega L/j\nu)
\end{bmatrix}$$

Making the ABCD matrix for a unit cell

$$M_{UC} = M_{CPW}(L_{lo}/2, Z_{lo})M_{CPW}(L_{hi}, Z_{hi})M_{CPW}(L_{lo}/2, Z_{lo})$$  \hspace{1cm} (4.11)$$

Using the ABCD matrix, we can calculate scattering parameter $S_{21} = \frac{2Z_0}{A+B/Z_0+CZ_0+B}$. In Figs. 4.4c and d, comparison of the measured $S_{21}$ for the bare crystal (taken at powers high enough to saturate qubit effects) and the calculated $S_{21}$ from transfer matrices show good agreement [76].

\subsection*{4.1.5 Obtaining crystal parameters - tradeoffs}

To integrate with the standard measurement setup and qubit parameters, we chose unit cell lengths such that the second band-edge would fall between 7-8 GHz. As seen in Fig. 4.4c, the second band had a smoother pass-band compared to the first and
Figure 4.5: A platform for interacting dressed bound states

A 16-site microwave photonic crystal is realized by alternating sections of high and low impedance coplanar waveguide. Two transmon qubits (multi-level, anharmonic energy ladder) are in neighboring unit cells in the middle of the device, centered in the high impedance sections for maximal coupling to the band edge at 7.8 GHz (all values presented in units of $(2\pi)$Hz, i.e. $\omega_{BE} = 7.8 \ (2\pi)$GHz). For this experiment, the pass band (band gap) refers to states above (below) the band-edge frequency. Each qubit is individually tunable in frequency via a local flux bias line. b and c offer closer looks at a qubit and the crystal.

thus we chose to study this band-edge. The frequency of the band edge was designed to be at 7.8 GHz to match with the traveling wave parametric amplifier (TWPA, dispersion feature around 8.3 GHz) to provide good amplification for frequencies in the vicinity of the band edge as well as deep in the bandgap. The width of the bandgap was from 4.75 GHz to 7.8 GHz and needed to be large enough such that we would have a wide range to tune the qubit frequency over, which in turn would result in a wide range of accessible localization lengths. The width of the (second) passband needed to be sufficiently large such that we could ignore the third band edge and we could make the approximation that the curvature of the band (near the band edge) was quadratic. Finally as the curvature of the band played a role in determining the localization length, to make the states more localized, we chose a shallower band curvature (compare red plots in Fig. 4.4 a and b). For this device,
one unit cell consisted of a high impedance section \((Z_{hi} = 124\Omega, L_{hi} = 7.8\ mm)\) and a low impedance section \((Z_{lo} = 25\Omega, L_{lo} = 1.2\ mm)\). Impedance estimates were determined both by measuring coplanar waveguide features after device fabrication and by fitting the measured spectrum with transfer matrix simulations; we find that the dispersion is robust to small impedance deviations in the fabricated sample. In this device, we fit 16 unit cells on a 10 mm x 10 mm sapphire chip. While more unit cells could fit on the chip, we saw experimentally that we must wire-bond extensively on-chip (to connect ground planes and reduce slot-line modes) to create clean band-gaps and pass-bands and included this requirement into the design. By switching to air or dielectric-supported bridges in the future we will be able to shrink the device footprint or include more unit cells in the same size device.

### 4.1.6 Bloch wavefunction

To determine where to place the qubits within the unit cell such that they maximally couple to the desired band, we must calculate the electric field distribution within the unit cell, distribution determined by the Bloch modes for the crystal [79]. We consider electric field because we will capacitively couple a transmon in this project. In comparison, when coupling a qubit to a cavity we look for the voltage antinode to similarly maximize coupling.

To obtain the Bloch wavefunction, we first relate voltage, \(V(x,t)\), and current, \(I(x,t)\), using inductance per unit length, \(l(x)\), and capacitance per unit length, \(c(x)\) in the follow differential equations.

\[
\frac{d}{dx} V(x, t) = -l(x) \frac{d}{dt} I(x, t) \tag{4.12}
\]

\[
\frac{d}{dx} I(x, t) = -c(x) \frac{d}{dt} V(x, t) \tag{4.13}
\]
Figure 4.6: Magnitude of Bloch wavefunction for first four energy bands: $Z_{lo} = 25\Omega$, $Z_{hi} = 124\Omega$, $L_{lo} = 1.2mm$, $L_{hi} = 7.8mm$. For maximal coupling to second band near the edge of the Brillouin zone, we must place the qubit in the middle of the high impedance section (center of the unit cell). Here, $a$ is the length of the unit cell.

We rewrite these to obtain the following wave equation,

$$\frac{\partial}{\partial x} \left[ \nu_p \frac{\nu_p}{Z_c(x)} \frac{\partial V(x,t)}{\partial x} \right] = \frac{1}{\nu_p Z_c(x)} \frac{\partial^2}{\partial t^2} V(x,t)$$  \hspace{1cm} (4.14)

where phase velocity is

$$\nu_p = \frac{1}{\sqrt{l_c}}$$ \hspace{1cm} (4.15)

and characteristic impedance is periodically modulated according to the unit cell

$$Z_c(x) = \sqrt{\frac{l(x)}{c(x)}}$$ \hspace{1cm} (4.16)
We can solve this numerically using Fourier transform techniques and matrix manipulation [79]. The simulated Bloch modes for the first four energy bands are shown in Fig. 4.6. These plots illustrate that for maximal coupling with the second band-edge (near wavevectors $\pm \pi/a$ in the top-right plot), we must place the qubit in the center of the unit cell which is the middle of the high impedance section. Simultaneously, this corresponds to minimal coupling to the first and third band-edges.

For these crystal parameters, maximally coupling to the second band edge (and minimally to the first band edge) corresponds to placing the qubit in the center of long high-impedance section. Other locations within a unit cell change coupling to each band edge, which is a potentially interesting regime for future experiments. However, here we are interested in reducing the effect of the other band as much as possible. We cannot completely eliminate this coupling; experimentally we can still detect a drop in transmission in the lower passband when the qubit is resonant but this change is orders of magnitude smaller than in the second band.

In this device, we capacitively couple a transmon qubit to each of the two central unit cells of the 16-cell crystal. A transmon’s anharmonic level structure is due to the nonlinear inductance of Josephson junctions and allows for selective addressing of energy level transitions. However, it is important to emphasize that our realization of a qubit does have higher energy levels set by transmon geometry, unlike the standard theoretical qubit which is synonymous with a two-level system. These higher levels are also coupled to the band edge and therefore accounting for these levels becomes important when looking beyond the first excitation sector.

Our qubits are fully patterned with a 125kV e-beam writer, with bridge-free junctions, and are made of evaporated aluminum. The qubits are designed to have a target charging energy (from electro-magnetic simulation) of approximately 450 MHz, and emphasis was placed on maximizing coupling between the qubit and photonic crystal
without significantly altering the unit cell. Finally, although identical in design, in reality the qubits do differ due to fabrication uncertainty/error. However, as coupling to the waveguide is designed to be the dominant decay channel for the qubits, bound states are robust to small variation in other parameters.

As mentioned, we place qubits in adjacent unit cells (9mm separation) at the center of the crystal such that we can see significant change in interaction strength with detuning. Each qubit has a local flux bias line for independent control (DC cross-talk is corrected for through standard calibration). These lines are low pass filtered; however, as the dominant decay of the qubit is via the crystal, this is not expected to be a limiting factor in coherence.

4.2 Investigating the dressed qubit-photon bound state

A qubit-photon dressed bound state, seeded by a single qubit in a superconducting crystal, was first directly detected by Liu et al[76]. These states are fundamentally distinct from both standard transmon qubits (isolated, in transmission lines, or in cavities) and harmonic defects in crystals. In this section we will share some of the unique properties of these states measured in experiment.

As stated previously, in our system the overlap of the photonic component of the dressed bound state with the “ends” (input and output) of the crystal results in “quasi-bound” states. This overlap enables photon transport across the crystal at otherwise forbidden frequencies. In experiment, this translates to detection via transmission measurement - a standard microwave measurement using a vector network analyzer. This transport will manifest in the (single photon) transmission measurement of a Lorentzian peak at the bound state frequency, where the linewidth of the peak will be determined by the magnitude of overlap of the state with the
input/output waveguides. Before embarking on a discussion of experimental observations, first let us gain some intuition by briefly studying the origin of the bound state and the importance of non-Markovianity in this system.

4.2.1 Bound state theory: comparison of exact and Born-Markov solutions

Here we examine the difference between the full solution and the Born-Markov approximation for a single qubit near a band-edge for the purpose of determining the bound state resonance. For now, let us consider the Hamiltonian

\[ H = \omega_{01}|1\rangle\langle 1| + \sum_k \omega_k a_k^\dagger a_k + \sum_k (g_k|1\rangle\langle 0|a_k + h.c.), \]

(4.17)

where \(\omega_{01}\) is the qubit frequency, and \(\omega_k\)'s are the continuum of photonic modes (band dispersion). In this context, the Born-Markov approximation consists of eliminating the photons to second order in perturbation theory to obtain an effective qubit with resonant frequency,

\[ \omega'_{01} = \omega_{01} - \sum_k \frac{g_k^2}{\omega_k - \omega_{01}}. \]

(4.18)

Replacing \(\sum_k\) with \(\int_{-\infty}^{\infty} dk\), and assuming \(\omega_k = \omega_0 + \alpha k^2\), \(g_k = g\), and \(\omega_0 > \omega_{01}\) (bare qubit frequency is below the band-edge),

\[ \omega'_{01} = \omega_{01} - \frac{g^2 \pi}{\sqrt{\alpha (\omega_0 - \omega_{01})}}. \]

(4.19)

We compare this to the solution which does not make any approximations [76]. Beginning with the state,

\[ |\psi\rangle = c_1|\text{vac}\rangle|1\rangle + \int dk c_k a_k^\dagger|\text{vac}\rangle|0\rangle \]

(4.20)
with energy $\omega_b$. The time-independent Schrödinger equation gives,

$$\omega_b c_1 = \omega_{01} c_1 + \sum_k g_k c_k$$  \hspace{1cm} (4.21)

$$\omega_b c_k = \omega_k c_k + g_k c_1$$  \hspace{1cm} (4.22)

$$\omega_b = \omega_{01} - \sum_k \frac{g_k^2}{\omega_k - \omega_b}$$  \hspace{1cm} (4.23)

Comparing Eq. 4.18 and 4.23, we see that the Born-Markov approximation consists of replacing the dressed (bound-state) energy $\omega_b$ in the denominator with the bare $\omega_{01}$ energy. Without making the Born-Markov approximation, but again taking $\sum_k \to \int_{-\infty}^{\infty} dk$, $\omega_k = \omega_0 + \alpha k^2$, $g_k = g$, and $\omega_0 > \omega_b$

$$\omega_b = \omega_{01} - \frac{g^2 \pi}{\sqrt{\alpha(\omega_0 - \omega_b)}}$$  \hspace{1cm} (4.24)

Therefore the bound state remaining within the band-gap rather than crossing over the band-edge is only captured by the full solution - one that does not take into account the standard Born-Markov approximation. Thus observation consistent with this prediction (see Fig. 4.7a) is itself direct evidence of Non-Markovianity. In Sec. 4.6.2 we will expand this simple derivation to a more generalized form, incorporating two qubits with arbitrary coupling and frequency.

### 4.2.2 Experimental detection of dressed qubit-photon bound state

In Fig. 4.7 we measure $S_{21}$ at low power to track the bound state as a function of qubit frequency. This crystal (see Fig. 4.4) has a bare (uninfluenced by the qubit)
Figure 4.7: a Experimental data and b hopping model simulation for $S_{21}$ vs. single-qubit frequency and probe frequency. The bare band edge is at 7.797GHz. The bright peak in the bandgap is the dressed qubit-photon bound state. The bound state always exists within the bandgap for qubit frequencies both above and below the band edge - a clear signature of non-Markovianity (see Sec. 4.2.1). In this figure, the other qubit is far detuned and has negligible effect. See Sec. 4.3 for discussion of modeling and simulation.

The band edge at 7.797GHz, delineating the bandgap (dark red/black) from the pass-band (bright yellow). The bound state shows up as a Lorentzian peak in transmission. As the qubit frequency, y-axis of Fig. 4.7a, increases in frequency to approach the band-edge, the bound state also increases monotonically. There is also a shift in the band-edge and change in the pass-band as the detuning between qubit and band-edge is reduced. While the bare qubit frequency can increase above the band-edge (apparent as a drop in transmission in the pass-band), the bound state will always be within the band-gap.

In addition to bound state resonance, in Fig. 4.7a we also obtain the linewidth of the bound state peak (Fig. 4.8). The linewidth of the bound state is set by the amplitude of the exponentially decaying photonic wavefunction at the ends of the crystal (ignoring other forms of loss). The envelope amplitude decays as $\sim e^{-x/L}$,
Figure 4.8: Bound state linewidth, an indirect measure of localization, varies with qubit frequency. The wide range over which photon localization can be tuned indicates the feasibility of realizing a chain of strongly interacting bound states. Experimentally measured and simulated linewidths are shown in red and black, respectively. Numerical simulation using hopping model (see Sec. 4.3).

where x is the distance from the qubit location and L is the localization length. For simplicity, we consider the case of a single qubit at the center of the crystal (total length d) such that the envelope is symmetric. This results in a linewidth proportional to $e^{-d/2L}$. Of course, this approximation is only valid in the limit where $e^{-d/2L} << 1$, meaning the bound state is sufficiently localized compared to the finite-length of the crystal.

State localization is tunable in situ with frequency through a range determined by device parameters, including qubit-waveguide coupling and band curvature. We realize stronger localization in this device than in Liu. et al (compare maximum linewidths measured in this work and Liu’s work of $\sim 10$ MHz and $\sim 100$ MHz, respectively) primarily due to a shallower band-curvature, realized by tailoring the unit cell of the photonic crystal. These more localized states still exhibit a wide range of tunability, critical for realizing strong, tunable interaction between spatially separated bound states. The ability to tune the localization with small sized crystals shows the versatility of this platform.

As the different coupling regimes translate to dramatically altered system behavior [63], it is important to determine which domain our system falls under. In systems
Figure 4.9: **Probing the bound state energy levels a** The anharmonicity of the bound state is dependent on bare-qubit frequency, demonstrating a tunable on-site interaction strength. In blue (red), the first (second) transition of the bound state is measured across a range of bare qubit frequencies (inset - simulation. See Sec. 4.3). **b** Decreasing anharmonicity with increasing bound state frequency shown in red for experimental data and black for simulation.

such as the one presented here, qubit emission into the waveguide being larger than the other decay rates (coherent atom-photon interaction rates being larger than decay rates) is the minimal coupling criterion, upon which the dressed bound state within the gap can be spectrally resolved [63]. The strong coupling criterion corresponds to the situation where a bare qubit resonant with the band edge gives rise to a bound state that is shifted from the band edge by more than the bound state’s linewidth [63, 76]. In our finite system, we observe \( \sim 250 \) MHz separation between the bound state and the band edge with bound state linewidth of 4 MHz when a qubit is resonant with the band edge, thus firmly reaching the strong coupling condition (see Fig. 4.8 and Fig. 4.7a). By fabricating two qubits in the photonic crystal (Fig. 4.5), we realize multiple, spectrally-resolvable bound states and can study inter-bound state interaction.

### 4.2.3 Bound state anharmonicity

In addition to determining localization length, the frequency of the bound state also determines on-site interaction strength. In Figs. 4.9a and 4.9b, we characterize the dependence of the transition frequencies between the three lowest levels of the bound
state on bare qubit frequency, and observe the steady reduction in bound state anharmonicity from over 350 MHz to 0 MHz as the qubit is tuned from deep in the bandgap to the passband. This is dramatically more than the \( \sim 10\% \) modification of qubit anharmonicity with frequency expected when a qubit is strongly coupled to a cavity mode \([86]\).

Therefore, while we may treat the one-excitation and two-excitation bound states as first \(|1\rangle_q\) and second \(|2\rangle_q\) excited states of a new effective anharmonic qubit \([76]\), it is important to note that this effective qubit differs in frequency and anharmonicity from the bare (multi-level transmon) qubit. Defining the three lowest bare qubit levels as \(|0\rangle_q\), \(|1\rangle_q\), and \(|2\rangle_q\), here the two-excitation bound state is largely due to the coupling of the second qubit transition \(|1\rangle_q \leftrightarrow |2\rangle_q\) with the band edge rather than other multi-photon effects \([64]\).

Numerical simulations - modeling the photonic crystal as a coupled cavity array with free parameters fit to match the band curvature from the dispersion relation \([87, 63]\) - show similar dependence of anharmonicity on detuning (see Fig. 4.9a inset and Fig. 4.9b). Unlike the transfer matrix method \([78, 88, 89]\), this approach can extend beyond the single-excitation manifold to capture the higher levels of the bound state, as well as the Lamb shift of the qubit frequency, observed when including next-nearest neighbor hopping between coupled cavities. Each qubit is modeled as a three-level ladder with negative anharmonicity, and with the \(|0\rangle_q \leftrightarrow |1\rangle_q\) and \(|1\rangle_q \leftrightarrow |2\rangle_q\) transitions coupled with amplitudes \(g\) and \(g\sqrt{2}\), respectively, to its local cavity-site. It is critical to include level \(|2\rangle_q\) to accurately reproduce the two-excitation manifold observed in experiment.

### 4.2.4 Theory of two-photon bound state

To understand the significance of the higher bound state transition, here we take a closer look at the two-excitation bound state formed by a single qubit. For a single
The population of qubit levels in the two-excitation ground state of $H_{\text{tot}}$ as a function of bare qubit frequency.

qubit, the most general two-excitation wave function is

$$|\psi_{2B}\rangle = b|2\rangle|0\rangle + \sum_i d_i |1\rangle|0\rangle + \sum_{i>j} f_{i,j} a_i^\dagger a_j^\dagger |0\rangle|0\rangle + \sum_i f_i (a_i^\dagger)^2 \frac{|0\rangle}{\sqrt{2}}|0\rangle.$$  \hspace{1cm} (4.25)

Here the basis states are labeled as $|\text{qubit}\rangle|\text{photon}\rangle$. For $i < j$, it is convenient to define $f_{i,j} = f_{j,i}$. In Fig. 4.10, we plot $|d_i|^2$ and $|f_{i,j}|^2$, which are obtained via exact diagonalization of the two-excitation sector for 16 sites. (As a technical aside, we note that our two-excitation numerical simulations involve two qubits unless explicitly noted. For this section, the qubit on site eight is detuned to 4.25 GHz for our numerical simulations and thus has negligible effect.)

We observe that the photons are localized around the qubit. In Fig. 4.10c, we plot the populations of qubit levels in the two-excitation ground state of $H_{\text{tot}}$, which
are given by

\[ |\langle 0|\psi_{2B}\rangle|^2 = |b|^2, \quad |\langle 1|\psi_{2B}\rangle|^2 = \sum_i |d_i|^2, \quad |\langle 2|\psi_{2B}\rangle|^2 = \sum_{i \geq j} |f_{ij}|^2, \]  

(4.26)

to illustrate which terms in Eq. 4.25 are important for a given bare qubit frequency. For example, when the bare qubit frequency is deep in the gap, the ground state of the two-excitation sector is mostly in the \(|2\rangle|0\rangle\) state as seen in Fig. 4.10c. Upon increasing the bare qubit frequency (while still in the band gap), the population of \(|1\rangle\) increases, while the population of \(|0\rangle\) stays relatively small. This is because two photons must be exchanged to couple the dominant \(|2\rangle|0\rangle\) state and any two-photon state. Since there are no terms in \(H_{\text{tot}}\) that directly exchange two photons, this makes it a higher order process. On the other hand, coupling \(|2\rangle|0\rangle\) and \(a^\dagger_i|1\rangle|0\rangle\) only requires exchanging one photon. When the bare qubit frequency is at or near the band edge, each qubit level in Eq. 4.25 contributes significantly to the bound-state wavefunction.

Unfortunately, we are unaware of an exact solution similar to the one in Sec. 4.6.2. To make analytical progress, we assume \(f_{ij} = 0\) which is a valid approximation when the bare qubit frequency is deep in the band gap (as seen in Fig. 4.10c). Solving the eigenvalue equation, \(H|\tilde{\psi}_{2B}\rangle = E_{2B}|\tilde{\psi}_{2B}\rangle\), for the following wave-function ansatz (in momentum-space),

\[ |\tilde{\psi}_{2B}\rangle = \tilde{b}|2\rangle|0\rangle + \sum_k \tilde{d}_k a^\dagger_k |1\rangle|0\rangle, \]  

(4.27)
yields the following equations,

\[ \tilde{b}E_{2B} = \tilde{\omega}_{02}\tilde{b} + \frac{\sqrt{2g}}{\sqrt{N}} \sum_k e^{ikaz} \tilde{d}_k, \]  

(4.28)

\[ \tilde{d}_k E_{2B} = (\tilde{\omega}_k + \tilde{\omega}_{01})\tilde{d}_k + \frac{\sqrt{2g}}{\sqrt{N}} e^{-ikaz} \tilde{b}. \]  

(4.29)
These are similar to equations for the single photon case. Thus, we have

\[ E_{2B} - \omega_0 = -\frac{g^2}{\sqrt{\omega_0 + \omega_0 - E_{2B}}}, \]  

(4.30)

and

\[ d_j \propto \sqrt{\frac{2b}{N}} \sum_k \frac{e^{ika(j - z_2)}}{E_{2B} - \omega_0 - \omega_k} = -\frac{\sqrt{2b} \cos(\pi (j - z_2))}{2\sqrt{\alpha(\omega_0 + \omega_0 - E_{2B})}} e^{\sqrt{\omega_0 + \omega_0 - E_{2B}}|j - z_2|}. \]  

(4.31)

We see that the photon is localized around the qubit, consistent with the exact finite-size numerical results seen in Fig. 4.10a. We note this ansatz breaks down when the bare qubit frequency is near the passband as the states become more photonic, in which case we can no longer neglect \( f_{i,j} \).

4.3 Modeling the bound state - hopping model

Given these key experimental observations, we seek a theoretical model that simultaneously captures them all. We represent the system using the hopping model, comprising three main parts: the crystal, the qubit(s), and interaction between the two. This platform offers us the ability to (1) simulate transmission in the single excitation sector by introducing a weak drive and loss, (2) calculate eigenstates of the coupled system in higher excitation manifolds, and (3) simulate inter-bound state interaction.

4.3.1 Photonic crystal Hamiltonian

The Hamiltonian for the one-dimensional photonic crystal is given by \( H_c = \sum_k \omega_k a_k^\dagger a_k \), where \( a_k^\dagger \) creates a bosonic excitation with momentum \( k \), and \( \omega_k \) is the dispersion relation of the second band of the photonic crystal, which is discussed in Sec. 4.10. Here, we have ignored the other bands of the photonic crystal.
as the qubits couple predominantly to the second band. Fourier transforming

\[ a_k = \sqrt{\frac{2}{L}} \sum_j N a_j^\dagger e^{ikx_j} , \]

where \( L \) is the system size, \( a \) is the unit cell size, \( N \) is the number of unit cells, \( x_j = aj \), and \( k = \frac{2\pi}{L} n \), where \( n \) is an integer) gives a hopping model with periodic boundary conditions, \( H_c = \sum_{i,j} J_{i,j} a_i^\dagger a_j \), where

\[ J_{i,j} = J_{|i-j|} = \lim_{N \to \infty} \frac{1}{N} \sum_k e^{ik(x_i - x_j)} \omega_k = \int_{-\pi}^{\pi} \frac{d\tilde{k}}{2\pi} e^{i\tilde{k}(x_i - x_j)/a} \omega_{\tilde{k}}/a. \]  (4.32)

Here, \( \tilde{k} \) is a dimensionless integration variable, and we have used the fact that \( J_{i,j} = J_{j,i} \) since \( \omega_k = \omega_{-k} \). In Eq. 4.32 we have taken \( N \to \infty \), as we only know \( \omega_k \) in that limit (see Sec. 4.10). To model our finite system, which has open boundary conditions and 16 unit cells, we use a 16 site hopping model with open boundary conditions with hopping strengths determined by Eq. 4.32. Using the photonic crystal parameters in Sec. 4.1.5, we find (by numerical integration) \( J_0 = 9.3272 \text{ GHz}, J_1 = 0.7288 \text{ GHz}, J_2 = -0.0344 \text{ GHz}, J_3 = 0.0178 \text{ GHz}, J_4 = -0.0034 \text{ GHz}, \) and \( J_5 = 0.0014 \text{ GHz} \). Unfortunately, we are unaware of an exact analytical solution for \( J_{i,j} \) for our system. In our numerical simulations, we keep hopping terms up to \( J_5 \). We have calculated the hopping parameters for a given set of photonic crystal parameters. A different choice of photonic crystal parameters would have given a different set of hopping parameters. As such, these parameters should only be understood as estimates. We briefly comment on the change in theory parameters that arises from using different photonic crystal parameters at the end of this section.

### 4.3.2 Qubit Hamiltonian

Each qubit is modeled as a multi-level ladder with negative anharmonicity as it is critical to include the higher qubit levels to reproduce the second excitation manifold observed in experiment.
The Hamiltonian for the isolated qubits is given by

\[ H_q = \sum_{i=1,2} \sum_{n=0}^{\infty} \omega_{0n;i} |n\rangle_i \langle n|_i. \]

(4.33)

Here, \( i \) labels the qubit, \( n \) labels the level of the qubit and \( \omega_{0n;i} \) are the bare energy levels of the qubits. In our simulation, the number of qubit levels is truncated at five (i.e., \( |0\rangle \) through \( |4\rangle \)). For our experiment, \( \omega_{00;i} = 0, \omega_{02;i} = 2\omega_{01;i} - \Delta, \omega_{03;i} = 3\omega_{01;i} - 3\Delta \) and \( \omega_{04;i} = 4\omega_{01;i} - 6\Delta \), where \( \Delta \) is the bare anharmonicity of the qubits, which is taken to be the same for both qubits.

### 4.3.3 Interaction Hamiltonian

We now turn to the coupling of the qubits to the photonic crystal. To an excellent approximation, the coupling between the qubit and the photonic crystal takes place within a single unit cell. Thus, in the rotating-wave approximation, we can write the coupling term of the Hamiltonian as

\[ H_{qc} = \sum_{i=1,2} g_i a_{z_i}^\dagger (|0\rangle_i \langle 1|_i + \sqrt{2}|1\rangle_i \langle 2|_i + \sqrt{3}|2\rangle_i \langle 3|_i + \sqrt{4}|3\rangle_i \langle 4|_i) + h.c., \]

(4.34)

where \( z_i \) labels the position of the two qubits. In our system, the qubits are on neighboring unit cells, i.e., \( z_1 = \frac{N}{2} \) and \( z_2 = \frac{N}{2} + 1 \), and the coupling for each qubit, \( g_i \), is different due to small experimental imperfections. The total Hamiltonian of the system is then

\[ H_{\text{tot}} = H_c + H_q + H_{qc}. \]

(4.35)

Finally, we note that this Hamiltonian conserves total excitation number.
4.3.4 Modeling transmission

We now discuss the two theoretical methods we use to calculate transmission in the linear drive regime. Neither method relies on a weak coupling approximation between the qubits and the photonic crystal. The first method involves treating the system as an open quantum system, with loss on each site (that is site-dependent), subject to a weak drive on the first site. The largest loss terms are at the ends of the one-dimensional photonic crystal. The system can then be described by the following effective non-Hermitian Hamiltonian (in the rotating frame) with driving frequency $\omega_d$ and strength $\epsilon$,

$$H_{\text{eff}} = \sum_{i,j=1}^{N} \left( J_{i,j} - \omega_d \delta_{i,j} - i\kappa_0 \delta_{i,j} \right) a_j^\dagger a_j + \sum_{i=1,2} (\omega_{01;i} - \omega_d - i\kappa_q) |1\rangle_i \langle 1|_i + \sum_{i=1,2} g_i (a_{z_i}^\dagger |0\rangle_i \langle 1|_i + a_{z_i} |1\rangle_i \langle 0|_i) - i\kappa (a_1^\dagger a_1 + a_N^\dagger a_N) + \epsilon (a_1^\dagger + a_1),$$

(4.36)

where $\kappa_q$ is the qubit halfwidth, $\kappa_0$ is a uniform contribution to photonic halfwidth, and $\kappa$ is a decay rate on the first and last sites. While there are certainly other forms of loss (such as non-uniform loss on each site), our goal is to reproduce the key features (for example, the locations of the bound state and of the transmission dip, as well as the linewidth of the bound state) using as few parameters as possible. The equations of motion for the quantum operators are

$$\frac{\partial a_y}{\partial t} = -i \left( \sum_{j} (J_{y,j} - \omega_d \delta_{y,j}) a_j + \epsilon \delta_{y,1} + \sum_{i=1,2} \delta_{y,z_i} g_i |0\rangle_i \langle 1|_i \right) - \left( \kappa_0 + \kappa (\delta_{y,1} + \delta_{y,N}) \right) a_y,$$

(4.37)

$$\frac{\partial |0\rangle_i \langle 1|_i}{\partial t} = (-i(\omega_{01;i} - \omega_d) - \kappa_q) |0\rangle_i \langle 1|_i - i g_i a_{z_i} (|0\rangle_i \langle 0|_i - |1\rangle_i \langle 1|_i).$$

(4.38)
We have omitted vacuum Langevin noise from the equations of motion as this noise does not affect our calculations. Solving for the steady state of $a_N$ in the weak drive limit ($\langle |1_i\rangle_i\langle 1_i|_s = 0$) yields the transmission. More specifically, $S_{21} \propto \langle a_N \rangle_{ss}/\epsilon$.

### 4.3.5 Fitting the parameters of the hopping model

The unknown parameters in the Hamiltonian that we must fit to the data include $g_i$, $\kappa_0$, $\kappa_q$, and $\kappa_x$ and $\Delta$. First we will limit ourselves to fitting parameters of the single excitation sector, and then incorporate $\Delta$ in the next section.

It is important to note that while $\omega_{01;i}$ is tunable its exact value is unknown. This is because neither transmission nor spectroscopic measurement permits direct detection of the qubit frequency as the qubit has already hybridized with the crystal to create the bound state, a new effective qubit. The transmission dip that occurs in the pass-band when the qubit is in the pass-band (see Fig. 4.7) also does not occur at the bare qubit frequency - from simulation we see that there is a finite difference between the two that is due to the next nearest (and beyond) neighbor coupling. From simulation we see that the transmission dip due to the shifted qubit frequency persists inside the gap although we cannot detect it using transmission. We can however, use the second qubit/bound state as a beacon to hone in on the dip of the first qubit when inside the gap by tuning the second bound state until it becomes extinguished by the dip. This will be discussed in more detail in Sec. 4.6. For the purpose of fitting the numerical model with experimental data, we will simply acknowledge that the estimated $\omega_{01;i}$ in experiment has a finite uncertainty on the order of few to tens of MHz.

The unknown parameters include $g_i$ and $\Delta$, and, for the first method, also $\kappa_0$, $\kappa_q$, and $\kappa$. Furthermore, $\omega_{01;i}$ is tunable but its value is unknown, and the transmission dip (visible when the bare qubit frequency is in the passband) does not, in general,
Figure 4.11: Dependence of transmission $S_{21}$ on drive frequency, dependence used for determining the coupling strength of the second qubit, i.e., the one at site $N/2+1 = 9$. 

a Solid blue line is theoretical data for $\omega_{01;2} = 7.9875$ GHz while blue dots are experimental data. We choose parameters of the Hamiltonian such that the bound state frequency, the transmission dip frequency, and the linewidth of the bound state match the experimental data. 

b Solid blue line is theoretical data for $\omega_{01;2} = 7.941$ GHz and blue dots are experimental data. Solid red line is theoretical data for $\omega_{01;2} = 8.038$ GHz and red dots are experimental data. 

c Comparison of transmission methods for $\omega_{01;2} = 7.9875$ GHz. The solid blue line is from method one, while the solid red line is from method two. The bound state and transmission dip occur at the same frequencies for both methods.

occur at the bare qubit frequency unless hopping amplitudes $J_{i,j}$ beyond nearest-neighbor are negligible.

The first parameters we determine are the coupling strength for each qubit along with $\kappa_x$, $\kappa_0$ and $\kappa_q$. We detune the qubit at site $N/2$ far away from the pass-band and then fix the other bare qubit frequency near the band-edge. Transmission is then measured as a function of driving frequency. We choose parameters such that our numerical simulations match the transmission dip and experimentally measured frequency and line-width of the bound state for a given bare qubit frequency, as seen in Fig. 4.11a. To make sure we have chosen suitable parameters, we tune the bare qubit frequency. If we have chosen the correct parameters, we should accurately capture the location of the bound state and transmission dip along with the line-width for different bare qubit values, while keeping the other parameters fixed. Indeed, as seen in Fig. 4.11b and Fig. 4.8, we find this is the case for $g_2 = 548$ MHz, $\kappa_q = 0.5$ MHz,
\( \kappa_0 = 2.27 \text{ MHz}, \kappa_{1,L} = 600 \text{ MHz}, \kappa_{2,L-1} = 120 \text{ MHz}, \kappa_{3,L-2} = 20 \text{ MHz} \) and \( \kappa_x = 0 \) for \( x \in 3, \ldots, N-3 \). In Fig. 4.7 we compare the experimental transmission measurement with numerical simulation of this model and find convincing agreement. Repeating the process to determine the coupling strength for the first qubit we find \( g_1 = 505 \text{ MHz} \).

The first parameters we determine are \( \kappa \) and \( \kappa_0 \) (using the first transmission method). We turn off the coupling of the qubits to the photonic crystal (in the experiment, this is accomplished by saturating the qubits using a drive tone with large photon number). We set \( \kappa_0 \) and \( \kappa_q \) to zero and fit \( \kappa \). Given that the largest losses occur at the ends of the photonic crystal, fitting \( \kappa \) first is reasonable. \( \kappa \) controls the linewidth of the photonic modes and the transmission amplitude difference between the transmission dips and peaks in the passband. We find that a reasonable estimate for \( \kappa \) (for the experimental data in Fig. 4.4d) is 1 GHz, although any \( \kappa \) in the range of 0.5 to 1.5 GHz also gives a reasonable fit. We then turn on \( \kappa_0 \), which further reduces the transmission amplitude difference between the transmission dips and peaks in the passband, and lowers the transmission peak of the lowest photonic mode. We estimate that \( \kappa_0 = 4 \text{ MHz} \) (although any \( \kappa_0 \) in the range of 3 MHz to 5 MHz also fits the data well). Fig. 4.4d shows that simulated transmission is in good agreement with the experimental data. Given that there are other losses in the system that we have not included, these numbers should be understood as estimates.

We now turn to determining \( g_i \). While \( \kappa_q \) is set to zero for now, we find that varying it or the other loss parameters does not noticeably change the frequency of the bound state or transmission dip, thus making our estimate of the coupling strength independent of the decay parameters. To begin, we detune the qubit at site \( N/2 \) far away from the passband (in the experiment, the detuned qubit is at 4.5 GHz) and then fix the other (i.e., second) bare qubit frequency.
Though far detuned, the detuned qubit will shift the frequency of the bound state. To account for this effect, we estimate the ratio of coupling strengths. When the bare qubit frequency is resonant with the band edge, the ratio of coupling strengths can be estimated as $g_1/g_2 \approx (\Delta_1/\Delta_2)^{3/4}$ (see Ref. [76] or Eq. 4.55), where $\Delta_i$ is the frequency difference between the band edge and the bound state for the $i$th qubit. Experimental data indicates $\Delta_2 \approx 250$ MHz and $\Delta_2 - \Delta_1 \approx 25$ MHz, which corresponds to $g_1/g_2 = .93$. Upon fitting the data, we estimate that $g_2 = 0.55$ GHz (and hence, $g_1 \approx 0.512$ GHz).

Given that our value of $g_1$ is only an estimate, one may wonder about the effect of fine-tuning the coupling strength of the far detuned qubit. We find that even if one changes the coupling strength of the detuned qubit, $g_1$, by 25 MHz away from 0.512 GHz, the bound state will only move around half a MHz. In other words, the effect of any fine tuning of $g_1$ can be safely ignored.

Transmission is then calculated as a function of driving frequency. We find that $g_2 = 0.55$ GHz and $\omega_{01;2} = 7.9875$ GHz match the experimental data well when the bound state is at 7.605 GHz, as seen in Fig. 4.11a. Calculating transmission when the first qubit frequency is near the pass band and the second qubit frequency is detuned and comparing it to experimental data, we find $g_1 = 0.505$. To make sure we have chosen suitable coupling strengths, we tune the bare qubit frequency (the detuned bare qubit frequency is kept fixed). If we have chosen the correct parameters, we should accurately capture the locations of the bound state and the transmission dip for different bare qubit frequencies, while keeping the other parameters fixed. Indeed, as seen in Fig. 4.11b, we find this is the case for the chosen coupling strengths.

Our next goal is to obtain an estimate for $\kappa_q$. To do so, we increase $\kappa_q$, which increases the linewidth of both the transmission dip and the bound state, until the linewidth of the bound state matches the experimental value well for a fixed bare qubit frequency (we note increasing $\kappa_0$ also increases the linewidth of the bound
state, however $\kappa_0$ is already fixed). We found that $\kappa_q = 0.5$ MHz accomplishes this task for $\omega_{01:2} = 7.9875$. To make sure we have chosen a suitable qubit halfwidth, we again tune the second bare qubit frequency (while keeping the detuned bare qubit frequency fixed). If we have chosen a reasonable qubit halfwidth, we should be able to accurately estimate the linewidth of the bound state for different bare qubit frequencies (while keeping all other parameters fixed). Fig. 4.8 shows that our estimate of $\kappa_q$ is reasonable.

4.3.6 Simulating anharmonicity

We now fit the last remaining parameter, $\Delta$. We first diagonalize $H_{tot}$ in the two-excitation sector for fixed $\omega_{01;i}$ (with the other qubit detuned far away). The theoretical prediction for the dressed anharmonicity is found by taking the lowest eigenvalue of $H_{tot}$ in the two-excitation sector and subtracting two times the lowest single-excitation eigenvalue. We vary $\Delta$ until the theoretically predicted dressed anharmonicity matches the experimentally measured dressed anharmonicity for a given bare qubit frequency (we choose our bare qubit frequency such that the single-particle bound state is at 7 GHz). In doing so, we find, to a good approximation, that $\Delta = 0.365$ GHz for both qubits. We then vary the bare qubit frequency and make sure the theoretically predicted dressed anharmonicity is still consistent with the experimentally measured value for different bare qubit frequencies. We find excellent agreement for a wide range of bare qubit values as shown in Fig. 4.9.

Before we close this section, we estimate errors in our parameters. To begin, we estimate what change in hopping parameters (we call these different hopping parameters $J'$) we would get if we choose $Z_{\text{high}} = 123.5 \Omega$ instead of $124 \Omega$. Both of these choices fit the experimental data well in transmission matrix simulations. This choice of $Z_{\text{high}}$ gives $J'_0 = 9.331$ GHz, $J'_1 = 0.7308$ GHz, $J'_2 = -0.0345$ GHz, $J'_3 = 0.0179$ GHz, $J'_4 = -0.0035$ GHz, and $J'_5 = 0.0014$ GHz. We see that the ratio of
these hopping parameters to the previous set is not less than .97 for any term, so we expect the other parameters in our model will not differ by more than 5 percent from their given predictions. We also expect this to hold true if one uses any reasonable set of photonic crystal parameters. To test this, we estimate \( g_2 \) and the range of decay parameters for the second set of hopping parameters. We find \( g_2 = 0.555 \text{ GHz} \) and that the same range of decay parameters fit the data well, consistent with our expectation.

### 4.3.7 Alternate simulation method

For comparison, we looked at two other methods to model our system. In comparison, each falls short of the hopping model in being able to reproduce actual system behavior.

**Closed system model**

The second method we use was introduced by Biondi et al [87]. Here, we treat the system (which is taken to be the photonic crystal and qubits) as being connected to waveguides with linear dispersions, with velocity \( v_g \), at the ends of the photonic crystal. In this method, we take \( \kappa_q = \kappa_0 = \kappa = 0 \), so that the single-excitation transmission through the system can be expressed in terms of eigenvalues and eigenvectors of the system described by \( H_{\text{tot}} \) (Eq. 4.35) [87]. More explicitly, the transmission for a given frequency \( \omega \) is given by \( |T(\omega)|^2 \), where

\[
T(\omega) = \frac{-2i\beta}{\Gamma_l \Gamma_r + |\beta|^2}, \quad \Gamma_{l,r} = 1 + \frac{i}{2v_g} \sum_n \frac{|V^l_n|^2}{\omega - \Omega_n}, \quad \beta = \frac{1}{2v_g} \sum_n \frac{V^l_n(V^r_n)^*}{\omega - \Omega_n}.
\](4.39)

Here, \( V^l_r = \sqrt{v_g g_w} |0| a_{1,N} |n\rangle \), \( \Omega_n \) and \( |n\rangle \) are the eigenvalues and eigenvectors of \( H_{\text{tot}} \) in the single-excitation sector, and \( g_w \) is the coupling between the waveguide and the photonic crystal. Intuitively, transmission occurs when the single-excitation
eigenstates have the probability of the photon being on both ends of the photonic crystal.

Fig. 4.11c shows theoretical data from both simulations for $g_2 = 0.55$ GHz and $\omega_{01;2} = 7.9875$ GHz. The locations of the bound state and transmission dip occur at the same spot for both methods. The key difference is that the second method does not accurately predict the magnitude of the linewidth of the bound state as it assumes $\kappa_q = \kappa_0 = \kappa = 0$ (but instead has coherent coupling of the crystal to the waveguide). In these simulations, we have taken $g_w = 2$ GHz as that fits the data when the qubits are saturated well (not shown). We note that any value of $g_w$ in the range of 1.5 to 2.5 GHz also gives a reasonable fit to the saturated qubit data and that the frequencies of the bound state and the transmission dip are not sensitive to $g_w$.

**ABCD matrix simulation**

We can also obtain an approximate numerical simulation of the one-excitation sector of the coupled qubit-crystal system using ABCD matrices. (see Sec. 4.1.4 for simulation of bare crystal). The matrix for a qubit in the single photon regime is $[88, 76]$}

$$M_q = \begin{bmatrix} 1 & 0 \\ -j \gamma(\omega_q) \frac{1}{\omega - \omega_q Z_0} & 1 \end{bmatrix}$$

where $\gamma(\omega_q)$ is set by the coupling strength between qubit and a waveguide of impedance $Z_0$ and for simplicity is assumed to be constant for all $\omega_q$. It is important to note that due to the nature of the calculation, $\omega_q$ is not the bare qubit frequency but an effective frequency that is shifted from the bare qubit frequency due to coupling with the band-edge. This distinction becomes more significant when the qubit frequency is in the pass-band (where the Born-Markov approximation breaks down), where we see
a transmission dip corresponding to $\omega_q$. Knowing only the effective frequency, it is non-trivial to recover the bare qubit frequency as the magnitude of the shift depends on qubit frequency. This is a relevant challenge when trying to fit device parameters for calibration and numerical simulation. This is another reason why the hopping model is preferred; when including next-nearest neighbor interaction and beyond, that model takes as input the bare qubit frequency without assumptions regarding the frequency of the transmission dip.

Despite this, the ABCD simulation method is a useful technique that takes into account the exact design of the device and allows one to numerically study the impact of experimental variation - such as non-homogenous impedance, variations in length, or qubit location - and provides easy comparison with experimental data.

Thus overall the hopping model is the most successful method we explored that reproduces all of the key experimental observations presented - bound state resonance, linewidth, anharmonicity, and Lamb-shifted qubit frequency.

### 4.4 Strongly driving the bound state

The tunable level structure also emerges in the emission spectrum of a continuously driven bound state (Fig. 4.12), induced by a single qubit with bare frequency above the band edge. At low drive amplitude or Rabi frequency, transmission across the crystal via the bound state exhibits antibunching [91], consistent with single photon transport of a two-level system and resonant pump [29, 92, 43]. When the Rabi frequency is on the same order as the anharmonicity, the bound state can no longer be approximated as a two-level system. In this domain, the steady state will be a mixture of the three eigenstates obtained by diagonalizing the drive Hamiltonian in the Hilbert space spanned by $|0\rangle$, $|1\rangle$, and $|2\rangle$. Transitions between all three eigenstates
Figure 4.12: Response of a resonantly driven (∼ 7.59 GHz) bound state (induced by a qubit at 7.9 GHz, which is above the band edge located at 7.8 GHz) as a function of drive power. At low drive power, only the Mollow triplet is observed. With increasing power we see four additional sidebands, two on either side of the original Rabi sidebands, which together are the transitions between the three lowest levels of the anharmonic bound state ($|0\rangle$, $|1\rangle$, $|2\rangle$)

(a) Pump-probe spectroscopic measurement of bound state response, sweeping weak tone (x-axis) to detect resonances that appear as function of increasing pump power (y-axis). As resonances are detected as a change in transmission amplitude at the band-edge, the sign of the change (bright vs. dark in color-scheme) is not significant and depends on the exact frequency monitored. The bright feature circa 7.8 GHz is due to the pass-band and is not therefore a result of the strong drive. 

(b) Power or emission spectrum of resonantly driven bound state for increasing drive power. The white crosses are from numerical simulations (see Sec. 4.4.1). We have included five effective qubit (bound state) levels in our simulation. See text for the discussion of the seventh sideband around 7.25 GHz. In both (a) and (b) we see the Rabi sidebands, linearly displaced from the central peak with increasing drive amplitude, characteristic of the Mollow triplet. The remaining 4 sidebands (two at lower frequency and two at higher frequency) are due to the involvement of the third level of the bound state coupling to the drive field. At strong drive, the generalized eigenstates thus include the lowest three levels of the dressed bound state, resulting in the six transitions [90]. While qualitatively similar, the two detection methods vary in the exact quantity they measure - the Fourier transform of the same-time and two-time autocorrelation functions respectively.

result in six sidebands [90]. These six sidebands are visible in Fig. 4.12, though emission intensity varies greatly among them due to eigenstate population.

A seventh transition is evident in the data (7.25 GHz in Fig. 4.12b). This additional transition is due to the fourth effective qubit level ($|3\rangle$) while its curvature
Figure 4.13: Theoretical simulations of the emission spectrum for different pump powers. Here, the blue squares are numerical results obtained from the total Hamiltonian Eq. 4.40, the green squares are from the dressed-qubit Hamiltonian Eq. 4.41, and the red squares are from Eq. 4.41 but with $\cos \theta = 1$. a Here, $\omega_{01} = 7.97$ GHz, and the bound-state frequency is 7.591 GHz. Using the appropriately reduced matrix element ($\cos \theta < 1$, blue squares) is crucial in obtaining accurate results using Eq. 4.41. b Here, the bare qubit frequency of 7 GHz and the bound-state frequency of 6.847 GHz are both far from the band edge, so that $\cos \theta \approx 1$ and the reduction in the matrix element can be neglected, so all three data sets lie on top of each other.

is reproduced by including a fifth effective qubit level ($|4\rangle$) in our numerical simulations. Crucial to reproducing this transition in our theoretical simulations is taking into account that the bound state level structure cannot be defined by a single anharmonicity, i.e., given the anharmonicity, $\Delta = \omega_{12} - \omega_{01}$, of the bound state, the frequency of the fourth level of the bound state is not simply given by $3\omega_{01} - 3\Delta$ as is expected for a transmon [4].

### 4.4.1 Emission theory

Unfortunately, due to the large dimension of the Hilbert space, we found that a direct approach of calculating the emission spectrum using the master equation for our sixteen-unit-cell system is not numerically feasible. Instead, we diagonalize the Hamiltonian and investigate energy differences. While this approach does not predict
the widths and the driving-strength-dependent intensities of the sidebands, it does predict the frequencies of the sidebands. The Hamiltonian of a single qubit with driving frequency \( \omega_d \) equal to the bound-state frequency is given by (in the rotating frame)

\[
H = \sum_{i,j} (J_{i,j} - \omega_d \delta_{i,j}) a_i^\dagger a_j + g_2 (a_{z_2}^\dagger (|0\rangle\langle 1| + \sqrt{2}|1\rangle\langle 2| + \sqrt{3}|2\rangle\langle 3| + \sqrt{4}|3\rangle\langle 4|) + h.c.) + \\
\sum_{n=0}^{4} (\omega_{0n} - n\omega_d)|n\rangle \langle n| + \Omega (|0\rangle\langle 1| + \sqrt{2}|1\rangle\langle 2| + \sqrt{3}|2\rangle\langle 3| + \sqrt{4}|3\rangle\langle 4|) + h.c.),
\]

where \( \Omega \) is the bare Rabi frequency of the drive and is the only unknown parameter. (While in numerical simulations with a drive we only consider one qubit, this results in differences of up to 10 MHz when compared to simply detuning one of the qubits.) We stress that \( \omega_d \) is not at the bare qubit frequency but at the frequency of the bound state. In the presence of a drive, excitation number is no longer conserved, and thus, to make progress, one must implement a cut-off. In our numerical simulations, we have implemented a cut-off of five qubit levels and 3 photons. Diagonalizing the system, we take the differences of the eigenvalues of states corresponding to large occupation of atomic states with no photons.

We now compare the results obtained by diagonalizing Eq. 4.40 to the results obtained by driving a dressed qubit (without explicitly including the photonic crystal). The latter approach was used in Ref. [76]. The Hamiltonian for the dressed qubit is

\[
H = \sum_{n=0}^{4} (\tilde{\omega}_{0n} - n\omega_d)|n\rangle \langle n| + \tilde{\Omega} (|0\rangle\langle 1| + \sqrt{2}|1\rangle\langle 2| + \sqrt{3}|2\rangle\langle 3| + \sqrt{4}|3\rangle\langle 4| + h.c.).
\]
Here, $\tilde{\omega}_{0n}$ are the dressed qubit frequencies, $\omega_d = \tilde{\omega}_{01}$, and $\tilde{\Omega}$ is the Rabi frequency seen by the dressed qubit. If the exact wavefunction for the bound state is $|\psi\rangle = \cos \theta |1\rangle |0\rangle + \sin \theta \sum_k c_k a_k^\dagger |0\rangle |0\rangle$ with $\sum_k |c_k|^2 = 1$ (here, our basis states are labeled as $|\text{qubit}\rangle |\text{photon}\rangle$), we have $\tilde{\Omega} \approx \Omega \cos \theta$, where $\theta$ is given by

$$\tan^2 \theta = \frac{g^2}{N} \sum_k \frac{1}{(E_{1B} - \omega_k)^2},$$

(4.42)

which, for an infinite system, simplifies to

$$\tan^2 \theta = \frac{g^2}{4} \frac{1}{(E_{1B} - \omega_0)^{3/2} \sqrt{\alpha}}.$$  

(4.43)

When the bound state is approximately at 7.59 GHz, we find $\cos \theta \approx .68$ for our finite system. Fig. 4.13 compares the results obtained from Eqs. 4.40 and 4.41. We see that, upon taking into account the reduction of the matrix element due to the dressing, the two methods agree. We also see (Fig. 4.13b) that, as expected, as the bare qubit frequency moves deeper into the gap, $\theta$ approaches zero and $\tilde{\Omega}$ approaches $\Omega$. In Fig. 4.13, we have used the anharmonicity value predicted by theory. In Fig. 2c of the main text, we use the experimental values of anharmonicity, which is given by $\tilde{\omega}_{02} - 2\omega_d = -.11$ GHz.

We assume that the feature around 7.22 GHz in Fig. 4.12b is approximately $\omega_{23}$ (which gives $\tilde{\omega}_{03} - 3\omega_d = -.48$ GHz). This assumption is in decent agreement (around 50 MHz off) with results obtained by diagonalizing the full system when the bound state is at 7.59 GHz. This 50 MHz disagreement can be traced back to the 20 MHz disagreement in $\Delta$ (anharmonicity) between theory and experiment when the bound state is at 7.59 GHz (if $\Delta$ is off by 20 MHz, level $|3\rangle$ is expected to be off from its value by around 3 times this amount as $\tilde{\omega}_{03} \approx 3\tilde{\omega}_{01} - 3\Delta$). Finally, we find that $\tilde{\omega}_{04} - 4\omega_d = -1.78$ GHz (this value is also consistent with results obtained by diagonalizing Eq. 4.40) matches the experimental data well as seen by overlaying the
theoretical data from the dressed qubit with the experimental data (Fig. 4.12b). In particular, we have captured the feature that appears around 7.22 GHz and −10 dB. The unique bending of this feature can be traced back to the fact that the level structure of the dressed qubit (Eq. 4.41) does not behave like a normal transmon due to the strong coupling to the photonic crystal.

4.5 Single photon transport via the bound state

As discussed, a bound state mediates transport across the crystal, at the otherwise forbidden frequencies inside the bandgap, via the overlap of the photonic mode with the ends of the crystal. However, unlike a cavity mode which accommodates many photons (of the same frequency) due to its harmonic nature, the bound state inherits an anharmonic level structure from the qubit. This will result in single-photon, blockaded transport. For a definitive confirmation, we measure the second-order autocorrelation of the transmitted component of a weak, resonant, continuous drive. In Fig. 4.14, we plot the emission spectrum of the resonantly driven bound state for low drive amplitudes. Here we see the familiar Mollow triplet structure featuring sidebands that are linearly displaced from the center peak with increasing drive amplitude. We measure second-order autocorrelation (Fig. 4.14 inset) for a drive amplitude below the threshold for incoherent triplet emission such that the qubit is not saturated by the drive. This measurement (see [93, 94, 44, 95, 43] for concept) was made possible by a TWPA (MIT Lincoln Labs) to improve SNR and a GPU (CUDA-Matlab) for significant computational speed-up. See Appendix A and B for extensive details on the autocorrelation measurement algorithm and relevant digital signal processing theory.
Figure 4.14: Power spectrum of a resonantly driven bound state for increasing drive amplitude. Sidebands are linearly displaced from the central peak with increasing drive amplitude, characteristic of the Mollow triplet. Inset - second order autocorrelation measurement for drive amplitude = 0.2 is consistent with single photon, anti-bunched transport.

4.6 Interacting bound states

The nature of inter-bound state interaction makes this platform intrinsically well-suited for investigating one-dimensional chains of bound states (see Fig. 1c). Realizing sizable chains is possible by increasing the number of unit cells - a property that does not impact the Bloch mode distribution or band-dispersion. Thus qubits can be in separate unit cells but realize near identical coupling to the band-edge. As the strength of inter-bound state interaction depends on the spatial overlap of the photonic wave-functions with the qubits, the distance separating qubits (set by device design) is directly mapped into the interactions of the system, maintaining the chain-like interaction pattern.

Controlling interaction between spatially separated qubits is an essential ingredient for quantum computation and simulation. In circuit QED, the popular choice for interfacing two qubits is via a cavity mode - a robust, well-understood interaction
Other experiments have demonstrated interaction between qubits embedded in a linear waveguide. However, in both of these cases the distance between the qubits was effectively eliminated (standing wave interaction in a cavity) or otherwise reduced (modulo wavelength in a linear dispersion waveguide). Thus photonic crystals and tunable bound states offer a fundamentally distinct avenue of interaction where interaction directly depends on distance between qubits in the crystal.

4.6.1 Experiment: observing interacting single-excitation bound states

We observe the flip-flop interaction between the two spatially separated bound states by measuring the avoided crossing in transmission when the bound states are tuned into resonance. As these qubits are a fixed distance apart (9 mm) and there is negligible direct capacitive coupling, the strength of the flip-flop interaction will be entirely determined by the overlap of the localized photonic mode of one qubit with the other qubit, controllable here via the qubit frequencies.

In Fig. 4.15a, the frequency of one qubit is held constant while the other is tuned through resonance. Measuring transmission at the single photon level reveals an avoided crossing between the $|01\rangle$ and $|10\rangle$ levels of the coupled dressed bound states. Transmission amplitude of a bound state dims when the bound state and bare qubit are near resonance (see Fig. 4.15a inset). From this plot, we can extract a resonant bound state – bound state interaction of 120 MHz for a 7.73 GHz bare qubit frequency. In comparison, Figs. 4.15b-d shows reduced interaction strength when both qubits are further detuned from the band edge, 6.125, 6.75, and 7.625 GHz, respectively, for the fixed qubit frequency.

To characterize this aspect of the two bound state interaction, we map the magnitude of the avoided crossing as a function of detuning. In Figs. 4.15e and 4.15f, the qubits are maintained on resonance with one another while being simultaneously
Figure 4.15: **Interacting Bound States** - Interaction between bound states is characterized by the avoided crossing seen in transmission while tuning one qubit (y-axis) through resonance with the other (fixed). a An avoided crossing of 240 MHz is observed when the fixed qubit is at 7.73 GHz. The two points where bound state transmission amplitude is dimmed are understood as a bound state peak being resonant with the qubit frequency. a (inset) Hopping model simulation of the one-excitation manifold is consistent with experimental observation. The lamb shift in the hopping model originates from next-nearest neighbor interaction between coupled cavities. b, c, d Tunable bound state interaction strength is illustrated in example bound state avoided level crossings for a fixed qubit whose bare frequency is circa 6.125, 6.75, and 7.625 GHz. As qubits are detuned further from the band edge, bound states are more tightly localized, reducing overlap and thus reducing interaction. e Measuring bound state separation as qubits are simultaneously tuned, maintaining resonance, shows changing bound state interaction strength with frequency. f Bound state avoided crossing as a function of average bound state frequency. A steady reduction in interaction strength occurs with increasing detuning from the band edge (moving deeper into the bandgap) due to increasing localization of the bound states. Hopping model simulation (black) captures this detuning-dependent behavior.
tuned through the bandgap. Theoretical modeling (Fig. 4.15f) shows experimental
data to be consistent with localized photonic states and with interaction via wave-
function overlap. In the limit where the qubit is deep in the gap, the Markovian
approximation holds. Here the localized mode and flip-flop interaction both have
the same distance dependence $e^{-x/L}$ where $L = a\sqrt{2\delta}$ is the localization length, $\delta$
is the detuning between the bare qubit and the band edge, $a$ is the unit cell size,
and the band-edge dispersion is $\omega_k = \omega_0 + \alpha a^2(k - k_0)^2$. The corresponding flip-flop
interaction Hamiltonian is $H \propto \sum_{j,l} S_1^+ S_2^- (-1)^{|x_1-x_2|/a} e^{-|x_1-x_2|/L}$.

### 4.6.2 Generalized bound state theory: comparison of exact
and Born-Markov approximated solutions

**Exact solution**

In this section we expand on (see Sec. 4.2.1) the theoretical discussion of qubit-photon
bound states in the single excitation sector for an infinite photonic crystal coupled
to two qubits. While our system is of course finite, these results provide an intuitive
understanding of our system and emphasize the importance of Non-Markovianity for
inter-bound state interaction near the band-edge. We note that a similar calculation
for two qubits was done in Ref. [63] for the case when the two qubits have equal
coupling strengths and equal qubit frequencies. The results below generalize that
work to unequal coupling strengths and unequal qubit frequencies. To begin, we first
write the Fourier transformed Hamiltonian (ignoring decay and ignoring terms that
do not affect the single-excitation bound states),

$$H = \sum_k \omega_k a_k^+ a_k + \sum_{i=1,2} \omega_{01;2} |1\rangle_i \langle 1|_i +$$

$$\frac{1}{\sqrt{N}} \sum_{i=1,2} \left( \sum_k g_i (a_k^+ e^{ikaz_i} |0\rangle_i \langle 1|_i + a_k e^{-ikaz_i} |1\rangle_i \langle 0|_i) \right).$$

(4.44)
To make analytical progress, we assume that the dispersion relation is $\omega_k = \omega_0 + \alpha a^2 (k \mp \frac{\pi}{a})^2$, which is valid around $k = \pm \pi/a$. While we have chosen a quadratic dispersion, these results are qualitatively similar for a cosine dispersion. The most general single-excitation wavefunction is

$$|\psi_{1B}\rangle = a_1 |1\rangle_1 |0\rangle_2 + a_2 |0\rangle_1 |1\rangle_2 + \sum_k c_k a_k^\dagger |0\rangle_1 |0\rangle_2 |0\rangle. \quad (4.45)$$

Here, the basis states are labeled as $|qubit\ one\rangle_1 |qubit\ two\rangle_2 |photon\rangle$. Solving the eigenvalue equation, $H|\psi_{1B}\rangle = E_{1B}|\psi_{1B}\rangle$, yields the following coupled equations,

$$E_{1B}a_1 = \omega_{01;1} a_1 + \frac{g_1}{\sqrt{N}} \sum_k c_k e^{-ikaz_1}, \quad (4.46)$$

$$E_{1B}a_2 = \omega_{01;2} a_2 + \frac{g_2}{\sqrt{N}} \sum_k c_k e^{-ikaz_2}, \quad (4.47)$$

$$E_{1B}c_k = \omega_k c_k + a_1 \frac{g_1}{\sqrt{N}} e^{ikaz_1} + a_2 \frac{g_2}{\sqrt{N}} e^{ikaz_2}. \quad (4.48)$$

Solving for $c_k$ from Eq. 4.48 and inserting the result into Eq. 4.46 yields

$$E_{1B}a_1 = \omega_{01;1} a_1 + a_1 \frac{g_1}{N} \sum_k \frac{1}{E_{1B} - \omega_k} + a_2 \frac{g_2}{N} \sum_k \frac{e^{-ika(z_1-z_2)}}{E_{1B} - \omega_k}. \quad (4.49)$$

The sums are evaluated as follows,

$$a \int_0^{\pi/a} \frac{dk}{2\pi} \frac{1}{E_{1B} - \omega_0 - \alpha a^2 (k - \frac{\pi}{a})^2} + a \int_{-\pi/a}^0 \frac{dk}{2\pi} \frac{1}{E_{1B} - \omega_0 - \alpha a^2 (k + \frac{\pi}{a})^2}. \quad (4.50)$$
Shifting the integrals by $\pi/a$, making the integrals dimensionless, and extending the limits to infinity gives,

$$
\frac{1}{N} \sum_k \frac{1}{E_{1B} - \omega_k} = \int_{-\infty}^{\infty} \frac{d\tilde{k}}{2\pi} \frac{1}{E_{1B} - \omega_0 - \alpha k^2} = -\frac{1}{2\sqrt{\alpha(\omega_0 - E_{1B})}}.
$$

(4.51)

Here, we have assumed that $E_{1B} < \omega_0$. Following the same steps for the remaining integral gives

$$
\frac{1}{N} \sum_k e^{-ika(z_1-z_2)} \frac{1}{E_{1B} - \omega_k} = -\frac{\cos(\pi(z_1-z_2))}{2\sqrt{\alpha(\omega_0 - E_{1B})}} e^{-\sqrt{\frac{\omega_0 - E_{1B}}{\alpha}|z_1-z_2|}}.
$$

(4.52)

Here, we used the fact that $(z_1 - z_2)$ is an integer. We then have

$$
E_{1B}a_1 = \omega_{01,1}a_1 - \frac{1}{2\sqrt{\alpha(\omega_0 - E_{1B})}} \left(a_1g_1^2 + a_2g_1g_2 \cos(\pi(z_1-z_2))e^{-\sqrt{\frac{\omega_0 - E_{1B}}{\alpha}|z_1-z_2|}}\right).
$$

(4.53)

Repeating these steps for $a_2$, gives the following equation for the bound state energy,

$$
\left(E_{1B} - \omega_{01;1} + \frac{g_1^2}{2\sqrt{\alpha(\omega_0 - E_{1B})}}\right)\left(E_{1B} - \omega_{01;2} + \frac{g_2^2}{2\sqrt{\alpha(\omega_0 - E_{1B})}}\right) =
\frac{g_1^2g_2^2 e^{-2\sqrt{\frac{\omega_0 - E_{1B}}{\alpha}|z_1-z_2|}}}{4\alpha(\omega_0 - E_{1B})},
$$

(4.54)

where we used the fact that $(z_1 - z_2)/a$ is an integer again. We note that when the qubits are infinitely far away from each other, we recover the well-known bound state energy for a single qubit (see, for example, Ref. [63] or Ref. [76]),

$$
E_{1B} - \omega_{01} = -\frac{g^2}{2\sqrt{\alpha(\omega_0 - E_{1B})}}.
$$

(4.55)

Generically, Eq. 4.54 yields one or two bound states depending on the coupling strength, qubit frequencies, distance between qubits and $\alpha$ [63].
To illustrate this point, we consider the case when $g_1 = g_2 = g$ and $\omega_{01;1} = \omega_{01;2} = \omega_{01}$ (which is relevant to the case in Fig. 4.15). While the coupling strengths are not exactly equal in our experimental system, it is a decent approximation to consider them equal. In this case, we expect a symmetric and an antisymmetric solution, i.e., $a_1^r = a_2^r$ or $a_1^a = -a_2^a$. The difference of the bound-state energy and the energy of the band edge, $E_{1B} - \omega_0 = \delta E_{1B} < 0$, is then given by

$$
\left( \delta E_{1B} - (\omega_{01} - \omega_0) \right) = \Sigma_{\pm}(\delta E_{1B}) = -\frac{g^2}{2\sqrt{-\alpha \delta E_{1B}}} \left( 1 \pm (-1)^{|z_1 - z_2|} e^{-\sqrt{-\frac{2\delta E_{1B}}{\alpha}} |z_1 - z_2|} \right),
$$

where $+$ is for the symmetric state and $-$ is for the antisymmetric state and $\Sigma_{\pm}(\delta E_{1B})$ is the self-energy. The condition for the presence of a bound state, as derived in Ref. [63] is $-(\omega_{01} - \omega_0) > \Sigma_{\pm}(0)$.

We explicitly consider the experimentally relevant case when $|z_1 - z_2|$ is odd. In this case, we have $\Sigma_+(0) = -\frac{g^2}{2\alpha} |z_1 - z_2|$ and $\Sigma_-(0) = -\infty$. For the antisymmetric state, the condition is always satisfied, while for the symmetric state, we only have a bound state if $g > \sqrt{2\alpha(\omega_{01} - \omega_0)} |z_1 - z_2|$. We now apply this formalism to our experimental system. For our experimental system, $\alpha = 1.155$ GHz and $|z_1 - z_2| = 1$. We also take $g$ to be the average of the two coupling strengths determined in the previous section, i.e., $g = (g_1 + g_2)/2 = .5275$ GHz. Using these numbers, we estimate that we have two bound states for $\omega_{01} - \omega_0 < 120$ MHz. We remind the reader that this result is only an estimate, as our experimental system is finite and has unequal coupling strengths.
Finally, one can investigate the real-space wave function. Fourier transforming $c_k$ gives

$$c_j \propto \frac{1}{N} \sum_k c_k e^{ikax} = a_1 g_1 \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{i\omega(j-z_1)}}{E_{1B} - \omega_k} + a_2 g_2 \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{i\omega(j-z_2)}}{E_{1B} - \omega_k} =$$

$$-a_1 g_1 \frac{\cos(\pi(j-z_1))}{2\sqrt{\alpha(\omega_0 - E_{1B})}} e^{-\sqrt{\frac{\omega_0 - E_{1B}}{\alpha}}|j-z_1|} - a_2 g_2 \frac{\cos(\pi(j-z_2))}{2\sqrt{\alpha(\omega_0 - E_{1B})}} e^{-\sqrt{\frac{\omega_0 - E_{1B}}{\alpha}}|j-z_2|}. \quad (4.57)$$

We see that the photon is exponentially localized around the qubits with localization length $a\sqrt{\frac{\alpha}{\omega_0 - E_{1B}}}$, as in the case of a single qubit (see Fig. 4.1). We remind the reader that we can have two different bound state energies (one for the symmetric bound state and one for the antisymmetric one), thus two different localization lengths. In other words, the linewidths of the bound states will, in general, be different, with the bound state closer to the band edge having a larger linewidth. In our system, the symmetric bound state, whenever it exists, is closer to the band edge and thus has a larger linewidth.

**Born-Markov approximation**

We now briefly compare these exact results to the Born-Markov approximation. For simplicity, we restrict ourselves to the case when the qubit frequencies and coupling strengths are the same. Using a second-order Schrieffer-Wolff transformation to eliminate the high-energy subspace gives the following effective Hamiltonian for the two qubits,
Figure 4.16: Exact solution versus Born-Markov Approximation. Here, the red lines are the exact solution while the blue lines are the Born-Markov approximation. The dashed black lines mark the band edge and the thick black line is the bare qubit frequency. Here we take, $\omega_0 = 7.8$ GHz, $\alpha = 1.155$ GHz and $g = 0.5275$ GHz. a Single qubit. b Two qubits for $|z_1 - z_2| = 1$.

$$H_{BM} = \left(\omega_{01} + \frac{g^2}{N} \sum_k \frac{1}{\omega_{01} - \omega_k}\right) \left(|1\rangle_1|1\rangle_1 + |1\rangle_2|1\rangle_2\right) +$$

$$\frac{g^2}{N} \sum_k e^{ika(z_1 - z_2)} \frac{1}{\omega_{01} - \omega_k} \left(|0\rangle_1|1\rangle_1|0\rangle_2 + |1\rangle_1|0\rangle_1|0\rangle_2|1\rangle_2\right) =$$

$$\left(\omega_{01} - \frac{g^2}{2\sqrt{\alpha (\omega_0 - \omega_{01})}}\right) \left(|1\rangle_1|1\rangle_1 + |1\rangle_2|1\rangle_2\right) -$$

$$\frac{g^2}{2\sqrt{\alpha (\omega_0 - \omega_{01})}} \cos(\pi (z_1 - z_2)) e^{-\sqrt{\frac{\omega_0 - \omega_{01}}{\alpha}} |z_1 - z_2|} \left(|0\rangle_1|1\rangle_1|0\rangle_2 + |1\rangle_1|0\rangle_1|0\rangle_2|1\rangle_2\right).$$

(4.58)

We stress that this formula is only valid for $\omega_{01} < \omega_0$. Diagonalizing $H_{BM}$, we have the following eigenvalues,

$$E_1 = \omega_{01} - \frac{g^2 e^{-\frac{1}{2} \sqrt{\frac{\omega_0 - \omega_{01}}{\alpha}} |z_1 - z_2|}}{\sqrt{\alpha (\omega_0 - \omega_{01})}} \sinh \left(\frac{1}{2} \sqrt{\frac{\omega_0 - \omega_{01}}{\alpha}} |z_1 - z_2|\right),$$

(4.59)
\[ E_2 = \omega_{01} - g^2 e^{-\frac{1}{2} \sqrt{\frac{\omega_0 - \omega_{01}}{\alpha}} |z_1 - z_2|} \cosh \left( \frac{1}{2} \sqrt{\frac{\omega_0 - \omega_{01}}{\alpha}} |z_1 - z_2| \right). \]  \hspace{1cm} (4.60)

In the limit where the qubits are infinitely far apart, we recover the standard expression for the dressed qubit frequency,

\[ \omega'_{01} = \omega_{01} - \frac{g^2}{2\sqrt{\alpha(\omega_0 - \omega_{01})}}. \]  \hspace{1cm} (4.61)

In Fig. 4.16, we compare the results obtained in the Born-Markov approximation to the exact analytical results. Fig. 4.16a shows these results for a single qubit and Fig. 4.16b shows these results for two qubits with \(|z_1 - z_2| = 1\). As expected, the Born-Markov approximation is a good approximation when the qubit frequency is away from the band edge. Closer to the band edge, the Born-Markov approximation fails, particularly for the lower-energy (i.e., antisymmetric) state. Furthermore, by comparing the blue curve in Fig. 4.16a to the experimentally measured bound state in Fig. 4.7, we clearly see that the experiment is not well-described by the Born-Markov approximation. We note that the higher energy red line in Fig. 4.16b ends abruptly at \(\omega_{01} \approx 7.920 \text{ GHz}\) as there is only one bound state for \(\omega_{01} > \omega_0 + .120 \text{ GHz}\).

We now analytically show that the Born-Markov approximation is excellent for one of the dressed states close to the band edge. We begin by expanding Eq. 4.56 (for the symmetric case, when \(|z_1 - z_2| = 1\)) in the limit that \(\omega_0 - E_{1B} \ll \alpha\), i.e., when the bound-state energy is close the band edge. This gives

\[ E_{1B} = \omega_{01} - \frac{g^2}{2\alpha}(1 + O\left( \frac{E_{1B} - \omega_0}{\alpha} \right)). \]  \hspace{1cm} (4.62)

Now comparing to the Born-Markov solution for \(E_1\) in Eq. 4.59 around \(\omega_0 \approx \omega_{01}\), we have \(E_1 \approx \omega_{01} - \frac{g^2}{2\alpha}\). We thus see that one of the dressed states (the symmetric one) is well captured by the Born-Markov approximation, while the other is not as seen in Fig. 4.16b.
Figure 4.17: Interaction between two-excitation levels of two bound states

a Spectroscopic measurement while tuning one bound state through the other (qubit fixed at 7.2 GHz), reveals survival of strong interaction into the two-excitation manifold. Crossed and dotted lines are guides to the eye to discern the levels belonging to the first (|01⟩ and |10⟩) and second (|02⟩, |20⟩, and |11⟩) excitation manifolds, respectively. In addition to the |02⟩⟨|20⟩⟩ and |11⟩ avoided level crossing, we also detect a two photon virtual interaction between |02⟩ and |20⟩ (white box). This interaction - fourth order in coupling $g$ - manifests itself in avoided level crossings up to and exceeding 20 MHz. For comparison, the |02⟩⟨|20⟩⟩ - |11⟩ and |01⟩ - |10⟩ interactions are second order in $g$ and thus both are significantly stronger.

b Numerical simulation for fixed bare qubit frequency of 7.27 GHz, with the one (two) excitation manifold in black (red).

### 4.6.3 Observation of interaction in the second excitation sector

To further study tunable on-site interaction, we probe the interacting bound states beyond the one-excitation manifold using spectroscopic measurements (see Fig. 4.17a). Similar to spectroscopy of qubits in cavities, we can use transmission at the band edge to help detect bound state transitions, a technique that provides sharper contrast compared to transmission measurement for the more highly localized bound states and allows detection of higher dressed transitions, such as the transition between |0⟩ and |2⟩ driven by two photons of frequency $\omega_{02}/2$. 
With this technique we detect interaction between $|02\rangle$, $|20\rangle$, and $|11\rangle$ of the coupled bound states, observed as avoided level crossings. In addition to the single-photon exchange interaction between $|02\rangle$ ($|20\rangle$) and $|11\rangle$ [97], remarkably we measure the two-photon virtual interaction between $|20\rangle$ and $|02\rangle$, despite the fact that this process is 4th order in coupling $g$. This two-photon interaction shows consistent dependence on detuning: increasing in strength (from 0 to over 10 MHz) as the bound states shift towards the band edge and the states become more delocalized. Numerical simulations (Fig. 4.17) are consistent with experimental data and capture the relative magnitudes of interaction between levels as well as frequency dependence on coupling strengths. Observation of this small interaction highlights the overall strength of inter-bound state coupling possible via overlap alone.

### 4.6.4 Theory behind two photon avoided crossing

In this section, we discuss the two-photon avoided crossing seen in Fig. 4.17. As in previous sections, we assume the two qubits have equal coupling strengths and equal bare frequencies. To begin, we first write the total Hamiltonian in the two-excitation sector (in the rotating frame), using a different notation,

$$H_2 = H_{0x} + H_{0y} + H_{1x} + H_{1y},$$  \hspace{1cm} (4.63)
where

\[
H_{0x} = \sum_k (\omega_k + \omega_{12})(|0, 1; k\rangle \langle 0, 1; k| + |1, 0; k\rangle \langle 1, 0; k|),
\]

\[
H_{0y} = \sum_{k,p} (\omega_k + \omega_p - \omega_{02})|0, 0; k, p\rangle \langle 0, 0; k, p|,
\]

\[
H_{1x} = \frac{\sqrt{2}g}{\sqrt{N}} \sum_k (e^{i k a z_1}|1, 0; k\rangle \langle 2, 0; 0| + e^{i k a z_2}|0, 1; k\rangle \langle 0, 2; 0| + \text{h.c.}),
\]

\[
H_{1y} = \frac{g}{\sqrt{N}} \sum_{k,p; k \neq p} \left( e^{i p a z_1}|0, 0; k, p\rangle \langle 1, 0; k| + e^{i p a z_2}|0, 0; k, p\rangle \langle 0, 1; k| + \text{h.c.} \right) + \frac{\sqrt{2}g}{\sqrt{N}} \sum_k \left( e^{i k a z_1}|0, 0; k\rangle \langle 1, 0; k| + e^{i k a z_2}|0, 0; k\rangle \langle 0, 1; k| + \text{h.c.} \right).
\]

Here the basis states are labeled as $|\text{qubit}_1, \text{qubit}_2; \text{photonic field}\rangle$. To proceed, we neglect the second line in $H_{1y}$ as there are many photonic modes, thus the probability of both photons going into the same mode is negligible. Using a unitary Schrieffer-Wolff transformation, we find the fourth order term in coupling strength, $g$, to be

\[
H_4 = \frac{1}{2} H_{1x} \bar{H}_0 (\bar{H}_0 H_{1x}^2 + H_{1x}^2 \bar{H}_0) \bar{H}_0 H_{1x} - H_{1x} \bar{H}_0 H_{1y} \bar{H}_0 H_{1y} \bar{H}_0 H_{1x},
\]

where $H_0 = H_{0x} + H_{0y}$ and $\bar{H}_0 = H_0^{-1}$ (here, $H_0^{-1}$ is taken to be zero outside the support of $H_0$). We are only interested in terms that involve interactions between the $|0, 2; 0\rangle$ and $|2, 0; 0\rangle$ states, i.e., terms like $|2, 0; 0\rangle \langle 0, 2; 0|$. Only the last term in Eq. 4.68 contributes such a term. Ignoring contributions of the last term that are diagonal in the $\{|0, 2; 0\rangle, |2, 0; 0\rangle\}$ basis, the effective interaction between the $|2, 0\rangle$
and the $|0, 2\rangle$ states is (after projecting out the photonic degrees of freedom),

$$H_{|2, 0\rangle \leftrightarrow |0, 2\rangle} = -4g^4/\mathcal{N}^2 |2, 0\rangle \langle 0, 2| \sum_{k,p} \frac{e^{i(k+p)a(z_2-z_1)}}{(\omega_k + \omega_p - \omega_{02})(\omega_k - \omega_{12})} \left( \frac{1}{\omega_k - \omega_{12}} + \frac{1}{\omega_p - \omega_{12}} \right) + h.c.$$
Evaluating the remaining integral gives,

\[ H_{|2,0\rangle\leftrightarrow|0,2\rangle} \approx -2g^4 \langle 2,0 | \langle 0,2 | \delta k e^{-|z_2 - z_1|} \frac{1}{\sqrt{\alpha}} \frac{\sqrt{\omega_0 \omega_1}}{\sqrt{\omega_0 - \omega_1}} \left( \frac{1}{\omega_0 - \omega_1} - \frac{1}{\omega_0 + \omega_1 - \omega_0} \right) \]

\[ + \frac{1}{\sqrt{\alpha} (\omega_{02} - 2\omega_{12})} \left( e^{-|z_2 - z_1|} \frac{1}{\sqrt{\omega_0 - \omega_1}} - e^{-|z_2 - z_1|} \frac{1}{\sqrt{\omega_0 + \omega_1 - \omega_0}} \right) \times \frac{e^{-|z_2 - z_1|} \sqrt{\omega_0 - \omega_1}}{\sqrt{\alpha} \sqrt{\omega_0 - \omega_1}} + h.c. \]

We see that every term decays exponentially as a function of \(|z_2 - z_1|\), thus the effective interaction between the \(|2,0\rangle\) and the \(|0,2\rangle\) states decays exponentially as well.

### 4.7 Summary and outlook

The widely tunable on-site and inter-bound state interactions demonstrated with this device and consistent theoretical simulations are promising benchmarks towards realizing larger, more complex systems of bound states that can mediate both local and long-range interactions. Beyond stepped impedance coplanar waveguides, there are undoubtedly numerous ways to realize superconducting microwave photonic crystals, including lumped element or Josephson junction based designs, that are equally compatible with superconducting qubits. Regardless of the platform, behavior of bound states due to qubit-band edge coupling will mirror the behavior characterized in this work, elevating this platform above any single experimental design choice.

While the bound states were centered in neighboring unit cells in this device, this is not a limitation or requirement for future experiments as the range of localization can be accordingly set via the basic crystal parameters, as seen by comparing bound state linewidths measured here with those reported previously [76]. Therefore, one can realize a one-dimensional chain of bound states in a moderately-sized photonic
crystal, where individual control over the qubits would allow dialing up or down long-distance interaction between sets of qubits.

In future iterations, one may consider altering boundary conditions specific to the desired application. For example, methods for impedance matching such as tapers or quarter-wave transformers [78] are straightforward additions that will modify impedance matching at specific frequencies (such as at a band edge). These options were not pursued in this work as we wanted to study bound state properties across a range of frequencies. If one were interested in only specific frequencies or ranges, then this is a promising improvement. The device is symmetric, so one end is chosen arbitrarily to serve as the input. As detection of the bound state is due to scattering, one may consider modifying the symmetry of the device or detecting signal from both ends of the crystal to improve collection efficiency.

We resorted to two-tone spectroscopy over direct transmission measurement to detect the bound state when the qubit was deep in the bandgap due to strong localization and poor signal-to-noise ratio (SNR). Choosing a less shallow band curvature will make it possible to see the bound state all the way through the gap (see Liu et al. [76]); however, this is a trade-off as the bound-state linewidths will increase accordingly. Thus, choosing curvature and crystal parameters such that the linewidth remains as narrow as possible without internal Q or loss effects is essential.

Beyond the standard transmon qubit, one can consider incorporating other qubit designs to study a diverse array of phenomena. For example, a tunable coupling qubit would allow control of qubit-crystal coupling while maintaining qubit frequency [7]. Inductively coupling a fluxonium qubit [6] could lead to greatly increased coupling strength between qubit and crystal as well as large bare qubit anharmonicities. With a giant atom [99], one could couple a single qubit to two separate unit cells - a system likely to host more novel bound states.
In this work the interactions were in situ tunable via qubit frequency (DC flux), a static quantity on the timescale of the bound state lifetime. Dynamically controllable interactions would introduce an additional tool for designing and manipulating spin Hamiltonians [69]. One method for realizing this type of fast timescale control is flux-pumping, a technique involving microwave frequency modulation of the qubit frequency along the flux bias line [100, 9, 101, 102]. Another potential pathway would use an auxiliary microwave field through the crystal itself. Here the qubits could be maintained on resonance deep in the bandgap such that there is minimal interaction via bound state overlap. A single RF control tone could then be turned on to induce a transition close to the passband, thus re-dressing the bound states into new, effective bound states with interaction strength depending on properties of the microwave drive. The addition of several drives or precisely shaped microwave pulses (made possible by commercial high-speed arbitrary microwave waveform generators [103]) promises not only changing interaction strength but also modification of the shape of the interaction itself - from an exponential to a sum of exponentials - leading to a wide range of possibilities including power-law-decaying interactions [69]. These supplementary forms of tunable control would expand the ability of the qubit-photonic crystal platform to realize a broader class of tunable spin models.
Chapter 5

Conclusion

In this dissertation we presented a glimpse into two avenues of strong light-matter interaction, seeking to push our understanding further beyond the well-studied single-qubit single-mode limit. Each project presented marked a new venture, creatively using simple superconducting circuit elements to design and realize complex quantum systems.

We explored the domain of multimode strong coupling by simultaneously strongly coupling a single qubit to many longitudinal modes of a microwave cavity. Through experiment we learned some of the different pathways through which multimode phenomena manifests. We similarly studied the qubit-photonic crystal strong coupling regime and characterized interacting dressed bound states. In doing so, we furthered this platform as a tool for future study of one-dimensional quantum many-body physics.

These unique domains of light-matter interaction discussed in this dissertation are a subset of exciting research initiatives seeking to grow our general understanding of complex, strongly coupled quantum systems. In the grand scheme of this endeavor, this work is a small step - hopefully contributing to the growing foundation upon which future scientists can build and continually advance.
Appendix A

Correlation

A.1 Background on photon statistics

Predominantly, the signals we are concerned with in cQED are governed by stochastic or random processes, such as spontaneous emission. Rather than trying to reconstruct the full underlying probability density function, we focus on learning specific, intrinsic statistical properties of the light created by the process. For example, quasi-probability functions or representation (Husimi-Q, Wigner, Glauber-Sudarshan P) are practical metrics that have been demonstrated to be useful tools for state characterization.

Autocorrelation of a time signal is another statistical metric that is useful when trying to understand origin or mechanism behind an emission process. Second-order autocorrelation (intensity correlation) provides a means to distinguish Poissonian (coherent), super-Poissonian (thermal), and sub-Poissonian (non-classical, i.e. squeezed) statistics, as well as identify bunching or antibunching. This makes autocorrelation of general interest in quantum experiments where we want to identify non-classical light, such as single photon or correlated emission. Despite the lack of broad-band, reliable, photon counters in the microwave regime, reconstruction of autocorrelation
statistics has been demonstrated with linear detectors using a variety of techniques. This appendix outlines the procedure used in this thesis to measure \( g_2(\tau) \) in Chapter 4. In Appendix B, further details regarding signal processing are provided.

### A.2 Stochastic signals

Prior to detailing the approach, it is beneficial to highlight a few properties of stochastic signals that are relevant to our measurement. As a concrete example, let us consider resonance fluorescence of a single emitter. Emission is a stochastic or random process, which mathematically is a random variable with an additional time dependence.

#### A.2.1 Stationarity

In experiment, we obtain a sample function of this process when we acquire a finite-length data set (a trace) on a digitizer. With a single trace, there is not much we can discern statistically, and so we repeat the experiment many times and collect an ensemble of traces sampling this process. In doing so we have made the implicit assumption that the process we are studying is stationary, having the same behavior at different times, such that absolute time is unimportant.

There are varying levels with which we can characterize the order of stationarity, but for our purposes the requirement is for weak or wide-sense stationarity (WSS). The criteria for WSS is that the mean and covariance of the signal does not change with time. If this is met then our assumption that all the data, regardless of which trace it is from, samples the same probability density function is valid.

While this may seem trivial, in practice this has more subtle implications; the signal we acquire is not purely from the single emitter but also includes the influence of the emitter’s changing environment, emitter stability, instrument stability, noise,
etc. As our signals very often have very low SNR, large ensembles (gathered over minutes or hours) are required for averaging purposes and so noise must also be WSS. To this end, interleaving acquisition of signal traces with noise traces to characterize the noise in the signal is necessary (as compared to acquiring signal and noise in separate, bulk ensembles). As covered in Appendix B, WSS is also an essential requirement in many digital signal processing algorithms, such as those needed to compute autocorrelation. Most signals are in fact non-stationary, such as speech, thus it is up to the experimentalist to confirm that the data they acquire meets the stationarity requirement.

A.2.2 Biased

When we estimate a statistical property, such as mean, from an ensemble of traces we seek convergence of the estimate. Estimates can be divided into two categories - unbiased and biased. An unbiased estimate of the mean will converge to the mean, while a biased mean estimator will not. While this may make biased estimators seem illogical, they are practically very useful for obtaining estimates that converge. Thus identifying whether and how your measurement is biased is necessary to figure out how to convert the biased to unbiased, if so required. The bias in the autocorrelation measurement is explained in later sections.

A.3 Approach

We seek to measure

\[ g_1(\tau) = \frac{\langle a^\dagger(t)a(t+\tau) \rangle}{\langle a^\dagger(t)a(t) \rangle} \]  

(A.1)
\[ g_2(\tau) = \frac{\langle a^\dagger(t)a^\dagger(t + \tau)a(t + \tau)a(t) \rangle}{\langle a^\dagger(t)a(t) \rangle^2} \] (A.2)

where \( a(a^\dagger) \) is the annihilation (creation) operator of the stationary light and the expectation values are averaged over time, \( t \). Second-order autocorrelation, \( g_2 \), is an intensity-intensity correlation. However, in the microwave regime we use linear detectors (high speed digitizers) to measure voltage on a coaxial line, a proxy for electric field not intensity. Thus the complexity of estimating \( g_2 \) arises in the digital signal processing and our ability to properly account for and subtract system noise which is usually orders of magnitude larger than the signal.

There are a few methods of measuring \( g_2 \) that have been successfully demonstrated, some targeting \( g_2(0) \) and others \( g_2(\tau) \). The procedure outlined in this appendix is derived from the method used in [93, 94, 44, 95, 43] and a good overview of which can be found in [104]. The main distinctions in the work presented here is the use of a single amplification chain with a TWPA, different microwave components, and a GPU rather than FPGA to aid in pseudo real-time analysis.

### A.4 Formalism

In chapter 5, we used the autocorrelation measurement to confirm single photon transport via the bound state. For this detection we applied a single continuous tone at the bound state frequency and measured the autocorrelation of the transmitted signal. As transmission is dependent on emission, this is a stochastic process.

The radiation we detect with the digitizer includes not only the signal from the device but also (necessarily) significant noise. Therefore to estimate the autocorrelation of the signal, we must be able to subtract the required correlations of the noise. To do this we must gain sufficient statistics regarding the noise - which is achieved by alternating traces of data taken with the drive tone on and off. These two data sets
("signal" and "noise") are then processed identically. This is an optimal detection of noise, catching both short time fluctuations and long time drifts as we average for around 20 hours.

A signal trace is written as $S(t) = a(t) + h^\dagger(t)$ and a noise trace is $h^\dagger(t)$, where $a$ is the signal we want to obtain the autocorrelation of. However, we cannot take one signal trace and subtract one noise trace to extract $a(t)$ because these are stochastic signals. Therefore we must obtain the expectation values of various moments of $S$ and $h^\dagger$ to extract moments of $a$. For this to succeed, we assume that noise at different times is uncorrelated and that the mean of the noise is zero (useful assumptions to confirm in experiment).

A.4.1 Note on normal ordering
While we seem to write $S$, $a$ and $h^\dagger$ as quantum mechanical operators, they are classical quantities we measure with classical equipment. We are restricted to detect normally ordered moments of $S$, $a$ and $h^\dagger$, such as $S^\dagger S$ rather than $SS^\dagger$ [93]. Numerically this is easily understood: multiplying a vector, $V$, with its complex conjugate, $V^*$ is equivalent to $V^*V$. Therefore it is not that $S^\dagger S = SS^\dagger$, but rather that we cannot directly compute the latter.

A.5 First order auto-correlation, $g_1(\tau)$

First-order autocorrelation is defined as,

$$g_1(\tau) = \frac{\langle a^\dagger(t)a(t + \tau) \rangle}{\langle a^\dagger(t)a(t) \rangle} \quad (A.3)$$

where we average over time $t$ such that the only time dependence left is the lag time, $\tau$. 

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As we do not have access to \(a(t)\) in experiment, the first step is to determine what ensemble averaged quantities we need given \(S(t)\) and \(h^\dagger(t)\) to construct \(g_1\).

The basic strategy is to write the autocorrelation function in terms of \(S\), where \(S = a + h^\dagger\). Then work backwards to figure out how to get autocorrelation in terms of \(a\).

\[
<S^\dagger(t)S(t + \tau) > = < (a^\dagger(t) + h(t))(a(t + \tau) + h^\dagger(t + \tau) > \\
= < a^\dagger(t)a(t + \tau) > + < a^\dagger(t)h^\dagger(t + \tau) > + < h(t)a(t + \tau) > + < h(t)h^\dagger(t + \tau) > \\
(A.4)
\]

We assume noise \((h)\) and signal \((a)\) are uncorrelated both at same time and different times.

\[
= < a^\dagger(t)a(t + \tau) > + < a^\dagger(t) > < h^\dagger(t + \tau) > + < h(t) > < a(t + \tau) > + < h(t)h^\dagger(t + \tau) > \\
(A.5)
\]

All the data taken is time-translationally invariant so \(< h(t) > = < h(t + \tau) > .\)

\[
= < a^\dagger(t)a(t + \tau) > + < a^\dagger(t) > < h^\dagger(t) > + < h(t) > < a(t) > + < h(t)h^\dagger(t + \tau) > \\
(A.6)
\]

Finally, it is usually accurate to assume that \(< h > = < h^\dagger > = 0\) and similar for odd moments of \(h\). It is a good experimental check to measure these and prove to yourself that this is true in your setup. Therefore to good approximation,

\[
<S^\dagger(t)S(t + \tau) > = < a^\dagger(t)a(t + \tau) > + < h(t)h^\dagger(t + \tau) > \\
(A.7)
\]

We can measure \(< S^\dagger(t)S(t + \tau) > \) and \(< h(t)h^\dagger(t + \tau) > \), and by subtracting the two we can obtain \(< a^\dagger(t)a(t + \tau) > \). Normalization, \(< a^\dagger(t)a(t) > \), is the entry for \(\tau = 0\).
While we can compute \(< S^\dagger(t)S(t + \tau) >\) in the time domain by multiplying together time-shifted S vectors, this is computationally inefficient. Instead we will use the Fourier Transform and correlation theorem. See Appendix B and Appendix A.8 for details.

\[
< F[S^\dagger(t)S(t + \tau)] > = < |F[S]|^2 > \quad (A.8)
\]

### A.6 Second-order autocorrelation, \(g_2(\tau)\)

Using the same strategy, let us turn to the second order autocorrelation:

\[
g_2(\tau) = \frac{< a^\dagger(t)a^\dagger(t + \tau)a(t + \tau)a(t) >}{< a^\dagger(t)a(t) >^2} \quad (A.9)
\]

Notation: \(\star\) is correlation, \(\ast\) is conjugation, and \(F[x]\) is the fourier transform of \(x\). For simplicity, I will replace \(x(t)\) with \(x\), and \(x(t + \tau)\) with \(x_\tau\).

\[
< S^\dagger S^\dagger(t)S(t + \tau) > = < (a^\dagger + h)(a^\dagger + h_\tau)(a_\tau + h_{\tau}^\dagger)(a + h^\dagger) > = < (a^\dagger a^\dagger_\tau + a^\dagger h_\tau + h a^\dagger_\tau + hh_\tau)(a_\tau a + a_\tau h^\dagger + h_{\tau}^\dagger a + h_{\tau}^\dagger h^\dagger) > = < a^\dagger a^\dagger_\tau a_\tau a > + < a^\dagger a^\dagger_\tau a_\tau h^\dagger > + < a^\dagger a^\dagger_\tau h_{\tau}^\dagger a > + < a^\dagger a^\dagger_\tau h_{\tau}^\dagger h^\dagger > + < a^\dagger h_\tau a_\tau a > + < a^\dagger h_\tau a_\tau h^\dagger > + < a^\dagger h_\tau h_{\tau}^\dagger a > + < a^\dagger h_\tau h_{\tau}^\dagger h^\dagger > + < h a^\dagger_\tau a_\tau a > + < h a^\dagger_\tau a_\tau h^\dagger > + < h a^\dagger_\tau h_{\tau}^\dagger a > + < h a^\dagger_\tau h_{\tau}^\dagger h^\dagger > + < h h_{\tau} a_\tau a > + < h h_{\tau} a_\tau h^\dagger > + < h h_{\tau} h_{\tau}^\dagger a > + < h h_{\tau} h_{\tau}^\dagger h^\dagger > \quad (A.10)
\]

As before, we assume all zero-lag, odd moments of the noise, such as \(< h >\) and \(< hhh^\dagger \rangle\), average to zero. Certain even moments of the noise - \(< hh >\), \(< h^\dagger h^\dagger \rangle\) -
also average to zero.

\[
< S^\dagger S^\dagger S > = < a^\dagger a^\dagger a > + < a^\dagger h_r a h^\dagger > + < a^\dagger h_r h^\dagger a > + < h a^\dagger a^\dagger h > + < h a^\dagger h^\dagger a > + < h h_r h^\dagger h^\dagger >
\]  

(A.11)

Rearranging this so we have the term we want to compute on the LHS and the terms on the RHS ordered by similarity of computation,

\[
< a^\dagger a^\dagger a > = < S^\dagger S^\dagger S > - < h h_r h^\dagger h^\dagger >
\]  

(A.12)

To determine how to compute each term we remind ourselves that the quantities we measure are normally ordered. For the following equations we purposefully rearrange the ordering of variables in each term for computational purposes, keeping in mind that this juggling does not change the quantity we compute (terms in the above equation).

\[
< S^\dagger S^\dagger S > = < (S^\dagger S)(S^\dagger S) > = < (S^\dagger S)^* \ast (S^\dagger S) >
\]  

(A.13)

\[
< F[S^\dagger S^* \ast S^\dagger S] > = < F[(S^\dagger S)^* F[S^\dagger S] > = < |F[S^\dagger S]|^2 >
\]

as \( S^\dagger S \) is a real quantity. Similarly,

\[
< h h_r h^\dagger h^\dagger > = < h_r h^\dagger h^\dagger > = < (h h^\dagger) \ast (h h^\dagger) >
\]  

(A.14)

\[
< F[h h^\dagger \ast h h^\dagger] > = < F[h h^\dagger] F[h h^\dagger] > = < |F[h h^\dagger]|^2 >
\]
The first two cross-terms can be rewritten into separable, first order correlators.

\[
\langle a^\dagger h \tau a^\dagger h^\dagger \rangle = \langle a^\dagger(t)a(t+\tau) \rangle \langle h(t+\tau)h^\dagger(t) \rangle
\]

(A.15)

The first term was calculated in the previous section for \(g_1(\tau)\). The second term however has reversed the delayed term.

\[
\langle h(t+\tau)h^\dagger(t) \rangle = \int_{-\infty}^{\infty} h(t+\tau)h^\dagger(t)\,dt = \int_{-\infty}^{\infty} h(t')h^\dagger(t'-\tau)\,dt'
\]

(A.16)

Computationally, we obtain this by computing \(\langle h^\dagger(t)h(t+\tau) \rangle\), previous section, and flipping the \(\tau\) axis. Similarly with the fourth term,

\[
\langle ha^\dagger \tau h^\dagger \tau a \rangle = \langle h^\dagger(t+\tau)a(t) \rangle \langle h(t)h^\dagger(t+\tau) \rangle.
\]

(A.17)

The last two terms needed for \(g_2(\tau)\) are same time, power-terms.

\[
\langle a^\dagger h \tau h^\dagger a \rangle = \langle h^\dagger \tau a^\dagger \tau h \rangle = \langle a^\dagger a \rangle \langle hh^\dagger \rangle
\]

(A.18)

A.7 Summary for implementation

We have established that we need well-averaged quantities for four terms - \(\langle S^\dagger S^\dagger \tau S \rangle\), \(\langle h h^\dagger \tau h^\dagger \rangle\), \(\langle S^\dagger S^\tau \rangle\), and \(\langle hh^\dagger \rangle\).

Outlined in Figs. A1, A2, and A3 are the practical details for implementation. See appendix B for more experimental details including relevant concepts from DSP.
Figure A.1: Fridge wiring for autocorrelation measurement in Chapter 5.

Figure A.2: Microwave hardware for autocorrelation measurement. An 80MHz IF was chosen for heterodyne due to availability of matching 90 degree hybrid coupler.
Figure A.3: Overview of digital signal processing for autocorrelation measurement.
A.8 Estimating the power spectrum

The goal of spectral analysis of a random signal is to tell us the frequency distribution of the signal. While we leave the practical considerations for computing a power spectral density (PSD) estimation to Appendix B, it is a priceless tool for monitoring the progression of data after each step and debugging an autocorrelation measurement.

Further, it would be negligent to conclude a summary of autocorrelation without mentioning that the PSD is the Discrete Time Fourier Transform (DTFT) of $g_1$. (We encourage the reader to read the derivations: Weiner-Khintchin theorem in continuous time and Wold’s theorem in discrete time.)

However, while the DTFT is discrete in the time-domain, it is continuous in frequency, therefore we cannot numerically compute the PSD. We can only estimate the PSD using the Discrete Fourier Transform (DFT) (which discretizes frequency, introducing time periodicity) using methods such as Welch, Periodogram, and Blackman-Tukey. The method we follow is a variant of the Periodogram where we compute the expectation value of the PSD estimate using many distinct traces. The Welch method adds an additional twist by allowing for overlapping traces in the computation, but was not advantageous for our measurement. We will not discuss the Blackman-Tukey method, which uses a biased autocorrelation as a stepping stone to obtaining the spectrum. In general, PSD estimation is divided into nonparametric and parametric methods (direct and indirect) and is highly sensitive to signal processing.

It is not always possible to estimate the PSD for arbitrary stochastic signals because the Fourier Transform (FT), in general, does not exist for signals that are not absolutely or square summable [105]. This means that while you can numerically compute the Fast Fourier Transform (FFT), the result you would obtain would be meaningless.

But as we are considering WSS signals in this section, we can invoke Parseval’s theorem and gain access to the FT and PSD estimate.
Two of the most important properties of the PSD are that it must be real and be non-negative. This last one is important when trying to perform spectral subtraction of noise from signal - as is done in this appendix. Further, when trying to estimate PSD (and therefore autocorrelation), our spectral content must be band-limited (either from a low-pass or a band-pass process) in order to obtain meaningful results.

Some other important parameters one must take into account for accurate estimation include sampling frequency, frequency resolution, windowing, zero-padding, spectral smoothing, and bias.

### A.8.1 Biased vs unbiased correlation

Computing autocorrelation using the correlation theorem includes an implicit bias due to finite trace lengths or windowing. Often, we deal with bias with how we normalize autocorrelation. This is apparent when we compare a biased autocorrelation

\[ C(k) = \frac{1}{N} \sum_{n=0}^{N-k-1} x(n) x(n+k). \]  

(A.19)

and unbiased autocorrelation,

\[ C(k) = \frac{1}{N-k} \sum_{n=0}^{N-k-1} x(n) x(n+k). \]  

(A.20)

Notice, this calculation implicitly used a rectangular window (\(x(n)\) is equal to zero outside range of 0 to \(N\)), so normalizing with \(\frac{1}{N-k}\) effectively removes the bias of the window. However, we can (and often will) choose other windows. In those cases we must take appropriate measures to remove the bias correctly if we are interested in unbiased correlation.

For example, let’s say \(w(n)\) is our window such that \(y(i) = x(i)w(i)\), where \(w\) has the same number of elements as \(x\). Computing the autocorrelation estimate for \(y\) will
therefore include the autocorrelation of w(n). However, because we can compute the autocorrelation of w(n), we can retrieve the unbiased autocorrelation estimate for x with a simple division. In the above case, the autocorrelation of a rectangular window is a triangle.

Biased autocorrelations are particularly useful for improving estimates of PSD in the Blackman-Tukey method. Long time lag values, which are poorly averaged, are weighted less thus reducing the high frequency noise and leakage in the PSD estimate.
Appendix B

Digital Signal Processing Basics

B.1 Motivation

Understanding the basics of digital signal processing (DSP) is a useful investment for any experimental work where one converts continuous signals (for example, radiation from the device) into discrete signals for processing and detection. While software, such as Python and Matlab, have many DSP algorithms pre-programmed, it leaves the job to the user to correctly use the functions and thus it is unfortunately very easy to do ”bad DSP” without knowing it. There are many excellent resources covering aspects of practical DSP to help you design your procedure [105, 106, 107, 108]. This appendix introduces the basics most relevant to microwave measurement and is intended as a starting point. If you are trying to optimize a particular low SNR measurement, I strongly encourage you to pick up a DSP textbook and read deeper into the concepts presented here.

B.2 Sampling a continuous signal

The first step of any signal processing algorithm is acquiring data. In our case, this comes from sampling and quantizing a continuous microwave signal using a high-speed
ADC or digitizer. A continuous signal has a few properties that make it subtly yet critically distinct from a discrete signal - it is defined continuously as a function of time and frequency. Therefore, it continues indefinitely in time and has infinite bandwidth regardless of the bandwidth set by analog filters or other physical components.

When we sample, or take snapshots of, a continuous signal, we have to determine a few things: how to quantize the input voltage, the sampling rate, and length of data acquisition.

Analog to digital high speed digitizers have a finite number of bits to describe the input voltage within the range set by the "full-scale," where more bits means better resolution. To avoid quantization errors, you want to use as much of your full-scale as possible without any data hitting the voltage limits. For this, we have to look at the raw data traces and pick appropriate analog amplification, attenuation, and filtering to meet this condition. In this process, you may find that it is beneficial to remove DC offset for heterodyne signals (via a DC-block or other high/band-pass filters) prior to data acquisition such that the full-scale is better used. Many commercial high-speed digitizers intrinsically have a high slew rate, which means they can quickly react to rapid changes in input voltage. They also have low aperture error such that each data point is closer to the instantaneous voltage at the time of acquisition rather than a time-average. The latter condition is known as impulse sampling and is a fundamental assumption typically made in DSP.

The other two specifications have implications beyond how many data points you want to process in code.

The sampling rate, $F_s$, is the rate at which your digitizer samples the data. Equivalently, we can define the sampling interval, $T = \frac{1}{F_s}$, as the time interval between data points. In the frequency domain, this translates to a detection bandwidth of $\pm F_s/2$. By Nyquist sampling [105, 106], this sets the maximum bandwidth of signal you can detect to $F_s/2$. In one ideal limit, you want to sample as quickly as possible. However
this increases data size, and due to low data transfer speeds when downloading data 
off of a digitizer, has run-time implications. Therefore we may tradeoff a smaller 
bandwidth window for faster downloads. From an experimental stand-point, we must 
remember that the digitizer is not intrinsically perfect at sampling at Fs, thus we 
provide it with an external clock reference to help synchronize it to the rest of the 
measurement chain. This deviation from the desired, constant sampling interval is 
the jitter of a digitizer.

The time duration of acquired data will ultimately set frequency resolution, or 
how well you can differentiate frequency components within the bandwidth set by 
$F_S$. It is beneficial to keep in mind for the following sections that while you only 
sample for a finite time duration, the original continuous signal is infinitely long. 
These together have important implications in the contrast between continuous and 
discrete time signal processing.

### B.2.1 Aliasing

When we periodically sample a signal at $F_S$, we are limited to a detection bandwidth 
of $\pm F_S/2$. However, content at frequencies outside this range are not simply ignored or 
discarded. Instead, they are mapped down to frequencies inside the detection window 
and incorporated into the detected signal. The result of this process, aliasing, is that 
one cannot determine the origin of a frequency component detected at $f_o$ as it could 
have originated from $f_o + k \times F_S$ for any positive or negative integer $k$. The fold-over 
frequency, $F_S/2$, marks the boundaries beyond which higher frequency content are 
folded down into the detection window. For example, a signal at $F_S + \delta$ will be 
detected at $\delta$, while a signal at $F_S/2 + \delta$ is folded over to $-F_S/2 + \delta$.

A classic example of aliasing in action can be seen in most car commercials - 
though a car is rapidly moving forward, its wheels appear to be rotating slowly, 
sometimes even backwards or even stationary. This occurs because the camera has a
finite sampling rate that is less than the rotation frequency of the wheels. In the case of stationary wheels, the wheel frequency is an exact multiple of the camera sampling rate. Similarly if the wheels appear the spin backwards or incongruously slowly, then the wheel frequency has been aliased down to frequency within the camera rate. Another example where we encounter aliasing is with strobe lights. Here the flashing light is sampling the scene for us so then we can directly witness the aliasing.

Therefore, prior to sampling the data, it is important to consider not only the spectral content in bandwidth of your signal, but also content that lies outside the sampling bandwidth, which may alias down and corrupt your detection. As an example, we often encounter measurements where the signal itself is band-limited to few MHz but the power of the noise background is significantly larger than the signal and spans > 2-3 GHz range (as is the case with a broad-band amplifier - TWPA). Without proper attention, this noise can alias down onto your signal to result in a significant reduction of SNR which can ruin a measurement.

To minimize this effect, anti-aliasing filters (aggressive, multi-stage, analog filters chosen to suppress spectral content above $Fs/2$) are employed prior to the digitizer. However as the cutoff of analog filters is not abrupt, often times we target suppression of all spectral content above a lower limit, such as $Fs/3$ or $Fs/4$, to ensure that aliasing is not occurring at significant levels. Regardless of how many filters are used, it is impossible to completely eliminate the high frequency content, but reduction by several orders of magnitude is sufficient for most applications. The higher the sampling rate, the more flexibility you have in choosing filters to reduce the effects of aliasing without introducing distortion or attenuation of your signal frequency.

Aliasing is not always synonymous with signal corruption. In cQED, we often use mixers to shift signal at several GHz to low frequency (baseband) for detection. However, with proper band-pass filters, it is possible to directly detect the several GHz signal using aliasing to your advantage - this is the band-pass sampling technique.
In this case, one should check whether the spectrum is inverted via the process of band-pass sampling (inverting shape of positive and negative frequency components) and correct for it appropriately. However, there are an abundance of inexpensive microwave components that operate at low frequencies - amplifiers, filters, mixers, hybrid couplers etc. - and thus bandpass sampling is not commonly used.

We’ve so far discussed how high frequencies have been mapped down to lower frequencies by aliasing. However, we equivalently should view this as the combined spectrum \((\pm Fs/2)\) being replicated periodically up to infinite frequency. This periodicity in frequency is a direct consequence of time discretization. Similarly, discretization of frequency (see Discrete Fourier transform) results in periodicity of the time domain signal.

### B.3 What is a signal?

In the physical world, all signals are real - for example microwave radiation traveling along coaxial lines. This simple statement is worth stating because we often choose to represent real signals in the complex plane. This choice, enabled by Euler’s formula, is motivated by mathematical simplicity and clarity.

Quadrature signals are two-dimensional signals (with time - three dimensions), meaning we can describe them by separating the signal into orthogonal components - in-phase (I) and quadrature (Q). Mathematically, it is convenient to use the complex plane (trigonometric or exponential form) to represent the relation between two orthogonal quadratures rather than rectangular or Cartesian coordinates. For example, multiplication by \(i\) is the same as a 90 degree counter-clockwise phase rotation.

Intuitively, real signals can be carried by a single cable while quadrature signals require two cables to carry the two orthogonal quadratures. We encounter quadrature signals with IQ mixers, in both pulse generation and down conversion operation
modes. In down conversion, we convert a single RF channel to I and Q channels via comparison with the LO. If we combine the I and Q channels then we regain a real, one-dimensional signal, both mathematically by Euler’s formula and in experiment as the output is a single channel.

The frequency spectrum of a discrete signal, whether that is an artificial signal or from sampling a real-world continuous signal, will have real and imaginary components as well as positive and negative frequency.

Negative frequency arises mathematically in the form of complex exponentials with negative exponents - $e^{-i\omega t}$ vs. $e^{i\omega t}$ where the former is a rotation clockwise and the latter counter-clockwise in the complex plane. To represent a real signal we need both positive and negative frequency, $\cos(\omega t) = \frac{e^{-i\omega t} + e^{i\omega t}}{2}$, therefore negative frequencies must be handled with care.

In the frequency domain, complex exponentials are represented as impulses with orientation in the complex plane depending on the coefficient - impulses along the positive, real-axis at $\pm \omega$ for $\cos(\omega t)$ and negative (positive) imaginary-axis at $+(-) \omega$ for $\sin(\omega t)$. Therefore, the spectrum of a real signal will be characterized by conjugate symmetry, where the real part of the spectrum has even symmetry while the imaginary has odd. This symmetry however is not required if the discrete signal is complex to begin with.

**B.4 Down conversion**

From the Fourier transform we know that multiplication of a time-domain signal with complex exponential is equivalent to a shift in frequency. When the complex exponential has a negative exponent ($e^{-i\omega_0 t}$), this shifts the spectrum towards lower frequency and, in literature, is called complex down-conversion or mixing to baseband. For this to be useful, the signal must have finite bandwidth.
We may choose to down-convert prior to detection depending on our signal properties and limitations or constraints set by microwave hardware, such as sampler bandwidth, or amplifier and filter availability. This will also determine what frequency we want to shift our high-frequency signal down to - the intermediate frequency (IF). Homodyne, the process of shifting to DC (IF = 0 Hz), and heterodyne, non-zero IF, are both accomplished in an experimental setup using dedicated microwave mixers (I/Q, image reject, etc.). Choice of mixer and IF will depend on application-specific trade-offs.

While DC may be the ultimate goal of a down conversion process, experimental challenges such as non-ideal analog components, DC drift, variation in amplification chains, and digitizer channel jitter may introduce substantial noise rendering homodyne problematic. A common workaround is a two-step down conversion where the signal is first shifted to baseband in a heterodyne method and then shifted to DC digitally. As is the case after any conversion, it is important to properly filter the signal between down-conversion steps.

Following down-conversion, the signal is a quadrature signal and, while each output channel individually is still real (and conjugate symmetric), the overall signal does not retain symmetry conditions. Digitally we can represent the signal as I + iQ, a complex signal. Furthermore, due to the periodicity of the spectrum of discrete signal, digital down-conversion results in a circular shift in frequency rather than the linear one that occurs for continuous signals. As was the case for aliasing, the wrap-around frequency is $F_s/2$.

See section B.7.1 for a related discussion on analog mixers for down-conversion.

**B.4.1 Fast digital down conversion**

Digital down conversion requires element by element multiplication of the data vector with a pre-defined vector of complex exponentials. While multiplication is optimized
on a GPU, on other platforms (such as FPGAs and CPUs) this task can be too slow. In these situations, there is a known, simple speed-up when IF is chosen to be exactly $F_S/4$. In this case the pre-defined vector consists of $\{1, 0, -1\}$ making the multiplication very simple. We found the speed-up intrinsic to GPUs is well beyond this simplification of multiplication and thus was not used - allowing for more flexibility in choosing anti-aliasing filters and matching the bandwidths of other microwave components.

### B.5 Discrete Fourier transform - DFT

The continuous Fourier transform translates the description of a signal from the time to the frequency domain and is defined

$$X(f) = \int_{-\infty}^{\infty} x(t) e^{-2\pi if t} dt$$

(B.1)

where $x(t)$ is continuous signal in the time domain and $X(f)$ in frequency. By definition, $X(f)$ is complex and conveys the magnitude and phase information of the individual spectral components of the signal.

In general, there are four "Fourier" categories: continuous Fourier transform, Fourier series, discrete time Fourier transform (DTFT), and discrete Fourier transform (DFT). For the purpose of this appendix we consider only the DFT which has discretization in both time and frequency and is of most practical use. While many FT properties translate when we move from continuous to discrete signals, there are many critical consequences that we will touch upon in this section.

The DFT is defined as,

$$X(m) = \sum_{n=0}^{N-1} x(n) e^{-2\pi jnm/N}$$

(B.2)
where $N$ is the number of samples in your discrete signal.

The frequency range of $X(m)$ is thus limited to $\pm F_s/2$ and, as there are $N$ points in $X(m)$ spanning positive and negative frequency, the frequency resolution is $F_s/N$. Finally, the frequency axis also takes into account whether $N$ is even or odd. For most cases the relative, rather than absolute, values of $X(m)$ are of interest and therefore we won’t discuss DFT normalization here.

The linearity of the transform tells us that the DFT of the sum of the signals is the sum of the DFT of each signal and is a powerful property as we most often average by accumulating data from independent traces.

As described previously, the DFT of a real signal is conjugate symmetric. The component at DC, $X(0) = \sum_n x(n)$, for real signals must therefore be real as well. If $X(m)$ is fully real, as is the case for power spectral density, then $x(n)$ must be real and even. Similarly, $X(m)$ being fully imaginary would be a consequence of a real and odd $x(n)$. These properties are useful to know when debugging a DSP algorithm, particularly when accounting for numerical round-off errors.

The inverse DFT is used to translate from the frequency to the time domain representation.

$$x(n) = \frac{1}{N} \sum_{m=0}^{N-1} X(m)e^{(2\pi inm)/N} \quad \text{(B.3)}$$

**B.5.1 Convolution and cross-correlation theorems**

One of the most fundamental concepts of signal processing is the convolution theorem. With this, the effect of any modification or transformation of the signal can be predicted. This in turn will inform you whether or not a particular operation is suitable for your application.

Convolution of two vectors, $f$ and $g$, is mathematically defined as

$$(f * g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau) d\tau. \quad \text{(B.4)}$$
for continuous signals. The convolution theorem then tells us that convolution in one
domain translates to multiplication in the other.

\[ F[f \ast g] = F[f]F[g] \]  

(B.5)

Cross-correlation is similar to convolution with the additional conjugation and
reversal of the time-axis.

\[ (f \ast g)(\tau) = \int_{-\infty}^{\infty} f^*(t)g(t + \tau)dt \]  

(B.6)

The cross-correlation theorem (of great importance for autocorrelation calculation
- see Appendix A) is then

\[ F[f \ast g] = F[f]^*F[g]. \]  

(B.7)

In practice, we must take extra care when using the convolution and correlation
theorems with discrete-time signals.

**B.5.2 Circular vs. linear correlation and convolution**

With discrete signals the theorems for cross-correlation and convolution still apply,
however we must take into account the periodicity of signals due to sampling.

The principle of circular convolution can be visualized in time domain when we
consider two time traces (for simplicity, the traces are the same length). When we
slide one trace across the other there will be elements at the end of one trace that do
not overlap with elements in the other. These elements wrap around to overlap with
the free elements at the start of the other trace. This occurs because our time signals
are implicitly periodic. Therefore, you can also visualize this as a finite convolution
between two traces - one that repeats indefinitely and one of finite length.

Therefore \( F[f]F[g] \) achieves a circular convolution.
In order to perform linear convolution and correlation, as is most often what we are interested in, we must first pad the signals with zeros before taking DFT. The act of zero-padding a time domain signal refers to adding a finite number of zero elements to the input sequence; in this case all the zeros are added to one end of the sequence. For the full linear convolution (correlation) of two traces, we must zero pad each trace to twice the length of the trace (or if the traces are not the same length, pad to the sum of the lengths of both traces -1). If we are concerned with only a small time window (near zero $\tau$) of the convolution our constraints on zero padding can be relaxed.

If desired, you can process the output of the convolution to eliminate side-effects of the zero-padding. This includes truncating extraneous elements and correcting implicit weighting by taking into account how many non-zero overlapping elements were involved in each output element.

**B.5.3 Zero padding and DFT resolution**

The second instance where zero padding is often used is for changing DFT resolution. As seen from the DFT, the DFT resolution is set by the sampling interval and total number of points (N) in the sequence. Therefore increasing the length of the sequence improves DFT resolution. However, there is a critical distinction between artificially increasing the length of the data sequence by adding zeros and taking a longer data trace. Qualitatively, while zero-padding decreases frequency spacing, the ability to resolve closely spaced signals in the frequency domain is ultimately limited by the length of the un-padded data sequence. The ability to resolve closely spaced signals is set by the the DTFT (continuous FT) of the data sequence and increasing the sequence length with zero entries improves our approximation of the DTFT with the DFT. In both cases, the length of the data, the window, is the same and thus we do not gain more information from the signal by zero-padding.
Therefore, the bottom line is that to increase our ability to detect weak signals we must take longer sequences of data. In practice there are often other, more dominant, technical limitations including spectral leakage that reduce our detection ability. While impossible to fully eliminate in all circumstances, there are steps to be taken to minimize the negative effects (see next section). Even in those situations, the final resolution will be limited by the length of the original data sequence.

B.5.4 Spectral leakage

In the previous sequence we related the finite length of the DFT sequence to frequency resolution. Now the question arises: what happens when the input sequence has a contribution from a frequency $f_1$ that is not specified by the granularity of the frequency axis? From a simple test, we can see that the DFT does not ignore the $f_1$ contribution entirely nor add it to the nearest frequency bin. This frequency contribution instead manifests as "spectral leakage" or an increase across all other bins, concentrated especially in the bins in the vicinity of $f_1$. The leakage leaves us with a poorer approximation of the correct spectrum. Before we can consider minimizing this effect, it is helpful to note that in the time-domain, signals such as $f_1$ have non-integer number of periods in the data sequence. Since the DFT’s discretization on frequency induces periodicity of the time domain sequence (periodic extension), this translates to abrupt discontinuities which in turn require the addition of artificial, higher frequency components to describe. This intuition leads us to the primary method to reduce spectral leakage - windowing the data. Previously, when we sampled the data, we implicitly applied a rectangular window to the data set; everything outside the length of our data sequence was multiplied by zero and the entries in our sequence were multiplied by one. However, we can change the window to taper both ends of the data set (most often, towards zero). If we apply a triangular window to reduce the magnitude of the data at the ends to zero, then under periodic extension,
the effect of the discontinuities is significantly reduced and thus leakage is abated. Of course, leakage can never be completely eliminated in practice as noise is continuous in frequency, and thus without infinite frequency resolution, there will always be some discontinuities causing leakage. We can predict the effect a window has on the spectrum by considering the DFT of the window. For example the Fourier transform of a rectangular window is a sinc function, characterized by a large main lobe and infinitely many side-lobes. The multiplication of the data with a rectangular window is equivalent to a convolution of the data’s intrinsic spectrum with a sinc function. The main-lobe width and height and the attenuation and roll-off of the side-lobes ultimately define the tradeoff between minimizing leakage and our ability to properly identify closely spaced or weak signals. There are many common windows (triangle, Hanning, Hamming, Bartlett, etc.) and significant resources available to help determine when each is helpful. As is the case with trade-offs, choice of window entirely depends on your application and your spectrum (for example, trying to detect a weak incoherent background next to a strong coherent signal for resonance fluorescence). In terms of reducing leakage, any non-rectangular window offers great improvement though it is recommended that you individually test windows with a metric such as SNR, or apparent distortion of the estimated spectrum, to choose the optimal one. Windows do reduce the energy of the signal by reducing the amplitude of the entries in the window’s tapered sections; this processing loss can be compensated, however we often only care about relative, rather than absolute, DFT values and so it can be neglected. Leakage also motivates ”detrending” of data prior to DFT calculation to remove strong, unwanted DC contributions that will leak across the bins. Spectral leakage is not the only potential pitfall from not correctly tailoring your process; other common issues include picket-fence effect and scalloping loss, which we encourage you to look into in a DSP guide.
Finally, we should always consider the impact of windowing on other calculations such as whether the window results in a biased PSD or autocorrelation estimate (see pg. 83 of Ref. [105] for a useful example). Similarly, if you use an additional window, it is essential that you apply the window first then zero-pad.

B.5.5 FFT

In practice, computing the DFT as it is defined is slow. Fast Fourier Transforms (FFTs) are algorithms that optimize calculation of the DFT (note: FFT is not an approximation; it exactly calculates DFT) and have pioneered the field of DSP. There are many popular FFT algorithms (FFTW, FFTPACK, Cooley-Tukey, etc.) though for the average user, often the in-built FFT function in any given programming language is sufficient and so only an understanding of the organization of input and output sequences is needed. However, if your application requires repeated FFT calculations of similar sequences, then you should consider using one of the optimized FFTs that are available. One of the subtle dangers of DSP is that while we may be able to do a numerical computation on our data, the output may not be what we intended and thus unintentional signal corruption may occur. Therefore, it is important to make the distinction here between the ability to calculate the FFT of a signal, the validity of taking the FFT, and what the FFT of a signal means.

Stochastic signals (see Appendix A) must meet the Wide Sense Stationary (WSS) requirement in order for the use of the FFT to be justified. Furthermore, spectral leakage, bias from windowing, zero-padding, and data sequence length can all contribute to distortion or corruption of the FFT output. When applied properly, the FFT is a priceless tool for data analysis and processing.
B.6 Digital filtering

The goal of filtering in signal processing is to change spectrum of the signal to reduce unwanted components. The ideal low pass filter is a box or brick-wall filter and its magnitude response consists of ones from DC to the cutoff frequency (to perfectly transmit all low frequencies) and zeros above the cutoff frequency.

You may think that you can easily implement the ideal low pass filter by taking the FFT, zeroing out all components above the cutoff frequency, and then taking the inverse FFT. While mathematically and computationally possible, it is highly inadvisable. The ideal low pass filter is non-causal - which can be seen using by interpreting this described method using the convolution theorem. Multiplication by a rectangular window in the frequency domain is equivalent to convolution with a sinc function in time, which means that the element at given time bin is influenced by all bins in the signal, past and future. Furthermore, there is necessarily a truncation of the infinite, continuous, sinc function in time domain which impacts the effectiveness of this attempt. For most situations, this type of distortion should be avoided. Fortunately, there are an assortment of digital filters that can be easily implemented or are already available in standard DSP software packages.

While there are many descriptors for characterizing filters, let us consider the two subsets: finite impulse response (FIR) and infinite impulse response (IIR) filters. The impulse response of a filter is the response (output) of the filter when the input is a single impulse (all zeros with one non-zero data point).

FIR filters are the most commonly used type of digital filter. As alluded to previously (in the misguided attempt to implement the ideal low pass filter), we can think of the act of filtering as a convolution of the signal in time domain with the filter’s impulse response, or multiplication of the signal spectrum with the filter’s frequency response.
Explicitly, the discrete convolution between $h(k)$ (filter coefficients) and $x(m)$ (input signal), yields the filtered output $y(n)$. The length of $y$ is $P + Q - 1$, where $P$ and $Q$ are the lengths of $h$ and $x$ respectively.

The "finite" descriptor for FIR filters refers to the criteria that only a finite number of input values are used to calculate the output of the filter. Therefore you can, if needed, design causal filters that require only a finite "memory" of the signal to produce the filtered output.

The filter is fully described by a finite number of coefficients (in this case, the impulse response), where higher order filters have more coefficients. The filter output is the convolution of the filter coefficients with input sequence; one may define filter coefficients manually and then perform the convolution, or use built-in digital filters that envelope the process (i.e., Matlab’s designfilt() and filter() methods). Increasing the order of a filter sharpens the roll-off between the pass-band and stop-band and increases the attenuation in the stop-band. However higher order filters also take more computational time and resources, defining the inevitable trade-off.

As was the case with windows for reducing spectral leakage, there are many established methods for designing filters, including the window design method, equi-ripple, and frequency sampling. DSP packages for Python and Matlab have well-documented functions and examples for how to visualize, create, and use a variety of filters. For our purpose here, there are three main considerations when choosing a digital filter: run time, amplitude response, and phase response. Since we generally want to use filtering as a step to processing large data sets, we want to use the fastest filter possible while still maintaining the integrity of the data and sufficiently attenuating the unwanted spectral components.
The amplitude response shows us the attenuation of the filter and is the most
recognizable filter property. For the phase response, it is often most desirable to
have a linear phase-frequency relationship in the pass-band of your filter. The phase
characteristic is often quoted in terms of group delay - the negative derivative of
phase response with response to frequency. For linear phase (constant group delay)
components, there will be an overall phase shift between the input and output of
the filter that can be easily corrected for, unlike a phase distortion. While you can
still design this relationship with other filters, FIR filters with symmetric-coefficients
intrinsically satisfy this criteria.

It is important to inspect filters (both digital and analog) to confirm that the
group delay is constant over the bandwidth of your signal. Furthermore the best test
of a filter is to compare the power spectrums before and after the filtering, as well as
to average the filtered data to ensure that the stop-band ripples do not accidentally
pass strong coherent signals (for example - multiples of your IF frequency in the case
of down-conversion). This is also true for analog filters, where you should measure
S21 amplitude and group delay across a filter using a vector network analyzer to
confirm that your signal band-width will not be corrupted.

You may find it more efficient to use combinations of digital filters to efficiently
suppress unwanted spectral content. For example, you may want to use a primary
filter designed to suppress multiples of your IF frequency and a secondary one to
suppress high frequency noise. See Appendix A for details on filters we chose for
calculating autocorrelation. This also is the case with analog filters (for example,
with anti-aliasing filters prior to the digitizer), though one must ensure that reflections
between filters do not arise in your measurement chain.

The simplest example of FIR filtering is the smoothing function (moving average)
where you slide a finite-length window across the input signal and average the values
enclosed by the box (by definition, the convolution of your signal with a rectangular
box). The length of the window determines the first cut-off frequency and the spacing between sidebands. For instance, smoothing data sampled at $F_s$ with a N-element window will have minima in the amplitude response at multiples of $\pm F_s/N$, however the sidebands of the filter have large amplitude and thus this filter does not suppress high frequency content well. However, because this filter is very efficient at suppressing multiples of IF quickly (i.e., implementation using cumulative sum) it is a highly useful filter to know.

Up until now, we have considered the finite size of the filter, but not the data set. For this explanation, let us assume that the original data set is itself a steady-state signal, with no abrupt changes. Since the data set is also finite in size, we can break up the response of the filter into two parts - transient and steady state. The transient period is readily observable as the ringing or distortion at the ends of the filtered output, while the steady state is the time-translationally invariant "bulk" in the center of the signal. At the ends of the signal, there are not sufficient neighboring elements to match the filter coefficients and thus while the entire signal is filtered, these edges may not be desirable for your application. One may consider discarding these end elements, which is acceptable. However, as truncating the signal is equivalent to multiplying by a rectangular window in time domain (convolution with a sinc function in frequency), you can expect to see an increase in high frequency spectral content.

In comparison, IIR filters describe almost all analog, electrical filters due to the inherent memory or feedback by inductors and capacitors. IIR filter coefficients are also not the same as the impulse response of the filter. While there are established IIR digital filter methods, improper use of them can produce unwanted phase distortion (for example, IIR filters can be made zero-phase by forward and backward filtering - filtfilt method of Matlab) or significant errors due to numerical rounding. We do not
use IIR filters in this thesis and so will not go into detail. For most situations, there are suitable FIR filters that can be applied.

### B.6.1 Decimation

If after filtering, digital down conversion, or other processing, your signal spectrum fills only a small fraction of the range set by the sampling rate then there is no reason to maintain the high sampling rate. Retaining a high sampling rate is both unnecessary and cumbersome, especially when computation resources are limited as is the case on an FPGA or GPU. For GPUs, linear reduction of data in memory can have nonlinear computational speedup!

There are two terms often used for reducing the sampling rate of a signal - decimation and down-sampling. Decimation describes the entire process of reducing sampling rate by a factor n: first low pass-filtering the data to ensure no unwanted aliasing can occur and then downsampling the data, or taking every nth point of the signal. DSP software packages in Matlab and Python have built in functions to handle the full decimation process, or you may do each step individually for customization.

As a rule of thumb for decimation, it is important to confirm that the magnitude of spectral content falls off to zero well before half of the new, reduced sampling frequency. Thus corruption due to aliasing can be successfully mediated by optimization of filtering and downsampling.

### B.7 Spectral subtraction

A sequence of data measured in experiment necessarily contains contributions from both the desired signal and noise. To reduce the effects of noise, we may consider subtracting an averaged noise spectrum. This process of spectral subtraction has been pioneered for audio processing where access to signal and noise is limited and sub-
traction is performed real-time, rather than on averaged data sets. In contrast, there are many cQED measurements where we are satisfied with detection improvement on averaged data sets, such as autocorrelation.

For example, we can use spectral subtraction for PSD estimation when noise power dominates. In the ideal limit, we can eliminate the contribution of noise by reconstructing the noise distribution. While this in general is not possible, a good estimate on noise statistics is sufficient to help improve detection of weak signals.

In practice, obtaining sufficient statistics for weak signals - such as signals in the roll-off or stop-band of a filter, or frequency ranges where noise is the only contribution - is a significant challenge. In these situations we encounter negative elements in a subtracted PSD estimate, an unphysical quality. Another signature of poor spectral subtraction is the emergence of "musical notes", the apparent re-emergence of signal at higher frequency (this phrase was coined for audio signals, where higher pitch carried an additional, musical fingerprint). Methods of nonlinear spectral subtraction including establishing a noise floor help reduce the effects of improper spectral subtraction, though as we can only estimate the noise and signal it can not be eliminated.

Regardless of whether subtraction occurs in the frequency or time-domain, it is imperative to confirm that basic principles of the signal (such as non-negativity of PSD estimates) are met.

B.7.1 Analog mixers

Basic mixers are nonlinear elements that multiply two signals to generate signals at the sum and difference frequency. We typically encounter mixers in cQED experiments in two places: during signal generation and prior to signal acquisition. In the first case, the mixer is used to up-convert a low frequency pulse to higher (many GHz) frequency. In the second, we use the mixer to shift a high frequency signal down to baseband in preparation for further amplification, filtering, and then sampling.
In cQED experiment, the IQ, image reject (IR), and single-sideband (SSB) mixers are among the most common. Though they operate using similar components, each is optimized for a different task. For example, the IR mixer is optimized for canceling the image - e.g., neglecting signal at LO − IF when LO + IF is the intended target for down-conversion (high side vs. low side injection). This can be a critical advantage when considering broad-band noise and a narrow-band signal or an otherwise densely populated spectrum. SSB provide similar function though usually with more relaxed requirements and therefore are generally less expensive. The IQ mixer is intended for modulating two distinct quadratures of a signal (I and Q) onto a carrier tone for up-conversion or retrieving two quadratures for down-conversion and is optimized for this function.

Non-ideality of the mixers enter in various forms including insertion loss, non-orthogonality of quadratures and leakage. While loss is typically not a concern at this stage of the measurement chain, there is still the potential to reduce SNR during down-conversion. This can happen with single-channel heterodyne (where one quadrature output is terminated) if the signal phase is not aligned with the correct output quadrature or if the signal has undefined phase. In this situation, we may choose to use a 90 degree hybrid coupler to recombine the quadrature outputs.

B.8 GPU for signal processing

All of the algorithms presented in this appendix have standard, optimized software implementations. However, when fast, real-time processing is required, DSP quickly becomes a bottle-neck. In these cases, we can turn from the standard CPU to specialized hardware.

While a custom FPGA is perhaps the most power efficient and fast platform, it can require significant overhead (time or cost) to implement correctly and integrate
successfully into a measurement setup. A more accessible alternative is to use a Graphics Processing Unit or GPU, hardware specifically designed for fast numerical computation with floating pointing numbers.

In recent years, GPU technology has made tremendous advances and off-the-shelf GPUs today feature high speeds, low cost, vast on-board resources, and simple user-interfaces. In particular, the NVIDIA CUDA package implements all the fundamental DSP operations and popular programming languages (Python and Matlab) already have wrapper functions programmed. Thus transitioning an algorithm programmed from the CPU to a GPU can be as simple as replacing CPU function calls with the corresponding GPU ones. Furthermore, it integrates seamlessly into existing measurement setups without attempting to replace timing-sensitive equipment such as AWGs or digitizers.

There are a few important considerations when working with GPUs for run-time optimization. First, there is an unavoidable overhead cost of transferring data between the CPU and the GPU. Secondly, the speed-up of a GPU has a nonlinear dependence on GPU memory or resource allocation. Fine-tuning algorithm parameters (such as data set size, data types, and memory storage) requires careful testing and iterative trouble-shooting by the user - as sometimes an unexpected drain on GPU resources such as a high resolution monitor may be impeding optimization efforts.

While GPUs are designed for floating point arithmetic, they further are specialized for single versus double precision speed and the consequences (accuracy, memory usage, speed) of each should be considered. Finally if GPU resources are not a limiting factor, one can consider multi-threading for further improvements.

In summary, affordable and accessible GPU technologies are powerful tools for computationally intensive algorithms such as an autocorrelation measurement on low SNR signals.
Appendix C

Device Fabrication

Devices shown in this thesis were fabricated in the Princeton Institute for the Science and Technology of Materials Micro/Nano Fabrication Laboratory and Princeton Quantum Device Nanofabrication Laboratory cleanroom facilities.

All devices were made on C-plane, single-side polished, sapphire substrates (approximately 500 microns thick) with 200nm of niobium sputtered on top. We patterned the niobium with a $SF_6$ reactive ion etch process following standard photolithography techniques. For the devices in the later section of the thesis, a direct write process on a Heidelberg laser writer was used in place of standard chrome-mask based lithography to realize a smaller critical dimension.

The transmon qubits were patterned using electron beam lithography. We used a bi-layer resist stack of MMA/PMMA and 40nm of evaporated aluminum for anti-charging purposes. Following development, devices were loaded into a Plassys for aluminum evaporation. The junctions for the multimode device and earlier devices were made using the Dolan Bridge technique. Since then we have transitioned to using the Manhattan Junction [109, 110], which does not depend on a resist bridge and thus had higher yield.
Bibliography


