Quantum Simulation with Circuit-QED Lattices: from Elementary Building Blocks to Many-Body Theory

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ABSTRACT

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Recent experimental and theoretical progress in superconducting circuits and circuit QED (quantum electrodynamics) has helped to develop high-precision techniques to control, manipulate, and detect individual mesoscopic quantum systems. A promising direction is hence to scale up from individual building blocks to form larger-scale quantum many-body systems. Although realizing a scalable fault-tolerant quantum computer still faces major barriers of decoherence and quantum error correction, it is feasible to realize scalable quantum simulators with state-of-the-art technology. From the technological point of view, this could serve as an intermediate stage towards the final goal of a large-scale quantum computer, and could help accumulating experience with the control of quantum systems with a large number of degrees of freedom. From the physical point of view, this opens up a new regime where condensed matter systems can be simulated and studied, here in the context of strongly correlated photons and two-level systems.
In this thesis, we mainly focus on two aspects of circuit-QED based quantum simulation. First, we discuss the elementary building blocks of the quantum simulator, in particular a fluxonium circuit coupled to a superconducting resonator. We show the interesting properties of the fluxonium circuit as a qubit, including the unusual structure of its charge matrix elements. We also employ perturbation theory to derive the effective Hamiltonian of the coupled system in the dispersive regime, where qubit and the photon frequencies are detuned. The observables predicted with our theory, including dispersive shifts and Kerr nonlinearity, are compared with data from experiments, such as homodyne transmission and two-tone spectroscopy. These studies also relate to the problem of detection in a circuit-QED quantum simulator.

Second, we study many-body physics of circuit-QED lattices, serving as quantum simulators. In particular, we focus on two different directions which complement each other. One is concerned with quantum phases, such as photon pairing states, arising from the specific nature of light-matter interaction not usually encountered in conventional condensed matter materials. The second deals with interacting photons in a very specific lattice, the Kagome lattice. In that case, interesting liquid-crystal-like quantum phases, such as a nematic superfluid and a Wigner crystal, arise from the geometric frustration of the lattice.
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to think about nematic states in frustrated Kagome lattices which had not been envisioned by existing theories before.

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Dedication

Dedicated to my mother Yuezhen Xu,

and my father Zhuoxin Zhu.
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CHAPTER 1

Introduction

1.1. Motivation

1.1.1. Quantum simulation

With the rapid development of quantum information science in the past decades, there has been significant experimental progress of controlling, manipulating and detecting individual quantum systems. Although realizing a full-fledged universal quantum computer may still need several decades of hard work, building a functioning quantum simulator is already possible and has been put into practice.

Interestingly, Richard Feynman’s original vision of a quantum computer from 1981 [24] is closely related to the idea of a universal quantum simulator. This idea was later further developed into the concept of a universal quantum computer by David Deutsch in 1985 [19]. In his seminal 1981 lecture ‘Simulating physics with computers’ [24], Feynman pointed out that a classical Turing machine (classical computer) would experience an exponential slowdown when simulating quantum phenomena. Indeed, to describe the most general quantum state, for example, of $N$ spin-1/2 particles, one has to store $2^N$ numbers. The computational power required grows exponentially and is practically impossible, for example, when $N > 50$. Instead, Feynman proposed that, to solve this problem, one could use a ‘quantum simulator’ which operates according to the laws of quantum mechanics. The central idea of quantum simulation is to map the Hamiltonian of a target quantum system $H_t$ to the Hamiltonian of a well-controlled quantum
simulator $H_s$. The mathematical equivalence allows one to study the quantum dynamics of the target quantum system through detecting relevant observables with the quantum simulator.

More specifically, there are two different types of quantum simulators, digital quantum simulators and analog quantum simulators [12]:

A digital quantum simulator is closer to Feynman’s original idea of a universal quantum simulator, which discretizes space and time and can also be reprogrammed to simulate other physical systems [24]. Such a digital quantum simulator usually involves a series of quantum gates which form a quantum circuit, in order to perform a unitary evolution from the system’s initial state to its final state. Therefore, a digital quantum simulator, to some extent, is similar to a quantum computer with a specific quantum algorithm. However, most of the time one may only be interested in certain physical observables of the system, such as particle density, magnetization or correlation functions, instead of the faithful representation or evolution of the complete many-body wavefunction. Hence a quantum simulator is expected to be less demanding and easier to build than a quantum computer.

An analog quantum simulator, on the other hand, evolves continuously in time. It is not as versatile as a digital quantum simulator, but specific to a certain type of physical systems. The essence of an analog quantum simulator is to use another well-controlled physical system (instead of a digital device) to mimic the behavior of a target physical system [12]. The underlying mathematical equivalence is encoded in the mapping between the Hamiltonians of the two systems. Although not being universal, the analog quantum simulator is less prone to imperfections and decoherence than the digital quantum simulator or the quantum computer, and

---

1 Certain versions of analog quantum simulators can also be continuous in space, while some others involve a lattice and hence spatial discretization.
2 Therefore, an analog quantum simulator can also be called a quantum emulator.
quantum error correction may not be needed. Also, the scale of an analog quantum simulator is less demanding. For example, although realizing Shor’s algorithm [97] with a quantum computer may need tens of thousands of qubits, tens or hundreds of qubits may already serve as a practical analog quantum simulator. Hence, a scalable analog quantum simulator is usually much easier to be build. In this thesis, we will focus on the discussion of analog quantum simulators, and in particular their usage in simulating condensed matter systems.

1.1.2. Analog quantum simulation of strongly correlated materials in condensed matter physics

In the area of condensed matter physics, it is usually possible to model a realistic material with a simple Hamiltonian, such as the Hubbard Hamiltonian of interacting electrons or the Heisenberg model of magnetism. However, exact analytical solutions are not available in most cases beyond one dimension. Conventional perturbative methods, such as diagrammatic techniques often fail in the strongly-correlated regime, namely when interaction effects dominate. Prominent examples of such strongly-correlated materials are high-temperature superconductors, for which the microscopic origin of superconductivity is still unclear. Exact numerical diagonalization is limited to small systems due to the exponentially growing memory ($d^N$ for a lattice model) needed to store the quantum state. Classical stochastic simulation methods, such as quantum Monte Carlo [77, 78, 101], have been developed. Unfortunately, they fail in many practical situations due to the so-called sign problem (sampling with negative weights), which includes the fermion sign problem, and the sign problem arising in frustrated spin or lattice models.

$^3$Here $d$ refers to the number of states on each site and $N$ refers to the number of sites.
An alternative is to build well-controlled quantum many-body systems which can emulate real materials. The benefit is two-fold. First, one can either use the quantum simulator to discover new physical phenomena, such as novel quantum phases. Second, one can compare the simulated results with those from existing analytical or numerical methods. This can verify theoretical predictions, improve existing theoretical methods, or inspire new theoretical techniques.

With the rapid experimental progress in the past decade, analog quantum simulation of strongly-correlated bosonic or fermionic many-body systems has been realized with ultracold atoms and trapped ions [5, 8, 58]. Interesting quantum phases, such as bosonic superfluids, Mott insulators, fermionic pairing superfluids, and quantum magnetism have been observed in these systems. Even more exotic models, which are hard to implement with real materials, can also be realized in these artificial systems, such as lattice models in the presence of synthetic gauge fields and observation of the Hofstadter butterfly spectrum [1, 39].

However, due to the specificity of the analog quantum simulator, the possible physical models which can be simulated with a given platform is limited to certain types. Also, different platforms have their own advantages and disadvantages. Therefore, investigating additional analog quantum simulators beyond the existing types is a worthwhile research direction. Furthermore, comparing simulation results for the same model but obtained with different platforms will also serve as a useful cross-check and may be necessary at the stage when independent theoretical calculations are not available.
1.1.3. Quantum simulation with superconducting circuits

Rapid experimental and theoretical developments in the area of superconducting circuits and circuit QED (Quantum Electrodynamics) \[7\] \[16\] \[21\] \[63\] \[91\] \[105\] during recent years have opened up a promising future for realizing a scalable solid-state quantum computer. In the route towards that ultimate goal, experimentalists have to develop and master the challenging techniques of controlling, manipulating and detecting a large-scale many-body system with high-precision. Quantum error correction needs to be implemented to ensure fault tolerance and is one of the biggest challenges. An intermediate stage, as one can imagine, is to realize an analog quantum simulator with superconducting circuits, where well-developed microchip fabrication can be used to engineer interesting many-body systems quickly and flexibly. Since a quantum simulator is less demanding to build, more fault tolerant, and may not need quantum error correction, realizing it will help physicists to accumulate experience of engineering well-controlled quantum many-body systems, and also provide a device with practical applications.

In a circuit-QED system, the microwave photons in the on-chip superconducting (SC) transmission line resonator interact with the SC “artificial atom”. This system realizes the Jaynes-Cummings (JC) model, which is the simplest model of light-matter interaction in the quantum regime \[45\]. The “atom” may also be called a “qubit” if only the first two levels play an important role. From now on, we will use the terminology “qubit” to represent atom/“artificial atom” for convenience.

With well-developed fabrication techniques, there has been experimental practice to engineer arrays of coupled SC resonators \[40\], with one qubit inside each resonator. In such a resonator array, photons can hop between different resonators. The combination of off-site photon hopping and onsite photon-qubit interaction of JC type lead to the Jaynes-Cummings lattice
model, in which interesting many-body phenomena can occur. Several recent theoretical works predict that polaritons, which are quantum superpositions of photons and qubit excitations, can undergo a superfluid-to-Mott insulator quantum phase transition \[35, 36, 52, 87, 88\] analogous to the one in the Bose-Hubbard model. This prediction motivates the application of circuit-QED lattices as quantum simulators of many-body physics \[12, 40\]. Prototypical experiments with SC resonator arrays have already been achieved by Andrew Houck’s group at Princeton \[40, 102\], and their ongoing efforts aim at placing SC qubits into the resonator array. Therefore, we are interested in the theoretical study of this type of systems, and make predictions of interesting many-body phenomena which may later be observed in the experiments.

The structure of the rest of the chapter is as follows. In Sec.\[1.2\] we introduce the elementary building blocks of the quantum simulator, namely a circuit-QED system which realizes the Jaynes-Cummings model. In Sec.\[1.3\] we show how the elementary building blocks can be scaled up into a circuit-QED lattice, which can, in turn, be used as a quantum simulator. In Sec.\[1.4\] we provide the outline of the entire thesis.

1.2. Circuit-QED and Jaynes-Cummings model

1.2.1. Superconducting circuits as qubits

It is quite remarkable that a superconducting circuit, which contains a macroscopic number of electrons, can actually behave like an “artificial atom” or qubit, with a discrete set of low-lying energy levels.

The underlying microscopic mechanism is that below the SC transition temperature, electrons with opposite spins in the superconductor pair up and macroscopically condense into a BCS ground state \[4\], with a substantial gap \(2\Delta\) from the excited spectrum. The existence of
the gap greatly reduces the number of effective degrees of freedom in the SC circuit and leads to zero resistance of the circuit. It turns out that the only effective dynamical variables of the SC circuit are charge $Q_i$ and generalized flux $\Phi_i$ (defined as the time integral of the voltage) on each node $i$ of the circuit [20]. After quantizing the Hamiltonian expressed by these dynamical variables, one can get a discrete set of energy levels of the SC circuit, resembling an “artificial atom”.

To form an actual qubit, having discrete energy levels is not enough. Another important requirement is the anharmonicity. With the usual circuit elements, namely capacitors and inductors (note that we no longer use resistors in the SC circuit), one can build an LC circuit, which is equivalent to a harmonic oscillator. In this case, the energy levels are equidistant and there is no possibility to operate the system only in the subspace of its ground and first-excited states. Thus, one needs to introduce another SC circuit element, the Josephson tunnel junction. It is described by the Hamiltonian: $H_J = -E_J \cos \varphi$, where $\varphi$ is the phase difference (proportional to the flux difference) across the junction. The above Hamiltonian tells us that the junction can be thought of as a nonlinear inductor. When combined with a capacitor or inductor, the resulting circuit has an anharmonic spectrum, and the first two levels can be used as a qubit.

All SC qubits consist of these three basic SC circuit elements (i.e. capacitor, inductor and Josephson junction), including the Cooper-pair box (CPB) in the charging [69] and transmon [54] regimes, the phase qubit, the flux qubit [15] and fluxonium [65]. Here, we use a CPB as a simple example for illustration. As shown in Fig. [1.1] the CPB contains two superconducting islands linked by two Josephson junctions and forms a SC loop. The loop is penetrated by an external magnetic flux $\Phi_{\text{ext}}$, which can be used to tune the qubit spectrum in situ. The
Figure 1.1. (Credit: A. A. Houck et al. [40]) Cooper-pair box. (a) Its circuit consists of two superconducting islands connected by two Josephson junctions, which forms a superconducting quantum interference device (SQUID). (b) The circuit is patterned onto a chip, typically by means of double-angle electron-beam evaporation of aluminum to obtain Al/AlOₓ tunneling junctions, shown magnified in (c). (d) Energy levels of the lowest three Cooper-pair-box eigenstates as a function of external flux. (In this example, the parameters are chosen as $E_J = 30 \text{ GHz}$ and $E_C = 2 \text{ GHz}$, respectively; the offset charge has been fixed to $n_g = 1/2$.)

Hamiltonian of this qubit is:

(1.1) \[ H = 4E_c(N - n_g)^2 - 2E_J \cos(\pi \Phi_{\text{ext}}/\Phi_0) \cos(\varphi + \pi \Phi_{\text{ext}}/\Phi_0) \]

Here, $N$ is the dimensionless charge operator, i.e. $N = Q/2e$; $\varphi$ is the phase operator which is proportional the generalized flux operator, i.e. $\varphi = 2\pi \Phi/\Phi_0$, where $\Phi_0 = h/2e$ is the flux
Figure 1.2. (Credit: A. A. Houck et al. [40]) Elementary circuit-QED building block. (a) Standard fabrication techniques are used for patterning the simplest circuit-QED elements onto a chip: superconducting qubit located in the transmission-line resonators and coupling capacitors on the two ends. The figure also illustrates the simplest measurement technique, which sends microwave photons in through one end and measures the transmitted photons through the heterodyne detector on the other end. (b) Capacitive coupling between a qubit and a resonator produces the Jaynes-Cummings model for a single lattice site.

quantum. The first term in the Hamiltonian comes from the charging energy of the capacitance, and the second terms comes from the Josephson energy of the two junctions. Figure 1.1(a) shows the circuit diagram of the CPB and Figure 1.1(b) a schematic image of the device. The junction loop is located in the middle and the long zig-zag pattern increases the geometric capacitance. Figure 1.1(c) shows the zoom-in version of the junction loop which appears in the middle of Fig. 1.1(b). Figure 1.1(d) shows the low-lying spectrum of the CPB, which contains a discrete set of low-lying energy levels. Note that the flux dependence of the spectrum suggests that one can tune the qubit level spacing $\epsilon_{01}$ continuously in situ.

1.2.2. Jaynes-Cummings model based on circuit-QED architecture

By capacitively coupling a SC qubit to a transmission line resonator, as shown in Fig. 1.2, the building block of the circuit-QED architecture is formed. The coupled system can be described
by the Jaynes-Cummings Hamiltonian, namely,

\begin{equation}
H^{JC} = \omega a^\dagger a + \epsilon \sigma^+ \sigma^- + g (a \sigma^+ + a^\dagger \sigma^-),
\end{equation}

where \( a^\dagger \) and \( a \) are the creation and annihilation operators of photons, and \( \sigma^+ \) and \( \sigma^- \) are raising and lowering Pauli operators of qubit levels. The first and second terms describe the decoupled resonator and qubit respectively, where \( \omega \) is the photon frequency and \( \epsilon \) is the qubit level spacing. The third term describes the JC coupling, which conserves the total excitation of the qubit and resonator, \( N_{\text{tot}} = a^\dagger a + \sigma^+ \sigma^- \).

When the JC coupling is turned off, each eigenstate of the system is a direct product state of bare photon and bare qubit states, denoted as \( |n, \sigma\rangle \). Here, \( n \) represents the number of photons in the resonator and \( \sigma = \uparrow \) or \( \downarrow \) represents the qubit state. When the JC coupling is turned on, the state \( |n, \downarrow\rangle \) is only hybridized with state \( |n - 1, \uparrow\rangle \) due to the photon-qubit interaction. There are only two states with total excitation number \( N_{\text{tot}} = n \). Thus, \( H^{JC} \) is block diagonal, i.e.,

\begin{equation}
H^{JC} = \bigotimes_{n=0}^{\infty} h_n,
\end{equation}

where \( h_0 = 0 \) and

\begin{equation}
h_n = \begin{pmatrix}
\frac{n \omega}{\sqrt{n}g} & \frac{\sqrt{n}g}{(n-1)\omega + \epsilon} \\
\frac{\sqrt{n}g}{(n-1)\omega + \epsilon} & \left(\frac{n - 1}{\omega} + \epsilon\right)
\end{pmatrix} \quad (n \geq 1).
\end{equation}

The ground state is not paired up and is unaffected by the interaction. By diagonalizing each \( 2 \times 2 \) matrix, one gets the excited-state energies \( (n \geq 1) \),

\begin{equation}
E_{n\pm} = n \omega + \Delta/2 \pm \sqrt{(\Delta/2)^2 + n g^2},
\end{equation}
where $\Delta \equiv \epsilon - \omega$ is defined as the detuning of the qubit-resonator system. The corresponding pair of eigenstates of each $2 \times 2$ block is:

\[(1.5) \quad | n, \pm \rangle = a_{n\pm} | n, \downarrow \rangle + b_{n\pm} | n - 1, \uparrow \rangle.\]

For $n \geq 1$, the coefficients are

\[(1.6) \quad a_{n+} = \sin \theta_n, \quad b_{n+} = \cos \theta_n;\]

\[(1.6) \quad a_{n-} = \cos \theta_n, \quad b_{n-} = -\sin \theta_n.\]

The mixing angle $\theta_n$ is given by

\[(1.7) \quad \theta_n = \frac{1}{2} \arctan \left( \frac{2g\sqrt{n}}{\Delta} \right).\]

The $| n, + \rangle$ and $| n, - \rangle$ are called upper and lower polariton states respectively, and both contain $n$ polaritons. Here, we use the Jaynes-Cummings ladder for the $\epsilon = \omega$ ($\Delta = 0$) case as an illustration, which is shown in Fig. 1.3. In this case, photon and qubit excitations are hybridized most strongly, since the pairing states are degenerate and the mixing angle is maximized at $45^\circ$.

1.3. Circuit-QED lattices

One way to generalize the JC model and to study many-body physics is to capacitively couple multiple qubit-resonator systems together. The building block of this array architecture is shown in Fig. 1.2, namely a single qubit-resonator system. These building blocks can be capacitively coupled to each other at their two ends and form lattices with different geometries and dimensions.
Figure 1.3. Jaynes-Cummings ladders for zero detuning ($\Delta = 0$). The left and right ladders represent the bare states and energy levels of the decoupled resonator-qubit system with qubit being $\downarrow$ and $\uparrow$ respectively. The middle ladder represents the eigenstates and energy levels when the JC interaction is turned on. Except for the ground state, the two degenerate bare states hybridize with each other and form lower (blue) and upper (red) polariton states. The doubly-degenerate bare energy levels are hence split into pairs.

As a specific example, we discuss the 2-D Kagome lattice [51], shown in Fig. 1.4, which is being built and studied in Andrew Houck’s experimental group in Princeton. Although the transmission line resonators form a honeycomb pattern, the actual photon lattice is a Kagome lattice as shown in Fig. 1.4(b). The realistic image of the experimental setup is shown in Fig. 1.5.

The Hamiltonian which describes the JC lattice model is hence:

$$(1.8) \quad H = \sum_j H_j^{JC} + t \sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j).$$

Here, the first term sums over the on-site JC Hamiltonian, while the second term describes the capacitive coupling between nearest-neighbor resonators. Due to the form of the JC coupling, the whole lattice system has a conserved total excitation number, $N_{tot} = \sum_j (a_j^\dagger a_j + \sigma_j^+ \sigma_j^-)$. 
Figure 1.4. (Credit: J. Koch et al. [51]) (a) Circuit-QED realization of a Jaynes-Cummings lattice. It consists of SC resonators (e.g., coplanar waveguides, schematically shown as rectangular boxes), each of which is coupled to a SC qubit (symbolized as dots centered in the resonators). Microwave photons hop between nearest-neighbor resonators, with the coupling strength $t$ set by the mutual capacitance between resonator ends. The onsite interaction between the photons and the superconducting qubits is of JC type with strength $g$. (b) Although the rectangular resonators form a honeycomb lattice, the photon lattice is actually a Kagome lattice.

Note that this particular Hamiltonian describes the general situation of JC lattices with different geometries and dimensions. Contrary to the case of a single-site JC Hamiltonian, no exact solution is known for the JC lattice Hamiltonian for $N_{\text{tot}} > 1$. The difficulty lies in the fact the JC lattice Hamiltonian actually describes a strongly-correlated many-body system.

The hopping amplitude $t$ (usually a real number) is determined by the mutual capacitance between resonators and is in general tunable during the fabrication process. The hopping sign can be varied when properly choosing the mode structures (e.g. $\lambda$-mode and $\lambda/2$-mode). Even
more surprisingly, when including a Josephson-junction ring on each three-way coupling vertex, the hopping amplitude $t$ can be made complex-valued, namely $t = |t| e^{i\phi}$, which is equivalent to introducing a synthetic gauge field coupling to the photons [51]. The schematic diagram of such a Josephson-junction ring is shown in Fig. 1.6. There, the external magnetic flux $\Phi$ can be used to tune the complex amplitude $t$ in situ.

1.4. Outline of the thesis

In this section, we give an overview of the structure of the entire thesis. Besides the Introduction (Chapter 1) and Conclusion and Outlook (Chapter 6), there are four main chapters with the following topics.
Figure 1.6. (Credit: J. Koch et al. [51]) Introducing synthetic gauge field and time-reversal symmetry breaking to circuit-QED lattices. In each vertex of the resonator lattice, three resonators are joined capacitively by a Josephson-junction ring. The time-reversal symmetry is broken by a perpendicular magnetic field, effecting a kind of Aharonov-Bohm loop which causes the clockwise path and the counter-clockwise path to acquire phases with opposite sign.

In Chapter 2, we discuss a novel superconducting qubit, the fluxonium, formed by shunting a single weak Josephson junction with a large Josephson junction array. For this type of qubit, the charge matrix (which determines the coupling to microwave photons) does not have a simple nearest-neighbor selection rule. This leads to the fact that a simple Jaynes-Cummings model is not sufficient enough to describe the coupling of this type of qubit to microwave photons. Instead, we use a generalized Jaynes-Cummings (Rabi) model to describe a multi-level qudit\(^4\) coupled to photons. In particular, we study the dispersive regime (when photon frequency and qudit level spacings are detuned) of such a model, and derive an effective Hamiltonian up to fourth order in interaction strength $g$. The effective Hamiltonian helps to give a quantitative match of the experimental measurements of dispersive shifts from homodyne measurement and

\(^4\)Here qudit refers to a multi-level generalization of a qubit, where quantum information can also be stored.
two-tone spectroscopy. Besides, we also use the effective Hamiltonian to identify the Kerr nonlinearity and two-photon vacuum Rabi resonance observed in the experiment.

In Chapter 3, we briefly discuss the analytical expressions of the charge matrix element in a certain parameter limit. Although no nearest-neighbor selection rule is present, there is still significant difference between certain charge matrix elements in the order of magnitudes. We use the classification of two distinct types of eigenstates, the persistent and metaplasmon states, to derive analytical expressions of the three types of charge matrix elements between them and find a quasi selection rule which reveals the underlying reason behind the relative magnitudes of different matrix elements. We also compare the analytical results with exact numerical diagonalization in the experimental regime and find qualitative agreement.

Starting from Chapter 4, we move from single-site light-matter interacting systems to the lattice system, i.e. the many-body problem with light-matter interaction. Chapters 4 and 5 explore different aspects of this problem. While Chapter 5 concentrates on the novel properties of the many-body system arising from the exotic property of light-matter interaction, Chapter 4 reveals the novelty arising from the lattice effect, i.e. frustration.

More specifically, in Chapter 4, we study the dispersive regime of Jaynes-Cummings (JC) lattice model and Rabi lattice model. We use a Schrieffer-Wolff transformation to derive the effective interaction, which includes qubit-qubit interactions mediated by virtual photons, photon-photon interaction (Hubbard-like) mediated by virtual qubit excitations, photon-qubit dressing, conditional photon hopping (determined by qubit states) and photon pairing. Novel many-body ground states appear for ultra-strong coupling (when the interaction strength is comparable to

5The difference between the two is that the Rabi lattice model contains additional counter-rotating terms which violate conservation of the total number of photonic and qubit excitations, and is a more precise description of light-matter interaction in the ultra-strong coupling regime.
either the photon or qubit frequency), including a ferromagnetic state of photon-dressed-qubit, and a photon pairing state.

In Chapter 5 we study the problem of interacting photons (in the simple dispersive JC limit where the effective photon-photon interaction mediated by qubits has the Hubbard form) in a Kagome lattice with geometric frustration or in the presence of a synthetic gauge field. In this case, the single-particle spectrum has a lowest flat band, and the usual picture, that macroscopic number of bosons condense into the lowest-energy single-particle state, breaks down. We identify novel nematic liquid-crystal like phases in such a lattice model, including a nematic Wigner crystal, nematic superfluid and nematic supersolid.

Some technical details related to the main chapters can be found in the appendices after the bibliography.
CHAPTER 2

Fluxonium I: fluxonium qubits interacting with photons

In this chapter, we discuss a specific example of an elementary building block for the circuit-QED quantum simulators, namely a fluxonium circuit coupled to a superconducting resonator. In contrast to the building block mentioned in Chapter 1 involving a Cooper-pair box, the fluxonium cannot easily be reduced to a simple two-level system. Even when the fluxonium is only operated in the subspace of its two lowest levels, observables such as dispersive shifts and Kerr nonlinearity acquire contribution by many low-lying levels. Thus, a theoretical description of a multi-level qudit\(^1\) coupled to the superconducting resonator is developed. In particular, we use a perturbation formalism (Schrieffer-Wolff transformation) to study the dispersive regime where the qudit level spacing and photon frequency are strongly detuned from each other. Such a dispersive regime and the corresponding perturbation formalism will also be generalized to the lattice case later in Chapter 4.

2.1. Introduction

As a member of the superconducting qubit family, the fluxonium qubit\(^6\) is composed of a small Josephson junction shunted by a large Josephson junction array (see Fig. 2.1). In this design, the junction array plays the role of a kinetic “super-inductance”. The super-inductance has a large value of inductance \((L > 100\text{nH})\)– so large that it is impossible to achieve with a

\(^1\)A qudit is a multi-level generalization of a qubit, where quantum information can be stored.
coiled wire\footnote{This is due to the parasitic capacitance in any coil. The inductance to capacitance ratio is fundamentally limited by the small value of the fine structure constant\cite{64}.} The fluxonium circuit is well described by the effective super-inductance model,

\begin{equation}
H_f = 4E_C N^2 - E_J \cos \varphi + \frac{1}{2}E_L (\varphi + 2\pi \Phi_{\text{ext}}/\Phi_0)^2.
\end{equation}

Here, the operator $\varphi$ describes the phase difference across the small junction; its conjugate operator $N = -i \frac{d}{d\varphi}$ describes the dimensionless charge on the small junction. The super-inductance model successfully reproduces most of the eigenstates and corresponding transitions observed in the experiment\cite{65}. Detailed analysis of the full model which takes into account the phase and charge variables across each junction in the array can be found in Ref.\cite{22}.

The fluxonium circuit has a rich level structure, which varies according to the various parameters in the Hamiltonian\footnote{This is due to the parasitic capacitance in any coil. The inductance to capacitance ratio is fundamentally limited by the small value of the fine structure constant\cite{64}.} i.e. $E_J$, $E_L$, $E_C$, and $\Phi_{\text{ext}}$. Figure\footnote{This is due to the parasitic capacitance in any coil. The inductance to capacitance ratio is fundamentally limited by the small value of the fine structure constant\cite{64}.} shows lowest three energy levels ($E_1$, $E_2$, and $E_3$) of the fluxonium circuit for the parameter values realized in the experiment. The spacing of the energy levels is tunable in situ by the external flux $\Phi_{\text{ext}}$. Here, we define the anharmonicity as $\kappa = (E_3 - E_2) - (E_2 - E_1)$. At $\Phi_{\text{ext}}/\Phi_0 = 1/2$, 1/4 and 0, $\kappa$ is positive, nearly zero, and negative respectively. The anharmonicity $\kappa$ at $\Phi_{\text{ext}}/\Phi_0 = 1/2$ and 0 is comparable to the energy spacing of the lowest two states, $E_2 - E_1$. This flexible tunability renders fluxonium a very useful artificial atom for the purposes of both quantum computation and quantum simulation.

For quantum state manipulation and readout, the fluxonium circuit can be capacitively coupled to a microwave resonator and thus integrated into the circuit QED architecture\cite{7,91}, as shown in Fig.\footnote{This is due to the parasitic capacitance in any coil. The inductance to capacitance ratio is fundamentally limited by the small value of the fine structure constant\cite{64}.} The amplitudes of photon-induced transitions between different energy levels are then determined by the charge matrix elements $N_{ll'} = \langle l | N | l' \rangle$ where $l$ and $l'$ denote...
Figure 2.1. Fluxonium circuit. (a) Image of the fluxonium circuit capacitively coupled to the superconducting resonator. The fluxonium circuit is composed of a small Josephson junction and an array of large Josephson junctions. (b) The effective circuit of the super-inductance model, where the large junction array is replaced by a kinetic super-inductance. The parameters in this model are the charging energy $E_C$ and Josephson energy $E_J$ of the small junction, and the effective inductive energy $E_L$ of the large junction array.

Figure 2.2. (Credit: V. Manucharyan [64]) Low-lying energy levels of the fluxonium circuit used in the experiment, with the external flux at $\Phi_{\text{ext}}/\Phi_0 =$1/2, 1/4 and 0. The black curves represent the potential well $V(\varphi) = -E_J \cos \varphi + \frac{1}{2} E_L (\varphi + 2\pi \Phi_{\text{ext}}/\Phi_0)^2$, with the horizontal and vertical axes representing phase $\varphi$ and energy $E$ respectively. The colored straight lines represent the lowest three energy levels.

the circuit’s eigenstates. For circuits like the Cooper pair box (CPB) in both charging [11, 69] and transmon regimes [54, 92], simple selection rules limiting the one-photon transitions to nearest-neighbor levels ($l \rightarrow l \pm 1$) give a very good approximation. For the fluxonium circuit, this selection rule is absent.
To be concrete, we analyze the situation of the CPB in the transmon regime (transmon qubit). The Hamiltonian is

\begin{equation}
H_t = 4E_C N^2 - E_J \cos \varphi,
\end{equation}

without the presence of the parabolic term in fluxonium, which comes from the shunted super-inductance. The transmon qubit is operated in the regime of \( E_J \gg E_C \). Hence, the charging term, which leads to quantum fluctuation of the phase variable, is relatively small. Therefore the phase variable is well localized at the bottom of the cosine potential well. Thus, one can expand the cosine term order by order in \( \varphi \) and rewrite the transmon Hamiltonian as

\begin{equation}
H_t = 4E_C N^2 + \frac{1}{2}E_J \varphi^2 - \frac{1}{24}E_J \varphi^4 + O(\varphi^6) - E_J.
\end{equation}

The first two terms in the above formula are nothing but a harmonic oscillator, while the third term leads to weak anharmonicity. This leads to the fact that the spectrum and matrix elements of a transmon are very close to a harmonic oscillator. Thus, the charge matrix element, \( \langle l | N | l' \rangle \) of the transmon has a nearest-neighbor selection rule, \( \langle l | N | l' \rangle \sim \delta_{l,l'\pm 1} \) in analogy to the momentum matrix element \( \langle l | p | l' \rangle \) of a harmonic oscillator. Here, \( p = -i \frac{d}{dx} \) is the momentum operator, which can be mapped to the charge operator \( N \), when mapping the position operator \( x \) to the phase variable \( \varphi \). However, the fluxonium Hamiltonian does not possess such similarity to a harmonic oscillator. In fact, as seen in Fig. 2.2 the spectrum can be quite anharmonic. Figure 2.4 also shows that the charge matrix elements \( \langle l | N | l' \rangle \) indeed do not obey a nearest-neighbor selection rule.\(^3\)

\[^3\)The level structures and selection rules of the CPB in the charging and transmon regimes, and of the fluxonium circuit are summarized in Table 2.1.
As a result, the usual Jaynes-Cummings model, which consists of a two-level qubit and a photon mode, is not sufficient to describe the coupling of fluxonium to microwave photons.

\[ \sum_l \chi_l |l\rangle \gg |l\rangle \]

Figure 2.3. (a) General scheme of circuit quantum electrodynamics with a charge-voltage coupling between one (or several) resonant mode(s) and a superconducting circuit acting as a qudit. Relevant examples of such artificial atoms are (b) the Cooper pair box in the charging and transmon regime, and (c) the fluxonium device.

Table 2.1. Level structure and selection rules for three different circuit QED systems, when coupling to a single resonator mode. For the transmon, \( \omega_p = \sqrt{8E_JE_C} \) denotes the plasma oscillation frequency, and \( E_J \) and \( E_C \) are the Josephson and charging energy, respectively. Here we set \( \hbar = 1 \) and, in the following, only deviate from this convention when discussing concrete experimental parameters and observables. For the Cooper pair box in both the charging \( (E_J \ll E_C) \) and transmon \( (E_J \gg E_C) \) regime, simplifying selection rules apply. No simple selection rules exist for the fluxonium device. (Abbreviations used: TLS – two-level system, MLS – multi-level system.)

<table>
<thead>
<tr>
<th>sc qubit</th>
<th>level structure</th>
<th>selection rules</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPB/charge</td>
<td>( \epsilon_0 = 0, \epsilon_1 ) (treated as TLS)</td>
<td>( g_{10} = g_{01} = g ) other ( g_{ll'} = 0 )</td>
</tr>
<tr>
<td>CPB/transmon</td>
<td>( \epsilon_l \simeq l \omega_p ) (-E_C(l^2 + l)/2) (weakly anharmonic MLS)</td>
<td>( g_{l,l\pm1} \neq 0 ) other ( g_{ll'} \simeq 0 )</td>
</tr>
<tr>
<td>fluxonium</td>
<td>( \epsilon_l ) (anharmonic MLS)</td>
<td>no simple selection rules</td>
</tr>
</tbody>
</table>
Figure 2.4. Charge matrix elements of the fluxonium circuit. (a) Magnitude of the charge matrix elements $|\langle l' | N | l \rangle|$ between fluxonium states $l$ and $l'$, at external magnetic flux $\Phi_{\text{ext}} = 0.4\Phi_0$. The parameters used are chosen in agreement with the experiment (footnote 8) and obtained by numerical diagonalization. Note the absence of the nearest-neighbor selection rules. (b) The magnitude of the charge matrix elements between ground state and low-lying excited states, plotted as a function of external magnetic flux. There exists even/odd selection rule on zero and half-integer flux quantum due to parity constraint. Away from these special flux values simple selection rules are absent. The vertical dashed line marks the flux value $0.4\Phi_0$ used in the plot shown in (a). The numerical methods used for exact diagonalization can be found in Appendix A.
Therefore, we discuss a generalized Jaynes-Cummings model which describes a multi-level qudit coupled to resonator modes. As we will see, higher levels of the qudit actually contribute to the virtual transitions and hence affect the dispersive shifts and nonlinearity in the dispersive regime, even when the qudit is only operated in the subspace of its ground and first-excited states. This leads to interesting and useful features including the surprisingly large and experimentally observed dispersive shifts (~5MHz) over a wide external flux range, despite strong detuning between the lowest fluxonium energy splitting and the photon frequency. Another interesting feature is the flux-tunable Kerr nonlinearity of photons when coupled to the fluxonium circuit, which can be captured by fourth-order perturbation theory and match spectroscopic measurements. The tunability of the Kerr nonlinearity of photons is particularly useful in the context of quantum simulation with interacting photons, which is studied in detail in Chapters 4 and 5.

In Sec. 2.2, we present the generalized Jaynes-Cummings model aimed at the systematic description of a generic circuit QED system consisting of a multi-level qudit coupled capacitively to one or multiple harmonic modes. In Sec. 2.3, we derive the general expression of the effective Hamiltonian describing the dispersive regime up to (and including) terms of fourth order in the coupling between qudit and the harmonic modes. We verify that our results correctly reproduce the well-known expressions for the dispersive regime of the Cooper pair box in the charging and transmon regime. In Sec. 2.4, we then apply our results to the fluxonium system where, different from the Cooper pair box case, the lack of selection rules allows for a large number of terms to contribute to the dispersive shifts. We compare our theoretical predictions

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4Here we consider the more general situation that the qudit is coupled to multiple resonator modes. This will be helpful for later discussions when two harmonic modes are considered.
with the data from reflection and spectroscopy experiments obtained previously \[64, 65, 66\] by the Yale group. We provide a summary in Sec. 2.5.

### 2.2. Generalized Jaynes-Cummings model for fluxonium qubits

The Jaynes-Cummings model, which treats the “atomic” part as a two-level system, is no longer sufficient to describe the coupled system of fluxonium and resonator. Instead, we use the generalized Jaynes-Cummings (Rabi\[^5\]) model \(H = H_0 + V\) to describe the coupled system with

\[
H_0 = \sum_j \omega_j a_j^\dagger a_j + \sum_l \epsilon_l |l \rangle \langle l |
\]

\[
V = \sum_j \sum_{l,l'} g_{j;ll'} |l \rangle \langle l' | (a_j + a_j^\dagger).
\]

Here, \(H_0\) is the bare Hamiltonian of the uncoupled resonator-qubit system, including multiple photon modes. The second term \(V\) represents the generalized JC coupling between the resonator and the qubit. Here, \(a_j (a_j^\dagger)\) is the usual annihilation (creation) operator for a photon in mode \(j\).

The interaction term describes the coupling between the relevant charge variable of the qudit, \((2e)N\), and the electric voltage of the resonator at the qudit position, \(V_j = V_j^{\text{rms}} (a_j^\dagger + a_j)\). The resulting coupling coefficients are given by

\[
g_{j;ll'} = g_j \langle l | N | l' \rangle,
\]

where \(g_j = 2e \beta_j V_j^{\text{rms}}\) abbreviates the qudit-independent part of the coupling strength and \(\beta_j\) is a dimensionless capacitance ratio, typically of order unity \[54\].

\[^5\]It might be more accurate to call this model a generalized Rabi model, since no rotating-wave approximation is applied and counter-rotating terms are not dropped.
The above Hamiltonian provides a generic model for simple, charge-coupled circuit QED systems. Adopting the appropriate qudit energy spectrum \( \{ \epsilon_l \} \) and coupling parameters \( g_{j,l,l'} \), Equations (2.4) and (2.5) may model, for instance, circuit QED systems based on the Cooper pair box, the transmon [54, 92], or the recently developed fluxonium device [65]. All three examples are summarized in Table 2.1. Note that the interaction will, in general, \textit{not} conserve the overall excitation number \( \sum_j a_j^\dagger a_j + \sum_l |l\langle l| \) unless special selection rules restrict the coupling \( g_{j,l,l'} \) to nearest-neighbor qudit levels and rotating wave approximation (RWA) is assumed.

\section*{2.3. Derivation of effective Hamiltonian in the dispersive regime}

In general, the qudit-photon interaction \( V \) facilitates transitions \( |l\rangle \rightarrow |l'\rangle \) between qudit states accompanied by the emission or absorption of photons. The dispersive regime of circuit QED [7, 9, 10, 75, 114] describes the situation when such transitions are suppressed due to large detuning between the transition frequencies and the relevant photon mode frequencies. The perturbative treatment of the coupling \( V \), appropriate when the energy mismatch is large compared to the coupling strength, has found many applications in different branches of physics and, depending on context, is known under several names including van-Vleck perturbation theory [103] and Schrieffer-Wolff transformation [93].

The perturbative treatment is illustrated most simply for an energy spectrum featuring a large gap between two groups of unperturbed states. By construction of an appropriate canonical transformation, one obtains an effective Hamiltonian in which the weak interaction between states above the gap to those below, is eliminated in favor of dressed states with energies slightly shifted relative to the unperturbed ones. The presence of two subspaces separated by a single
large gap, however, is not a necessary requirement for the approach, and the typical situation of
the dispersive limit in circuit QED indeed differs from that simple setting. Here, each unper-
turbed state $|n_l\rangle_0$ with $n = (n_1, n_2, \ldots)$ denoting the set of photon numbers in various modes
and $l$ the qudit state, forms its individual subspace as long as transitions from qudit state $l$ to
other states $l'$ remain sufficiently detuned from photon frequencies. The contribution of several
qudit transitions to each level shift can make the physics of the dispersive regime quite
rich. In part, this is already true for transmon-based circuit QED systems, where the $l = 2$
state gives rise to enhanced level shifts in the straddling regime [54]. Even more interesting
features emerge in the dispersive regime of the fluxonium device, which we discuss in detail in
subsection 2.4. Based on the lucid description given by Cohen-Tannoudji et al. [17], we next
summarize the systematic procedure for obtaining the effective dispersive Hamiltonian of the
circuit QED model specified in Eqs. (2.4) and (2.5).

As a necessary condition for the validity of the dispersive approximation, all one-photon
transitions among low-lying qudit states must be strongly detuned from the harmonic mode
frequencies. To formulate this condition quantitatively, we introduce compact notation for tran-
sition energies and detunings: $\epsilon_{ll'} \equiv \epsilon_l - \epsilon_{l'}$ abbreviates the energy released in the qudit transition
$l \rightarrow l'$ (note that $\epsilon_{ll'}$ is negative when $l' > l$), and $\Delta_{j, l, l'} \equiv \epsilon_{ll'} - \omega_j$ denotes the detuning between
this transition and resonator mode $j$. In this notation, the condition reads

$$|\Delta_{j, l, l'}| \gg |g_{j, l, l'}|\sqrt{n_j + 1},$$

where the relevant photon numbers are typically restricted to $n_j = 0$ (assuming dilution refrig-
erator temperatures $k_B T \ll \omega_j$), but may reach higher values when the system is driven with
microwave tones.
Condition (2.7) motivates the perturbative treatment of the interaction $V$ which couples the unperturbed $H_0$ eigenstates $|nl\rangle_0$. Each eigenstate of $H$ is a dressed state with the majority of all probability amplitudes in a single state $|nl\rangle_0$. As a result, the previous labeling of states can be maintained and dressed eigenstates be denoted by $|nl\rangle = e^{-iS} |nl\rangle_0$. The diagonalization of $H$, up to a specified order in $V$, is achieved by the unitary transformation $H' = e^{iS} H e^{-iS}$. Note that we have the following equivalence identity about the unitary transformation

$$\langle nl | H | nl \rangle = 0 \langle nl | H' | nl \rangle_0.$$  (2.8)

Such an equivalence suggests that finding the exact eigenstates $|nl\rangle$ is equivalent to finding the effective Hamiltonian $H'$, of which the eigenstates are just the unperturbed states $|nl\rangle_0$.

The procedure for obtaining the required hermitian generator $S$ [17] (see Appendix B for details) now follows from the two conditions that $H'$ be diagonal and the generator $S$ be off-diagonal in the unperturbed basis:

$$P_{nl} H' P_{n'l'} \sim \delta_{nn'} \delta_{ll'} \quad \text{and} \quad P_{nl} S P_{nl} = 0.$$  (2.9)

Here, $P_{nl} \equiv |nl\rangle_0 \langle nl|$ is the projector onto a single unperturbed state. Introducing an auxiliary parameter $\lambda$ for counting powers in $V$, one constructs $S = \sum_{m=1}^{\infty} \lambda^m S_m$ and $H' = H_0 + \sum_{m=1}^{\infty} \lambda^m H'_m$ order by order, by comparing with the nested commutator series.

$$H' = e^{iS} H e^{-iS} = \sum_{m=0}^{\infty} \frac{1}{m!} [iS, H]_m \equiv H + [iS, H] + \frac{1}{2!} [iS, [iS, H]] + \cdots.$$  (2.10)

Footnote: Its conjugate is denoted by $0\langle nl|$. Note that the subscript “0” for bare states is suppressed in the text up to Eq. (2.7), but is stated explicitly from here on to distinguish bare from dressed states.

Footnote: See Appendix B and Eq. (B.7) for details.
and enforcing the conditions \( \text{(2.9)} \).

In practice, this procedure quickly becomes cumbersome for terms beyond second order. Since terms of fourth order in the interaction will turn out to be relevant for the dispersive regime of fluxonium, we devise a way to bypass the evaluation of fourth-order nested commutators as follows. Note that there is a natural equivalence between the construction of the generator \( S \) on one hands, and the more ordinary form of time-independent perturbation theory (yielding corrections to energies and states) on the other hand. The two approaches simply differ in whether the basis change to the approximate eigenbasis is carried out as an active or passive transformation. In the first approach, the perturbation governs the generator \( S \) which brings the Hamiltonian into the diagonal form of \( H' \); in the second approach, the perturbation affects the dressed states which one explicitly constructs in the unperturbed basis as \( |nl⟩ = e^{-iS}|nl⟩_0 \).

Fortunately, obtaining higher-order corrections for eigenenergies in the second approach generally does not involve nested commutators. Thus, we first establish the generic structure of \( H' \) up to the desired order, leaving all energy coefficients of individual terms to be determined. We then apply the inverse unitary transformation (cut off at the same order) and obtain the effective Hamiltonian \( H_{\text{eff}} = e^{-iS}H'e^{iS} \). Finally, we employ ordinary perturbation theory to find the eigenenergy corrections and extract from them the undetermined energy coefficients to complete the effective Hamiltonian.

The generic form of \( H' \) is dictated by the conditions from Eq. \( \text{(2.9)} \), and is easily obtained as follows. Note that Eq. \( \text{(2.9)} \) excludes all coupling between different subspaces. Consequently, \( H' \) can be expressed as

\[
H' = \sum_{n,l} P_{nl}H'P_{nl} = \sum_{n,l} E_{nl}P_{nl},
\]

(2.11)
and any operator contributing to $H' = \sum_k H'_k$ must be diagonal in the unperturbed basis, i.e., $P_n H'_k P_n \neq 0$. Evidently, each such contribution can only consist of harmonic-mode number operators and qudit projectors. The resulting general form, after performing the inverse unitary transformation, is

$$H_{\text{eff},k} = \alpha_k \prod_j (a_j^\dagger a_j)^{N_{jk}} \vert l_k \rangle \langle l_k \vert,$$

where $N_{jk} \geq 0$ are integer exponents, $\alpha_k$ is an energy coefficient, and the harmonic oscillator and projection operators are dressed-state operators, i.e.,

$$a_j = e^{iS} a_j e^{-iS} \quad \text{and} \quad \vert l_k \rangle \langle l_k \vert = e^{iS} \vert l_k \rangle_0 \langle l_k \vert e^{-iS}.$$

Since the interaction $V$ is of order one and consists of a sum over operator terms with only one harmonic ladder operator each, the perturbation order of the contribution (2.12) cannot be smaller than the number of ladder operators, i.e., $\lambda \geq 2 \sum_j N_{jk}$. This provides us with the necessary information to obtain the generic structure of the effective Hamiltonian.

**Second-order terms.**—The generic structure of the effective Hamiltonian in second-order perturbation theory is

$$H_{\text{eff}} = \sum_j \omega_j a_j^\dagger a_j + \sum_l \epsilon_l \vert l \rangle \langle l \vert + \sum_{j,l} \chi_{j,l} a_j^\dagger a_j \vert l \rangle \langle l \vert + \sum_l \kappa_l \vert l \rangle \langle l \vert.$$

Here, the third and fourth terms describe dispersive shifts (of ac Stark type) and qudit level shifts (Lamb type). As usual, the ac Stark shifts may manifest as harmonic-mode frequency shifts which depend on the occupied qudit level $l$, $\omega_j \rightarrow \omega_j + \chi_{j,l}$, or as shifts in qudit energies which depend on photon numbers, $\epsilon_l \rightarrow \epsilon_l + \sum_j \chi_{j,l} a_j^\dagger a_j [25, 95]$. Note that terms of the form

$$\sum_j \chi_{j,l} a_j^\dagger a_j$$
\( \Delta \omega_j a_j^\dagger a_j \) corresponding to pure shifts of resonant mode frequencies may be absorbed by letting \( \chi_{j;l} \rightarrow \chi_{j;l} + \Delta \omega_j \). To determine the coefficients \( \chi_{j;l} \) and \( \kappa_l \) we use the ordinary expression for the second-order correction:

\[
E_n^{(2)} = \sum_{n' l'} \left( \langle n l | V | n' l' \rangle \delta_{00} \langle n' l' | V | n l \rangle \right) E_n^{(0)} - E_{n' l'}^{(0)},
\]

where the term \( n' l' = n l \) is to be omitted. For further evaluation, we separate the interaction into photon creation and annihilation terms of the individual modes, \( V = \sum_j (V_j^+ + V_j^-) \) where

\[
V_j^+ = \sum_{l, l'} g_{j;l; l'} a_j^\dagger \langle l' | l \rangle \quad \text{and} \quad V_j^- = (V_j^+)^\dagger.
\]

The product of transition matrix elements in the numerator of Eq. (2.15) selects the combinations \( V_j^+ V_j^- \) and \( V_j^- V_j^+ \), which change the photon number by one and subsequently undo the change. The virtual transitions affecting photon number and qudit levels are illustrated conveniently in the ladder diagram shown in Fig. 2.5. They yield

\[
E_n^{(2)} = \sum_{j, l'} (n_j [\chi_{j; l'} - \chi_{j; l}] + \chi_{j; l'})
\]

for the second-order energy correction, where

\[
\chi_{j; l'} = \frac{|g_{j; l'}|^2}{\Delta_{j; l'}}
\]
Figure 2.5. Second-order ladder diagram showing the contribution of harmonic mode $j$ to the eigenenergy correction. The two interfering paths correspond to virtual transitions which intermediately decrease $(V_j^+ V_j^-)$ and increase $(V_j^- V_j^+)$ the photon number in mode $j$. Without selection rules, summation includes all qudit levels $l_1$. $e_j$ denotes the unit vector for component $j$.

abbreviates partial dispersive shifts. The wanted energy coefficients can now be read off; the resulting expressions are given by

$$\chi_{j;l} = \sum_{l'} (\chi_{j;l'l'} - \chi_{j;l'l}) \quad \text{and} \quad \kappa_l = \sum_{j,l'} \chi_{j;l'l'}.$$  

Note that both expressions include a summation over all qudit levels $l'$. Thus, higher qudit levels – even when unoccupied – may contribute substantially to the dispersive shifts of photon frequencies and lower qudit levels. This fact is more clearly illustrated in a level diagram as shown in Fig. 2.6.

We have verified that the same expressions are obtained with the active Schrieffer-Wolff transformation method, see Appendix B. In addition, one can readily confirm that Eqs. (2.14) and (2.18) correctly reproduce the following well-known results. For the Jaynes-Cummings model with a two-level system (TLS) coupled to a single resonator mode we set $g_{1;l'l'} = g$ for $(l,l') = (1,0)$ or $(0,1)$. For all other choices, $g_{1;l'l'}$ vanishes. With this, one obtains

$$H_{\text{eff;JC}} = \omega a^\dagger a + \frac{\epsilon_{10} + \chi_{01}}{2} \sigma_z + \chi_{01} a^\dagger a \sigma_z + \text{const.}$$
which is in agreement with the standard result [7]. As the second case, we consider the multi-level transmon device coupled to one resonator mode [54]. In this case, there is a selection rule allowing only for coupling of nearest-neighbor transmon levels, i.e. $g_{l,l'} = 0$ for $l' \neq l \pm 1$. With this, we recover

$$H_{\text{eff, transmon}} = \omega a^\dagger a + \sum_l \epsilon_l |l\rangle\langle l| + \sum_l (\chi_{l,l-1} - \chi_{l+1,l}) a^\dagger a |l\rangle\langle l| + \sum_l \chi_{l,l-1} |l\rangle\langle l|,$$

which correctly leads to the expression $(\chi_{01} - \chi_{12}/2)a^\dagger a \sigma_z$ for the ac-Stark term upon projection on the subspace spanned by the $l = 0$ and 1 qudit states [54].
Fourth-order terms.—The fourth-order terms of the Hamiltonian take the form

\[
H_{\text{eff}} = \left[ \text{Eq. (2.14)} \right] + \sum_{j,l} \chi'_{jl} a_j^\dagger a_j | l \rangle \langle l | + \sum_{l} \kappa'_{l} | l \rangle \langle l |
\]

(2.21)

\[
+ \sum_{j,l} \eta_{jl} (a_j^\dagger a_j)^2 | l \rangle \langle l | + \sum_{i \neq j,l} \xi_{ijl} a_i^\dagger a_i a_j^\dagger a_j | l \rangle \langle l |.
\]

Beyond the corrections to terms already present in second order, the fourth-order terms also introduce interaction among harmonic modes of self-Kerr and cross-Kerr type. We denote the corresponding coefficients by \( \eta_{jl} \) and \( \xi_{ijl} \), respectively. For simplicity (and also motivated by the experimental data to be discussed in subsection 2.4) we will focus our discussion on a subset of two harmonic modes and refer to them as a and b modes.

Again, we use ordinary perturbation theory for the fourth-order corrections to the eigenenergies which are given by

\[
E^{(4)}_N = \sum_{M,P,Q} V_{NM} V_{MP} V_{PQ} V_{QN} E_{NM} E_{NP} E_{NQ} - \sum_{M} \left| V_{NM} \right|^2 E_{NM} \sum_{P} \left| V_{NP} \right|^2 E_{NP}.
\]

(2.22)

Here, \( N, M, P \) and \( Q \) are multi-indices of the form \( \{n, l\} \), energy differences in the denominators are given as \( E_{NM} \equiv E^{(0)}_N - E^{(0)}_M \), and matrix elements are abbreviated by \( V_{NN} \equiv \langle N | V | N' \rangle \). Note that additional terms in Eq. (2.22) involving diagonal matrix elements have been dropped since \( V_{NN} = 0 \) in the present case. We next sketch the evaluation of the fourth-order corrections and provide the relevant ladder diagrams.

We denote the two terms on the right-hand side of Eq. (2.22) by (I) and (II) and start with discussing the latter. Term (II) is the product of two factors with a structure nearly identical to
the expression (2.15) from second order and thus evaluates to

\[ E^{(4)(II)}_{nl} = - \sum_{j,l_1} |g_{j;l_1}|^2 \left( n_j [\Delta_j^{-2} - \Delta_{j;l_1}^{-2}] + \Delta_j^{-2} \right) \times \sum_{j',l_2} (n_{j'} [x_{j';l_2} - x_{j';l_2}] + x_{j';l_2}). \]

Expanding this expression, we identify contributions to each of the fourth-order terms given in Eq. (2.21). In addition to the simple poles like \((\epsilon_{ll'} - \omega_j)^{-1}\) which already appear in the second-order energy coefficients, new double and triple poles with the same denominators \((\epsilon_{ll'} - \omega_j)\) emerge.

Next, we turn to term (I) in Eq. (2.22) which cannot be factorized. We classify the contributions from (I) in terms of ladder diagrams. The rules governing these ladder diagrams are as follows.

1. Each ladder step is labeled by \((n_m, l_m)\) specifying the occupation of the harmonic modes and the qudit level.
2. Starting from the right, each subsequent ladder step is related to the previous one by a virtual transition effected by the operator \(V_j^{\pm}\) (label on the arrow).
3. The set of all possible paths is constrained by the condition that the left-most state must coincide with the right-most state \((n, l)\). Thus, each path must contain as many \(V_j^+\) as \(V_j^-\).
4. Each path traversing from right to left gives a contribution involving summation over all intermediate qudit levels \(l_1, l_2, l_3\).
5. The product of matrix elements in the numerator of each term is determined by the sequence of arrow labels in each path. For example, the sequence \(V_1^- V_2^- V_2^+ V_1^+\) results in the product \(g_{1;l_3} g_{2;l_2} g_{2;l_3} g_{1;l_1} l\).
(6) The denominator of each term consists of a product of three energy differences of the form \( E_{n}^{(0)} - E_{n'}^{(0)} \) where \((n', l')\) labels the virtual intermediate states on the inner three ladder steps.

The extraction of the various energy coefficients can further be simplified by noting that the ladder diagrams also allow the inference of the operator structure of the corresponding terms in the effective Hamiltonian. For example, the numerator \( V_{1}^{-}V_{2}^{+}V_{2}^{-}V_{1}^{+} \) is associated with terms of the structure \( a_{1}a_{2}a_{1} = (a_{1}^{+}a_{1} + 1)a_{2}^{+}a_{2} \).

We first treat the single-mode contributions shown in Fig. 2.7(a). For each given mode \( j \), the diagram gives rise to six different paths resulting in terms of the form

\[
(2.23) \quad \sum_{l} \sum_{t_{1},t_{2},t_{3}} \frac{g_{j}t_{3}g_{j}t_{2}g_{j}t_{1}g_{j}t_{1}}{E_{3}E_{2}E_{1}} \text{op}(a_{j}, a_{j}^{\dagger})|l \rangle \langle l |.
\]

The corresponding energy denominators and operators are specified in the table accompanying Fig. 2.7. The first and fourth terms in Fig. 2.7(b) exhibit new poles absent in second-order perturbation theory. In frequency space, these poles occur when the conditions \( \epsilon_{ll_{2}} \pm 2\omega_{j} \) are met and thus signal additional resonances when qudit transitions match the energy of two photons in mode \( j \). We will argue below that such resonances have indeed been observed in previous experiments [64, 65, 66].

With this motivation in mind, we turn to the remaining fourth-order contributions shown in Fig. 2.8. All of them are of dual-mode type, i.e., they include participation of two different harmonic modes in the virtual transitions. For clarity, we label the two modes \( j = a \) and
Figure 2.7. Single-mode 4th-order ladder diagram. (a) Single-mode ladder diagram involving only virtual excitations of mode \( j \). (b) The corresponding table specifies terms according to Eq. (2.23). An additional prime on \( E_2 \) signals exclusion of the term \( l_2 = l \) from the sum over \( l_2 \).

\[
j' = b \neq a \quad \text{in the following. All resulting contributions can be cast into the form}
\]

\[
(2.24) \quad \sum_{l} \sum_{l_1, l_2, l_3} \frac{g_4 g_3 g_2 g_1}{E_3 E_2 E_1} \text{op}(a, a^\dagger, b, b^\dagger) | l \rangle \langle l |.
\]

where \( g_{\nu} = g_{j_{\nu}, l_{\nu}, l_{\nu-1}} \) with \( j_{\nu} \in \{a, b\} \) and \( l_{\nu} \equiv l_0 \equiv l \). The harmonic lowering operators for the two modes are now simply denoted by \( a, b \). All the possible paths are listed in Fig. 2.8 and the corresponding coefficients and operators are summarized in Fig. 2.8(d).

New types of poles arise in the ladder diagrams of Fig. 2.8(b), (c) when one of the resonance conditions

\[
\epsilon_{ll_2} \pm (\omega_a + \omega_b) = 0 \quad \text{or} \quad \epsilon_{ll_2} \pm (\omega_b - \omega_a) = 0
\]

is met. Such resonances occur whenever a qudit transition matches either the energy required for placing one photon each in mode \( a \) and mode \( b \), or the energy required to convert an \( a \) photon...
Figure 2.8. Dual-mode ladder diagram. (a)–(c) Dual-mode ladder diagrams complete the contributions to fourth-order eigenenergy corrections. For a given selection of two modes, labeled $a$ and $b$, each diagram has an associated diagram obtained by interchanging the roles of $a$ and $b$. Only for (a) one finds that label interchange $(a \leftrightarrow b)$ yields an identical expression for the resulting contribution. (d) Table detailing the resulting contributions according to Eq. (2.24).

into a $b$ photon. We find that these additional resonances indeed lead to observable effects and can be pinpointed in the data from previous experiments [64, 65, 66], as we will discuss in the following section.
2.4. Dispersive shifts and spectroscopic measurements

Equipped with the general expressions for the effective Hamiltonian in the dispersive regime up to fourth order, we now study their concrete application to the fluxonium circuit. The fluxonium device is of particular interest in this context since experiments have shown surprisingly large dispersive shifts \[66\] and, as we will see, transitions between fluxonium states are not strongly restricted by selection rules. For fluxonium, the flux-dependent eigenenergies \(\epsilon_l(\Phi_{\text{ext}})\) and corresponding eigenstates \(|l\rangle\) are thus determined by the Hamiltonian Eq. (2.1).

Numerical diagonalization serves as a useful approach for the parameter values realized by the experiment \[65, 66\]. Employing the harmonic oscillator basis (which diagonalizes \(H_f\) for \(E_J = 0\)) and taking the necessary precautions for convergence with respect to the basis truncation, we obtain the energy spectrum and eigenstates and calculate the charge matrix elements \(\langle l | N | l' \rangle\) entering the coupling parameters \(g_{jl;ll'}\). For the interested reader, we provide details of the numerical diagonalization scheme in Appendix A. Figure 2.4 shows representative results for the charge matrix elements obtained in this way, using model parameters which match experimental parameters.

In previous circuit QED experiments \[65, 66\] the fluxonium device is coupled capacitively to one microwave resonator. To account for an additional harmonic mode observed in the experiment, we include coupling to two relevant harmonic modes in the generalized JC Hamiltonian. The first, associated with raising and lowering operators \(a^\dagger, a\), will describe the fundamental

---

8Experimental parameters: \(E_J/h = 8.91\,\text{GHz}; E_C/h = 2.48\,\text{GHz}; E_L/h = 0.53\,\text{GHz}; \omega_a/2\pi = 8.18\,\text{GHz}; \omega_b/2\pi = 10.78\,\text{GHz}; g_a/h = 0.18\,\text{GHz}; g_b/h = 0.39\,\text{GHz}.\) All the parameters are fit from the spectrum in fig. 2.12(a), by diagonalizing the coupled cQED system described by Eq. (2.4) and Eq. (2.5) (including the fluxonium qudit and the two harmonic modes).

9We speculate that this mode in fact represents one of the difference modes of the Josephson junction array, see D. G. Ferguson et al., Physical Review X, 3, 1, 011003 (2013) 22.
mode of the resonator, with frequency $\omega_a$. In the experiment, the resonator supports quarter-wavelength modes only. The lowest harmonic thus has a much higher frequency of $3\omega_a$, and we will neglect the corrections of higher harmonics in the following. The second mode will represent the observed array mode with frequency $\omega_b$ and coupling strength $g_b$ (both parameters are fit from spectrum in Fig. 2.12a and shown in footnote 8), and we will denote its raising and lowering operators by $b^\dagger$, $b$.

The generic form of the effective Hamiltonian derived in the previous section [see Eq. (2.21)] now takes the concrete form

\begin{equation}
H_{\text{eff}} = \omega_a a^\dagger a + \omega_b b^\dagger b + \sum_l (\epsilon_l + \kappa_l + \kappa'_l) |l\rangle\langle l| + \sum_l |l\rangle\langle l| \left[ (\chi_{a;l} + \chi'_{a;l}) a^\dagger a \\
+ (\chi_{b;l} + \chi'_{b;l}) b^\dagger b + \eta_{a;l}(a^\dagger a)^2 + \eta_{b;l}(b^\dagger b)^2 + \xi_{ab;l} a^\dagger a b^\dagger b \right],
\end{equation}

where the energies of fluxonium levels as well as their coupling strengths are tunable by the external magnetic flux, $\epsilon_l = \epsilon_l(\Phi_{\text{ext}})$ and $g_{j;l'j'} = g_{j;l'j'}(\Phi_{\text{ext}})$. The ordinary ac-Stark shifts $\chi_{a;l}$ were given in Eq. (2.18) and are now accompanied by additional fourth-order contributions. Fourth-order terms are also responsible for the interaction terms of Kerr type given by $\eta_{a;l}(a^\dagger a)^2 |l\rangle\langle l|$ (self-Kerr) and $\xi_{ab;l} a^\dagger a b^\dagger b |l\rangle\langle l|$ (cross-Kerr). These terms induce additional nonlinearity and result in dependence of the photon frequencies on the occupation numbers $n_a$ and $n_b$. The effective Hamiltonian for the dispersive regime of the fluxonium circuit enables us to study the two central types of measurements performed in Refs. [65, 66], and [64].
2.4.1. Measurements in the dispersive regime

The first measurement type corresponds to direct homodyne detection of the reflected amplitude. It employs a single microwave tone with frequency fixed close to the bare resonator frequency, and records the voltage of the reflected signal as a function of magnetic flux. This measurement primarily probes the dispersive shift of the resonator frequency (i.e., the \( \chi_a \) mode) given by \( \chi_{a;l} \) to second order, and by

\[
\mu_{a;l}(n_a, n_b) \equiv E_{n_a+1,n_b;l} - E_{n_a,n_b;l} - \omega_a = \chi_{a;l} + \chi'_{a;l} + (2n_a + 1)\eta_{a;l} + n_b\xi_{ab;l}
\]

when including fourth order corrections. Here, the energies \( E_{n_a,n_b;l} \) are obtained as the eigenvalues of the effective Hamiltonian, Eq. (2.25). We assume that the fluxonium circuit occupies a fixed level \( l \), where usually the ground state \( l = 0 \) is the appropriate state maintained during the measurement. Note that the Kerr terms in fourth order lead to an additional dependence of dispersive shifts on the excitations numbers \( n_a \) and \( n_b \).

The second measurement type corresponds to two-tone spectroscopy and probes the fluxonium transition frequencies via the \( l \) dependence of the resonator shift. Specifically, the first tone with frequency \( \omega_{d1} \) close to the bare resonator frequency is similar to the tone of the previous measurement type. As an alternative to the reflected amplitude, the phase shift \( \theta \) of the reflected tone may be recorded. The key to probing the fluxonium transition frequencies lies in the application of a second drive tone, the frequency of which, \( \omega_{d2} \), is varied over a wide range with the goal of inducing Rabi oscillations between the ground state and an excited state of the fluxonium circuit. The transfer of probability amplitude to a higher level is accompanied by a change in the dispersive shift of the resonator. In the simplest case, spectroscopy probes the
corresponding change in the dispersive shift given by \( \chi_{a;l} - \chi_{a;0} \) and \( \mu_{a;l} - \mu_{a;0} \) in second and fourth order, respectively.

The detected phase shift \( \theta_l \) has a characteristic dependence on the detuning between drive frequency \( \omega_d \) and the effective resonator frequency \( \omega_a + \chi_{a;l} \) (or \( \mu_{a;l} \)). To leading order, it follows the characteristic form \( \theta_l \approx 2 \arctan(\frac{2Q}{\omega_a} [\omega_d - \omega_a - \chi_{a;l}]) \).

(2.27)

Here, \( Q \) is the quality factor of the resonator and \( \chi \) may be replaced by \( \mu \) when considering fourth-order corrections.

In our subsequent discussion of direct homodyne detection and spectroscopy, the pole structure of the shifts \( \chi_{a;l} \) and \( \mu_{a;l} \) will play a crucial role. Poles are associated with resonances between fluxonium transitions and harmonic mode excitations, and signal the breakdown of perturbation theory within some frequency window centered at the pole. Since fluxonium levels are tuned by varying the external magnetic flux \( \Phi_{\text{ext}} \), frequency windows will correspond to flux windows in the experiments to be discussed next.

2.4.2. Direct homodyne detection of reflected signal

The specific quantity observed in direct homodyne detection is the quadrature voltage of the reflected signal \( [64] \). This voltage can be expressed in terms of the phase shift via

(2.28) \[ V = A \cos(\theta + \theta'_0) + C \approx A \cos(B\chi_{a;l} + \theta_0) + C. \]

Here, \( \theta_0 \) and \( \theta'_0 \) are offset phase shifts which may be present in experimental data, \( A \) is the amplitude of the reflected signal and \( C \) a constant voltage offset. The approximation in the
second step of Eq. (2.28) is obtained by Taylor expansion of Eq. (2.27) for the drive close to resonance, i.e., $|\omega_d - \omega_a - \chi_{a;0}| \ll \omega_a$.

We begin our comparison of theory with the experimental data from Ref. [65] with the expressions obtained in second-order perturbation theory. The predicted dispersive shift of the resonator $\chi_{a;0}$ (while maintaining the $l = 0$ ground state) is shown in Fig. 2.9(a). Its magnitude is of order 1 to 10 MHz except in the immediate vicinity of the poles where the fluxonium 0-1 transition crosses the resonator frequency (at flux values $\Phi_{\text{ext}}/\Phi_0 \approx \pm 0.06$).

Using Eq. (2.28), the dispersive shift is converted to homodyne voltage. We adjust the parameters $A$, $B$, $C$ and $\theta_0$ to minimize the mean-square deviations over the magnetic flux range $\Phi_{\text{ext}}/\Phi_0 \in [-0.3, 0]$, again assuming occupation of the fluxonium ground state only. We
compare the resulting fit with the experimental data in Fig. 2.9(b) and find good agreement in the mentioned flux range with the exception of the small peak-dip structure at $\Phi_{\text{ext}}/\Phi_0 \approx \pm 0.15$ [circled region in Panel (b)]. Our consideration of fourth-order corrections below will account for this feature. More significant deviations occur in the flux ranges close to half-integer $\Phi_{\text{ext}}/\Phi_0$. As we will see, fourth-order corrections from the effective Hamiltonian (2.25) alone do not lead to a satisfactory resolution, and we will discuss possible culprits for the persistence of deviations in this region.

As one cause for deviations, we note that the fluxonium 0-1 transition reaches a minimum frequency close to 300 MHz at half-integer flux [see Fig. 2.10(d)]. For a typical temperature of $T = 20$ mK = 0.42 $h$ GHz/$k_B$, thermal excitation of the $l = 1$ level indeed becomes relevant. (Thermal occupation of higher states $l > 1$ remains negligibly small.) We account for thermal excitation under the simplifying assumption that the measurement probes a statistical mixture of the lowest two fluxonium states with simple Boltzmann weights. In this case, the thermally averaged value of the dispersive shift of the resonator is given by

$$\langle \mu_{a;l}(n_a, n_b) \rangle = \frac{\mu_{a;0}(n_a, n_b) + e^{-\epsilon_{10}/k_B T} \mu_{a;1}(n_a, n_b)}{1 + e^{-\epsilon_{10}/k_B T}},$$

which we use for the remainder of this subsection. We expect thermal effects only to be significant for the flux range $0.35 \leq |\Phi_{\text{ext}}/\Phi_0| \leq 0.5$; outside this range, $\epsilon_{10}$ exceeds 2 GHz and thermal excitations of the fluxonium device should be negligible.

We now turn to the discussion of fourth-order corrections to the dispersive shifts. In Fig. 2.10(a), (b) and (c), we compare the same experimental data for the homodyne signal with the theoretical calculations which now include all fourth-order corrections and take into account thermal averaging. Specifically, we calculate the homodyne voltage [Eq. (2.28)] using the same
Figure 2.10. Homodyne voltage of reflected microwaves: comparison between experimental data from [65] and fourth-order theory for dispersive shifts, thermal averaging over fluxonium levels according to Eq. (2.29) included ($T = 20$ mK). (a) Theory curves show dispersive shifts of the resonator frequency for occupation numbers $n_a = n_b = 0$ and $n_a = 1$, $n_b = 0$ as indicated. The position of the additional pole at $\Phi_{\text{ext}}/\Phi_0 \approx \pm 0.15$ is in good agreement with that of the peak-dip structure observed in the experiment. (b) For mean photon number $\bar{n}_a = 0.05$ the theory prediction based on Eq. (2.31) also reasonably matches the amplitude of the peak-dip feature. (c) Additional poles are predicted if the b mode associated with the array is occupied. In each panel (a)–(c), significant deviations persist close to half-integer $\Phi_{\text{ext}}/\Phi_0$. (d) Fluxonium transition and harmonic mode frequencies, as specified by labels. Vertical dashed lines show alignment of resonances with corresponding poles in dispersive shifts and experimental features.
Figure 2.11. Level diagram illustrating a two-photon vacuum Rabi splitting. In this diagram, horizontal solid lines represent bare fluxonium levels which are coupled via a single photon mode. Here, the bare states with \( n_a = 0, l = 4 \) and \( n_a = 2, l = 0 \) are degenerate and coupled by an effective two-photon transition. The resulting two-photon vacuum Rabi splitting is represented by the dashed lines.

fit parameters as above and replace \( \chi \rightarrow \langle \mu \rangle \). For easy reference of resonances, panel (d) shows the fluxonium transition frequencies as well as integer combinations of the harmonic frequencies \( \omega_a \) and \( \omega_b \). Relevant resonances are circled and labeled by roman numerals. Their alignment with the corresponding poles in (a)–(c) is indicated by vertical dashed lines.

Figure 2.10(a) shows the thermally averaged homodyne voltage for the case of negligible harmonic mode excitations, \( n_a = 0, n_b = 0 \), and for the case of one initial excitation in the resonator mode, \( n_a = 1, n_b = 0 \). This choice of occupation numbers is motivated by the estimate of \( \langle n_a \rangle \approx 0.01 \) as given in Ref. [65]. In the flux region \( 0 \leq |\Phi_{\text{ext}}/\Phi_0| \leq 0.35 \), fourth-order contributions to the dispersive shift with initial state \( n_a = 0 \) have no significant effect as compared to the second order results [Fig. 2.9(b)]. The dispersive shift applicable to the \( n_a = 1 \) state, however, does show an additional pole close to \( |\Phi_{\text{ext}}/\Phi_0| \approx 0.15 \) labeled by \( \{v\} \) in Fig. 2.10(a). As indicated in panel (d), this pole occurs due to a resonance between two resonator photons, \( 2\omega_a \), and the 0-4 fluxonium transition, \( \epsilon_{40} \) which we illustrate in Fig. 2.11.
Specifically, the pole in $\mu$ originates from a fourth-order term in the effective Hamiltonian, which is associated with the $V_a^+ V_a^+ V_a^- V_a^-$ path of the ladder diagram [Fig. 2.7]:

$$\sum_{l_1,l_2} g_{a;0 l_1} g_{a;l_2} g_{a;l_1} g_{a;0 l_2} (\omega_a + \epsilon_{0 l_1})(2\omega_a - \epsilon_{40})(\omega_a + \epsilon_{0 l_1}) n_a (n_a - 1) |0\rangle \langle 0|.$$  

Note that this term vanishes for $n_a = 0$ or $n_a = 1$. Hence, according to Eq. (2.26) it contributes to $\mu_{a,0}(n_a = 1, n_b)$ which involves photon absorption $n_a = 1 \rightarrow 2$ but not to $\mu_{a,0}(n_a = 0, n_b)$ where photon absorption occurs as $n_a = 0 \rightarrow 1$. This fact is easily visible in the two theory curves shown in Fig. 2.10(a). The flux position of the pole is in excellent agreement with a similar feature in the experimental data. We note that this resonance also manifests as the two-photon vacuum Rabi splitting illustrated in Fig. 2.11, with splitting size $2\sqrt{2} \sum l' g_{a;0 l'} g_{a;l'} / \Delta_{a;0}$ (see Appendix C for derivation). As opposed to the usual vacuum Rabi splitting, the two-photon splitting is proportional to $g_a^2$ rather than $g_a$. As a direct consequence of the absence of strict selection rules for fluxonium, the summation of contributions from multiple intermediate states $l'$ can lead to a sizable splitting.

To compare the amplitude of the pole feature in Fig. 2.10(b) with the experimental reflection data, we show the weighted average of the dispersive shifts for $n_a = 0$ and $n_a = 1$. We parametrize the respective weights $P_0$ and $P_1 = 1 - P_0$ (probabilities for the two initial resonator states) in terms of the mean photon number $\bar{n}_a = 1 - P_0$. The weighted average is given by

$$\bar{\mu}_a(\bar{n}_a) = P_0 \langle \mu_{a,0}(0,0) \rangle + (1 - P_0) \langle \mu_{a,1}(1,0) \rangle.$$
For a mean photon number of $\bar{n}_a = 0.05$, slightly higher than the value 0.01 reported in Ref. [65], we find good agreement between theory and experiment for the amplitude of the resonance $\{v\}$.

In summary, for the flux region $0 < |\Phi_{\text{ext}}/\Phi_0| \leq 0.3$ we find very good agreement between theoretical prediction and the experimental data for the dispersive shifts, including the positions and amplitudes of the two resonances $\{v\}$ and $\{vi\}$. In the flux region closer to half-integer $\Phi_{\text{ext}}/\Phi_0$, however, agreement between experimental data and theory is weaker. As seen in Fig. 2.10(a), (b), the poles $\{ii\}$ and $\{iii\}$ due to resonances of $\epsilon_{40}$ and $\epsilon_{10}$ with $2\omega_a$ and $\omega_b - \omega_a$, respectively, do not quantitatively match the experimental data in this flux region, which are dominated by a pronounced minimum at $|\Phi_{\text{ext}}/\Phi_0| \approx 0.38$. The resonance features in the experimental data near $|\Phi_{\text{ext}}/\Phi_0| \approx 0.325$ and 0.44 are absent in the calculated dispersive shifts of panels (a) and (b). Vice versa, the pole $\{i\}$ predicted by theory has no correspondence in the experimental data. We next discuss the effects of b mode occupations, which could give partial explanations for some of the mismatches.

In panel (a) and (b), amplitudes predicted for the resonances $\{ii\}$ and $\{iii\}$ are dramatically smaller than features observed in the experiment at corresponding flux values. While thermal excitation of the b mode can be ruled out due to the large gap between the resonant frequency $\omega_b/2\pi = 10.79$ GHz and the frequency 0.42 GHz associated with a temperature of $T \sim 20$ mK, it is instructive to inspect the effects of non-equilibrium excitations of this mode. For this purpose, Fig. 2.10(c) shows the homodyne voltage in the presence of one b mode, as obtained from the dispersive shift $\langle \mu_{a,d}(0, n_b = 1) \rangle$. As an important result of this excitation, the amplitude of resonance $\{iii\}$ is amplified significantly. The enhancement of the resonance stems from four
terms. As an example, we write down the expression for one of them as

\[
\sum_{l_1,l_3} g_{a;0l_1} g_{b;l_1} g_{b;1l_3} g_{a;l_3} (n_a + 1) n_b \left( -\omega_a + \epsilon_{0l_1} \right) \left( \omega_b - \omega_a - \epsilon_{1l_3} \right) \left( -\omega_a + \epsilon_{0l_3} \right) |0\rangle \langle 0|
\]

which corresponds to the \( V_a^- V_b^+ V_b^- V_a^+ \) path. The other three terms come from the paths \( V_b^+ V_a^- V_a^- V_b^- \), \( V_b^+ V_a^- V_b^- V_a^+ \) and \( V_a^- V_b^+ V_b^+ V_b^- \), all of which also have the operator form \((n_a + 1)n_b|0\rangle \langle 0|\) and the specific denominator \((\omega_b - \omega_a - \epsilon_{10})\). The four terms are all associated with the dual-mode ladder diagram in Fig. 2.8(b) and (c) (including terms with \( a \leftrightarrow b \) exchange). All of these terms indeed vanish for \( n_b = 0 \) and hence did not contribute to the previous results in panels (a) and (b). It is thus possible that non-equilibrium \( b \) mode excitations are partly responsible for the deviations between theory and experiment in the half-integer flux region.

By a similar mechanism, \( b \) mode excitations also lead to an additional predicted resonance \{iv\} at a flux position fairly close to the resonance feature in the experimental data at \(|\Phi_{ext}/\Phi_0| \approx 0.325\). According to theory, this resonance occurs whenever the array mode excitation \( \omega_b \) matches the fluxonium 1-3 transition \( \epsilon_{31} \). The corresponding term in the effective Hamiltonian is

\[
\sum_{l_2,l_3} \frac{2 g_{a;13} g_{a;3l_2} g_{b;l_2} g_{b;l_3} g_{b;l_3} (n_a + 1) n_b}{(-\omega_a + \epsilon_{1l_2})(\omega_b - \epsilon_{31})} |1\rangle \langle 1|
\]

associated with the \( V_b^+ V_b^- V_a^+ V_a^- \) and \( V_a^+ V_a^- V_b^+ V_b^- \) paths in the dual-mode ladder diagram of Fig. 2.8(a).
Four both resonances \{iii\} and \{iv\}, we point out that, with occupation number $n_b$ larger than 1, the theoretically predicted poles become larger in a manner inconsistent with the experimental data. Hence, varying the occupation number $n_b$ does not help much to improve the quantitative match between theory and experiment.

In summary, we find that non-equilibrium array-mode excitations may produce significant changes in the dispersive shifts, some of which may point to resonance features observed in the experiment. Without a detailed understanding of the underlying non-equilibrium distribution and its dependence on magnetic flux, however, it is difficult to assess whether this explanation could ultimately give a consistent picture or whether additional array degrees of freedom, breakdown of perturbation theory, or dynamical effects under continuous driving are responsible for the observed deviations.

### 2.4.3. Two-tone spectroscopy

As explained in subsection 2.4.1, two-tone spectroscopy probes the change in the dispersive resonator shift due to induced Rabi oscillations between the fluxonium ground state and another fluxonium state (level $l$). When detected via the change in the phase of the reflected homodyne signal, the relevant observable is given by $\theta_{l0} \equiv \theta_l - \theta_0$ as obtained from Eq. (2.27). This phase difference is encoded by the color scale in Fig. 2.12(a), which shows experimental data from Refs. [65][66], and [64]. The observed transition lines correspond to the fluxonium 0-1, 0-2, 0-3 transitions and to an array-mode with frequency $\omega_b = 10.79$ GHz.

Interestingly, the spectroscopy data does not only reveal the frequencies of relevant transitions but also contains several distinct phase changes along these transition lines. In particular, the phase changes observed in the experiment can be classified into four types. We use
Figure 2.12. (a) Two-tone spectrum. The vertical axis represents the frequency of the sweeping tone, $\omega_d$, and the horizontal axis represents the external magnetic flux. The color-scale represents the phase difference between the ground state and the state $l$ excited by the sweeping tone, namely $\theta_l - \theta_0$, where red represents positive value and blue negative. The three types of color changing (I, II and III) are illustrated and magnified at the lower left corner. The dashed box illustrate a specific color change which is not associated with the above three types. (b) Plot of the nonlinear dispersive shifts $\mu_{a,1}(n_a, n_b) - \mu_{a,0}(n_a, n_b)$, where $n_b = 0$ for all the three curves. The three curves represent shifts with photon occupation $n_a = 0, 4, 9$ respectively. (c) Plot of the nonlinear dispersive shifts $\mu_{a,2}(n_a, n_b) - \mu_{a,0}(n_a, n_b)$, where the choices for occupation numbers $n_a$ and $n_b$ are the same as panel (b). (d) Plot of qudit transition frequencies and harmonic mode frequencies. Horizontal dashed lines represent harmonic frequencies and solid curves represent the qudit frequency differences. The three types of solid curves are used to distinguish transitions starting from level 0, 1, 2 respectively. The circles and squares of the corresponding crossings combined with vertical dashed lines through different panels are used to show alignment of the experimental features with theoretical poles and zero points.
the 0-2 transition line for illustrating these types and refer to the labels and magnified insets in Fig. 2.12(a): type I is an **abrupt red-blue change**, corresponding to a sudden jump from positive to negative phase difference $\theta_{l0}$; type II is a **gradual blue-white-red change**, corresponding to a continuous change of the phase difference from negative to positive values (or vice versa); type III is a **gradual blue-white-blue change**, corresponding to a the phase difference approaching zero and recovering without changing its sign. (In principle, red-white-red color changes may also occur under type IV but are not realized for this particular choice of parameters.)

In the following, we will show that dispersive shifts, when including fourth-order terms, explain these phase changes. The mathematical relation between the dispersive shift and the phase difference is given by

$$\theta_{l0} = 2 \arctan\left(\frac{2Q}{\omega_a}[\omega_{d1} - \omega_a - \mu_{a;d}]\right) - 2 \arctan\left(\frac{2Q}{\omega_a}[\omega_{d1} - \omega_a - \mu_{a;0}]\right).$$

(2.34)

This expression follows from Eq. (2.27) when setting $\omega_d = \omega_{d1}$. Our discussion of the different types of phase changes will be based on identifying magnetic flux values where the phase difference vanishes, $\theta_{l0} = 0$ (type II and III), and flux values where the dispersive shifts have poles such that the phase difference may jump from $\pi$ to $-\pi$ (type I). The first condition is satisfied whenever $\mu_{a;d} - \mu_{a;0} = 0$, the second condition whenever appropriate resonances between fluxonium transitions and harmonic modes occur. We note that in the linear regime of the two arctan functions, the phase difference is simply given by

$$\theta_{l0} = -4Q(\mu_{a;d} - \mu_{a;0})/\omega_a.$$

(2.35)

Thus, in the linear regime, the two-tone spectroscopy serves as a probe of the dispersive shifts.
For comparison with the experimental data, we calculate the nonlinear shifts for the fluxonium transitions $l = 0 \to 1$ and $l = 0 \to 2$, and show the corresponding differences $\mu_{a,1} - \mu_{a,0}$ and $\mu_{a,2} - \mu_{a,0}$ in Fig. 2.12(b) and (c), respectively. In each case, we consider dispersive shifts for different photon numbers $n_a = 0, 4, 9$ to illustrate the dependence of the detected phase response on the power of the microwave probe tone. We use vertical dashed lines with labels to emphasize the alignment of poles and zero points with the corresponding phase changes. According to Eq. (2.35), the color-encoded sign of the phase difference in panel (a) thus corresponds to the sign of $-(\mu_{a,l} - \mu_{a,0})$ in panels (b) and (c), respectively. We compare theoretical and experimental results for the 0-1 and 0-2 transitions in the flux regions $-0.22\Phi_0 \leq \Phi_{\text{ext}} \leq 0$ and $-0.5\Phi_0 \leq \Phi_{\text{ext}} \leq 0$ where experimental data is available [64, 65, 66]. The following discussion is organized according to the three different types of phase changes.

**Type I – abrupt red-blue phase change:**

The only type I phase change in Fig. 2.12 is marked by the vertical line with label \{4\}, and occurs due to a pole appearing in both $\mu_{a,1} - \mu_{a,0}$ and $\mu_{a,2} - \mu_{a,0}$. This pole originates from the fourth order contribution to $\mu_{a,0}$ given in Eq. (2.30) and corresponds to a resonance between two resonator photons and the fluxonium 0-4 transition, $2\omega_a = \epsilon_{40}$, see Fig. 2.12(d). (This is the same resonance that would also give rise to the two-photon vacuum Rabi splitting illustrated in Fig. 2.11.) As noted before in the discussion of the reflection measurements, this pole only occurs when $n_a \geq 1$. As a result, the $n_a = 0$ curves in panels (b) and (c) do not exhibit this pole and the pole becomes more pronounced as the photon number increases. We thus conclude that spectroscopy of the fluxonium transitions, in this case, also reveals information about photon population in the resonator.
Two clarifications are in order. First, the absence of a type I phase change in the 0-2 transition due to the pole in $\mu_{a;2} - \mu_{a;0}$ marked by the vertical line $\{2\}$ falls outside our current discussion: at this flux value, the 0-1 transition is resonant with $\omega_a$ and the discussion of the phase shift would need to include the hybridization of photon and fluxonium excitation. Second, we note that the abrupt phase change close to $\Phi_{\text{ext}} = -0.4\Phi_0$, marked by a dashed box in panel (a), is not associated with a pole and hence not of type I. Since phase changes in the experiment are defined in the interval $[-\pi, \pi]$, such additional phase jumps may simply occur when dispersive shifts become sufficiently large so that the magnitude of $\theta_{l0}$ exceeds $\pi$. These phase discontinuities do not involve sign changes in the dispersive shifts $\mu_{a;l} - \mu_{a;0}$. Indeed, the occurrence of such a phase discontinuity close to half-integer $\Phi_{\text{ext}}/\Phi_0$ is consistent with the large magnitude of the dispersive shifts $\mu_{a;2} - \mu_{a;0}$ predicted by theory in this region. The theoretically predicted pole corresponding to the resonance between $\epsilon_{21}$ and $\omega_a$ is slightly on the left of the dashed box. Close to $\Phi_{\text{ext}} = -0.41\Phi_0$, experimental evidence for the avoided crossing of the two spectral lines (the 0-2 transition and the 0-1 transition shifted by the photon frequency $\omega_a$) with better resolution can be found in Ref. [66].

**Type II – gradual blue-white-red change:**

Gradual phase changes of type II are present in both the 0-1 and the 0-2 transitions and are marked by the vertical line with label $\{5\}$. In both cases, the dispersive shift $\mu_{a;l} - \mu_{a;0}$ ($l = 1, 2$) smoothly crosses through zero so that the phase change is negative for flux values $< -0.18\Phi_0$, reaches zero, and then assumes positive values as $\mu_{a;l} - \mu_{a;0}$ approaches the pole at position $\{4\}$. As shown in panels (b) and (c), the precise zero-point crossing is, in fact, photon-number dependent. We note that the alignment between the predicted crossings for photon numbers as large as $n_a = 9$ is not perfect. Quite likely, this can be attributed to the breakdown
of perturbation theory in the immediate vicinity of poles and hence especially applies to the zero-crossing for $\mu_{a;2} - \mu_{a;0}$. As for the absence of pole $\{4\}$ for $n_a = 0$ discussed above, we also expect the crossing $\{5\}$ to disappear if no resonator photons are present.

An additional phase change of type II is present only in the fluxonium 0-1 transition and is marked by line $\{3\}$ and can be interpreted in a similar manner. Again, we find alignment of the zero crossing with the experimental feature only for rather large photon numbers, see the “$n_a = 9$” curve in panel (b). An experimental study of the power dependence of this phase change could help shed more light on the quantitative comparison with theory.

**Type III–gradual blue-white-blue color change:**

Type III phase changes occur for both the 0-1 and 0-2 transitions, and instances are marked by the vertical dashed lines labeled by $\{1\}$ and $\{3\}$ respectively. In both cases, we observe alignment with poles occurring in the corresponding dispersive shifts. A definite prediction for type III phase changes, however, appears difficult based on the perturbative results. In general, perturbation theory will break down at the position of the pole and will remain unreliable in a certain flux window in its vicinity. As a result, predictions in this case must likely be based on non-perturbative methods and may possibly also have to take into account the dynamical aspect of the two-tone measurement. Qualitatively, the type III phase changes are at least plausible given that the dispersive shifts $\mu_{a;l} - \mu_{a;0}$ are predominantly positive in the direct vicinity of both poles.

2.5. Summary

In conclusion, we have systematically discussed the fluxonium circuit, and its properties when coupled to microwave photons. One unique feature for this device is that its charge
matrix elements are not subject to the nearest-neighbor selection rule. We analyzed the detailed structure of the charge matrix elements and have set up a generalized Jaynes-Cummings model to describe its coupling to photons. The developed perturbation formalism allows one to study the coupled system in its dispersive regime and understand a variety of features observed in the experimental data for transmission and spectroscopy.

We have also presented a systematic treatment of fourth-order corrections to the dispersive regime of circuit QED. The results of this treatment are valid for a generic system consisting of a multi-level qudit capacitively coupled to one or several harmonic modes, and hence apply to a wide class of circuit QED systems. Our treatment, in particular, enables the description of dispersive shifts in systems lacking simplifying selection rules.

We have applied our results to the concrete case of the fluxonium device as realized in recent experiments \[64, 65, 66\]. Using numerical diagonalization, we have obtained the relevant charge matrix elements which confirm the lack of selection rules, and have incorporated them in the perturbative treatment of the dispersive regime, including corrections up to fourth order. The calculated dispersive shifts allow us to compare theoretical predictions with experimental data for homodyne reflection measurements and two-tone spectroscopy from Refs. \[65, 66\], and \[64\].

The absence of selection rules is an important mechanism for producing sizable dispersive shifts, even if the transition of interest is far detuned from the resonator used for readout. For the fluxonium system, our calculations show that dispersive shifts can indeed be as large as 10 MHz even when the corresponding 0-1 fluxonium transition is detuned by almost 8 GHz from the resonator. The lack of selection rules enables a multitude of virtual transitions to contribute to the dispersive shifts. Especially if such higher transition frequencies match photon resonance
conditions, dispersive shifts can be surprisingly large. We also note that the magnitudes of matrix elements are tunable with external magnetic flux, which in turn leads to the tunability of dispersive shifts.

Away from half-integer $\Phi_{\text{ext}}/\Phi_0$, we find good quantitative agreement for the homodyne reflection data with our theory prediction. This agreement also includes a resonance feature in the data which previously remained unexplained. The presence of this resonance indicates a small probability of a photon occupying the resonator, so that its amplitude may be used for extracting the mean photon number. Close to half-integer $\Phi_{\text{ext}}/\Phi_0$, even though we find tentative agreement between the flux positions of several resonance features in experimental data and theory, our calculation does not give a quantitative match. We note that the flux position coincidence of resonances points to non-equilibrium array-mode excitations of unknown origin.

Spectroscopy data of fluxonium samples show unusual phase changes (represented by color variations) along the transition lines. We identify three different types of phase changes, according to abrupt and gradual variations with or without sign change. Our calculations show that these phase changes are closely related to poles and zero points in the dispersive shifts and that their occurrence may sensitively depend on photon numbers in the resonator. Experimental studies of the power dependence of spectroscopy measurements are an interesting future option and may shed additional light on the origin of quantitative deviations between experiment and theory. Our results for spectroscopic phase changes show generally good agreement for the flux positions of such resonances. The prediction of the specific type of the phase change remains challenging since perturbative calculations break down at the positions where resonances occur. Nonperturbative calculations, taking into account the dynamics of the measurement protocol in a Master equation description, may be necessary to obtain such type of predictions
and to improve quantitative agreement. An additional source of quantitative deviations may lie in the presence of additional array modes not included in our description. The spectroscopy data indeed shows additional levels, especially close to $|Φ_{ext}/Φ_0| ≃ \frac{1}{2}$, which warrant further investigation.

For both types of experiments, we have identified a two-photon resonance near $±0.14 Φ_{ext}/Φ_0$ which manifests itself in the dispersive shifts in fourth order of perturbation theory and which should also lead to a two-photon vacuum Rabi splitting. Experimental verification would involve tuning the drive frequency $ω_d$ close to the $ε_{40}$ transition and directly observing the level splitting. (In previous experiments the $ε_{40}$ transition was outside the measured frequency range.) Further experimental verification could be achieved by detecting the correlated emission of photon pairs under vacuum Rabi oscillation.

The accumulation of contributions to dispersive shifts in the absence of selection rules does not only affect ac Stark shifts but can, similarly, lead to surprisingly large self-Kerr and cross-Kerr coefficients in fourth order which are tunable with magnetic flux. Making photon-photon interaction terms large while keeping the fundamental qudit transition off resonance, is particularly appealing for circuit QED lattices as a quantum simulator, which is discussed in Chapters 4 and 5.
CHAPTER 3

Fluxonium II: asymptotic expressions and quasi-selection rules of charge matrix elements

In the previous chapter, we have shown with numerical diagonalization\(^1\) that charge matrix elements indeed do not obey strict selection rules in the experimental parameter regime.

3.1. Introduction

The trend of certain matrix elements being up to an order of magnitude larger than others hints at the fact that a new set of selection rules emerges asymptotically in the limit of large Josephson energy and small inductive energy. In this limit, one can make use of the classification of fluxonium eigenstates into metaplasmon and persistent-current states\(^2\), and derive analytical expressions for the charge matrix elements. Based on the asymptotic selection rules, we finally shed light on the different magnitudes of charge matrix elements realized in the experimental parameter regime.

This short chapter is structured as follows. In Sec. 3.2, we briefly summarize the classification of the fluxonium eigenstates into metaplasmon and persistent-current states (previously presented in Ref. [53]) and derive analytical expressions for the charge matrix elements. Based on the resulting asymptotic selection rules, we distinguish matrix elements of different magnitudes and compare the analytical results with numerical results for the experimentally realized parameters in Sec. 3.3.

\(^1\)The matrix elements are illustrated in Fig. 2.4.
3.2. Analytical expressions for fluxonium charge matrix elements

As mentioned in the previous chapter, the fluxonium device is well described by the effective super-inductance model,

\[ H_f = 4E_C N^2 - E_J \cos \varphi + \frac{1}{2} E_L (\varphi + 2\pi \Phi_{\text{ext}} / \Phi_0)^2. \]  

(3.1)

It is instructive to view the Hamiltonian \( H_f \) [Eq. (3.1)] as describing a fictitious particle in a sinusoidal potential, deformed by an overall parabolic envelope. From this point of view, \( \varphi \) plays the role of the spatial coordinate. Hence, the Josephson and inductive energy terms in \( H_f \) determine the potential energy \( V(\varphi) \), while the charging term produces the kinetic energy contribution. The external magnetic flux \( \Phi_{\text{ext}} \) spatially shifts the parabolic envelope. Due to the presence of the inductive term, the appropriate boundary conditions supplementing the stationary Schrödinger equation for \( H_f \) are derived from normalizability of its eigenstates \( |\psi\rangle \), i.e.,

\[ \int_R d\varphi |\langle \varphi | \psi \rangle|^2 < \infty. \]

In the limit of large Josephson and small inductive energy (large inductance),

\[ E_J \gg E_C \gg E_L, \]

(3.2)

the low-lying eigenstates of the fluxonium circuit can be classified into two physically distinct types: metaplasmon states and persistent-current states [53]. The wavefunctions and localization properties of these two types of wavefunctions are illustrated in Fig. 3.1 with the parameters chosen as \( E_J / E_c = 2.5 \) and \( E_L / E_C = 10^{-3} \). For clarity and introduction of necessary notation, we briefly review this classification as obtained in Ref. [53]. To do so, we rewrite \( H_f \) in
a more suitable basis and start by separating off the inductive energy term, $H_f = H' + H_{\text{ind}}$. Despite the tempting appearance of $H'$, we must refrain from identifying it as the ordinary Cooper pair box Hamiltonian: in Eq. (3.1), the spatial coordinates $\varphi$ and $\varphi + 2\pi$ are distinct positions. Hence, $H'$ is not subject to periodic boundary conditions as the Cooper pair box, but rather obeys the quasi-periodic boundary conditions familiar from Bloch’s theorem, as appropriate for a particle in an infinitely extended periodic potential. Accordingly, the eigenstates of $H'$ are Bloch states,

\begin{equation}
H' | p, s \rangle = \epsilon_s(p) | p, s \rangle,
\end{equation}

where $s \in \mathbb{N}$ is the band index, $p \in [0, 1)$ the quasimomentum in the first Brillouin zone, and $\epsilon_s(p)$ denotes the band dispersion for the cosine potential (which coincides with the ordinary offset charge dispersion of the Cooper pair box levels [54]).

To rewrite the inductive contribution $H_{\text{ind}}$ in the Bloch basis, we re-interpret $p$ as a new spatial coordinate. Since it “lives” on a circle with circumference 1, the resulting expression $\varphi = i \frac{d}{dp} + \Omega$ for the phase operator must generally include an inter-band coupling operator $\Omega$ [59]. This inter-band coupling can be neglected for low-lying bands and sufficiently large $E_J/E_C$ [53]. In that limit, the Hamiltonian $H_f$ hence becomes block-diagonal, splitting into individual Hamiltonians for each band $s$, $H_f \approx \sum_s H_s | s \rangle \langle s |$ where

\begin{equation}
H_s = \frac{E_L}{2} \left( i \frac{d}{dp} + \frac{2\pi \Phi_{\text{ext}}}{\Phi_0} \right)^2 + \epsilon_s(p).
\end{equation}

Now, accompanied by periodic boundary conditions in $p$, each Hamiltonian $H_s$ indeed has the same structure as the Hamiltonian of a Cooper pair box. The only difference lies in the form of the periodic “potential” $\epsilon_s(p)$, which generally deviates from a pure cosine. To make the
analogy concrete, note that the variable \( 2\pi p \in [0, 2\pi) \) in \( H_s \) takes on the role of the periodic phase variable of the Cooper pair box, and the external flux \( \Phi_{\text{ext}}/\Phi_0 \) that of the Cooper pair box offset charge \( n_g \).

Next, two different types of low-lying fluxonium states can be distinguished for each band \( s \). First, eigenstates \( |\nu, s\rangle \) with energies below the maximum of the energy dispersion,

\[
E_{\nu s}(\Phi_{\text{ext}}) < \max_p \epsilon_s(p),
\]
are *metaplasmon states*. They are quasi-bound states\(^2\) in the \(\epsilon_s(p)\) potential analogous to the lowest states of the Cooper pair box in the transmon regime. The corresponding eigenenergies depend only weakly on the external flux \(\Phi_{\text{ext}}\), just as Cooper pair box levels are offset-charge insensitive in the transmon regime \([54]\). Second, eigenstates with energies above the maximum of the \(\epsilon_s(p)\) energy dispersion, are *persistent-current states*. Their energies strongly depend on the external flux \(\Phi_{\text{ext}}\), closely mimicking the offset-charge dependence of the high-lying transmon levels (for which, effectively, the charging regime holds). While quasi-itinerant in the \(\epsilon_s(p)\) potential, persistent-current states localize in the individual minima of the \(V(\varphi)\) potential \([\text{Eq. (3.1)}]\). They are conveniently expressed in terms of Wannier states

\[
|m, s\rangle = \int_{-\frac{1}{2}}^{\frac{1}{2}} dp \, e^{-2\pi i p} |p, s\rangle.
\]

Expressed in this basis, the Hamiltonian \([3.4]\) reads:

\[
H_s \approx \frac{(2\pi)^2}{2} E_L (m + \Phi / \Phi_0)^2 + \frac{1}{2} \sum_{m=-\infty}^{\infty} \epsilon_{s,1} \left[ |m, s\rangle \langle m+1, s| + \text{H.c.} \right] + \epsilon_{s,0},
\]

where we have approximated the potential \(\epsilon_s(p)\) by the truncated Fourier series

\[
\epsilon_s(p) \approx \epsilon_{s,0} + \epsilon_{s,1} \cos(2\pi p),
\]

and used \(\sum_{m=-\infty}^{\infty} |m, s\rangle \langle m+1, s| = e^{-i2\pi p}\) as well as \(m = i d/(2\pi p)\). Note that in the transmon regime \((E_J \gg E_C)\), \(\epsilon_{0,0}\) is just the plasmon energy \(\sqrt{8E_J E_C}\). Analytical approximations for \(\epsilon_{s,0}\) and \(\epsilon_{s,1}\) in the transmon regime are given in Ref. \([54]\). Based on the classification into metaplasmon and persistent-current states, we are ready to derive analytical expressions and

\(^2\)We speak of “quasi-bound” states to acknowledge that boundedness is not perfectly well-defined for wavefunctions defined on a closed space.
asymptotic selection rules for the charge matrix elements. Due to the two types of states involved, there are three possible types of charge matrix elements which we discuss one by one in the following.

**Matrix elements between persistent-current states.** The Wannier states $|m, s⟩$ provide good approximations for the persistent-current states (away from degeneracies which occur at integer and half-integer $\Phi_{\text{ext}}/\Phi_0$). The charge matrix elements between two persistent-current states, possibly from different bands $s$ and $s'$, are then given by

$$\langle m, s | N | m', s' \rangle \approx -i \left( \frac{E_J}{32E_C} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} d\varphi w^*_{ms}(\varphi) \times \left[ \sqrt{s'} w_{m's'1}(\varphi) - \sqrt{s'} + 1 w_{m's'+1}(\varphi) \right].$$

(3.9)

Here, $w_{ms}(\varphi) \equiv \langle \varphi | m, s \rangle$ is the approximate persistent-current state wavefunction in $\varphi$-space. Due to the strong localization in the minima of $V(\varphi)$, persistent-current states in adjacent minima are nearly orthogonal. One hence obtains the approximation

$$\langle m, s | N | m', s' \rangle \approx -i \left( \frac{E_J}{32E_C} \right)^{\frac{1}{4}} \delta_{m,m'} \left[ \sqrt{s'} \delta_{s,s'} - 1 \right].$$

(3.10)

To obtain nonzero values for the charge matrix elements in this limit, the two states involved must obey two asymptotic selection rules. The first is the neighboring-band selection rule, demanding $\Delta s = s' - s = \pm 1$. The second is the same-minimum selection rule, given by $\Delta m = m' - m = 0$. Accordingly, both states involved must belong to the same local minimum $m$ of the potential $V(\varphi)$. This rule implies that the circulating persistent current (and the flux it generates) cannot change its magnitude or direction during the transition. Both rules follow intuitively from considering the momentum matrix elements of local harmonic oscillators with negligible neighbor overlap.
Matrix elements between metaplasmon states. The charge matrix elements involving metaplasmon states only, can be brought into the form

\[
\langle \nu', s' | N | \nu, s \rangle \approx i \left( \frac{E_J}{32E_C} \right)^{\frac{1}{4}} (\sqrt{s}\delta_{s, s'+1} - \sqrt{s'}\delta_{s, s'-1}) \times \int_{-\frac{1}{2}}^{\frac{1}{2}} dp \chi^*_{\nu', s'}(p) \chi_{\nu s}(p).
\]

(3.11)

This expression was previously derived in Ref. [53], except for a misprint in the prefactor (fixed here). By \( \chi_{\nu s}(p) \equiv \langle p, s | \nu, s \rangle \), we denote the metaplasmon wavefunctions in the Bloch basis. The index \( \nu = 0, 1, 2, \ldots \) labels energy levels within a fixed band \( s \). The first asymptotic selection rule manifest in Eq. (3.11), is the neighboring-band selection rule \( \Delta s = \pm 1 \). The matrix elements still depend on the overlap between two metaplasmon states, see again Ref. [53] for analytic approximations and asymptotic selection rules in \( \nu, \nu' \).

Matrix elements between metaplasmon and persistent-current states. The last type of matrix elements involves both a metaplasmon and a persistent-current state. Its asymptotic expression is given by

\[
\langle \nu, s | N | m, s' \rangle \approx -i^{\nu+1} \left( \frac{E_J E_L}{32E_C |\epsilon_{s,1}|} \right)^{\frac{1}{4}} (\sqrt{s}\delta_{s, s'+1} - \sqrt{s'}\delta_{s, s'-1}) \times \exp \left[ -\pi F_{ms}^2(\Phi_{\text{ext}}) \right] H_\nu \left( \sqrt{2\pi F_{ms}(\Phi_{\text{ext}})} \right).
\]

(3.12)

Here, \( H_\nu(x) \) is the Hermite polynomial of order \( \nu \) and we have abbreviated \( F_{ms}(\Phi_{\text{ext}}) = (m + \Phi_{\text{ext}}/\Phi_0)(E_L/|\epsilon_{s,1}|)^{1/4} \). The only selection rule present is the one for neighboring bands. The magnitude of the matrix elements depends on both quantum numbers \( m \) and \( \nu \), and is conveniently tunable by magnetic flux \( \Phi_{\text{ext}} \).
3.3. Matrix elements realized in experiments

The values of Josephson, charging and inductive energy realized in recent experiments \( (E_J/h = 8.9 \text{ GHz}; E_C/h = 2.48 \text{ GHz}; E_L/h = 0.53 \text{ GHz} \) in Ref. 65) do not quite reach the asymptotic behavior predicted for \( E_J \gg E_C \gg E_L \). Hence, we cannot expect the asymptotic results from Sec. 3.2 to quantitatively match the experimental results and those obtained by exact diagonalization. Nonetheless, the asymptotic selection rules can still give valuable intuition and qualitative predictions for the different magnitudes of matrix elements, which will be of immediate use in the design of future fluxonium devices.

To apply the results derived in Sec. 3.2, we first need to establish the type of each low-lying fluxonium eigenstate (metaplasmon versus persistent-current), given the experimental parameters. As shown in Fig. 3.2(a), the energy dispersion of the lowest band, \( \epsilon_{s=0}(p) \), turns out to be too shallow to support any metaplasmon states. As a result, the ground state and first excited state are found to be \( s = 0 \) persistent-current states, lying in the gap between the lowest two bands \( \epsilon_{s=0}(p) \) and \( \epsilon_{s=1}(p) \). Due to inversion symmetry and periodicity in the magnetic flux, we may restrict our discussion in the following to the flux range \( 0 \leq \Phi_{\text{ext}}/\Phi_0 \leq 0.5 \) without loss of generality. Under these conditions and sufficiently away from integer and half-integer flux, the two lowest persistent-current states are well approximated by the Wannier states \( |m=0, s=0 \rangle \) and \( |m=0, s=1 \rangle \).

In the following, we focus on the example flux point \( \Phi_{\text{ext}}/\Phi_0 = 0.4 \). The exact wavefunctions at this point are illustrated in Fig. 3.2(b). Note that the ground state (first excited state) is indeed primarily localized in the minimum \( m=0 \) \( (m=-1) \). The second and third excited states are metaplasmon states with band indices \( s = 1 \) and \( s = 2 \), respectively. As expected, they delocalize over multiple minima of the potential \( V(\varphi) \). At \( \Phi_{\text{ext}}/\Phi_0 = 0.4 \), the fourth excited state
Figure 3.2. Fluxonium spectrum and wavefunctions. (a) Fluxonium energy levels (solid curves) as a function of external flux $\Phi_{\text{ext}}$, for the parameters realized experimentally [65]. Shaded regions in the background show position and width of the bands $\epsilon_s(p)$. The $s=0$ persistent-current states with parabolic flux dependence are labeled by their quantum number $m$. (b) Wavefunctions of the fluxonium eigenstates for $\Phi_{\text{ext}}/\Phi_0=0.4$ [vertical dashed line in (a)]. The bold black curve shows the fluxonium potential $V(\varphi)$. Local minima are labeled by the quantum numbers $m$. The fluxonium wavefunctions (thin curves) are offset by their eigenenergies. The lowest three eigenstates approximately form a Λ-system, suggested by the red arrows. The solid arrows represents relatively large transition rates, while the dashed arrow represents relatively small transition rate.

can easily be identified as a persistent-current state of the $s=0$ band, by noting its quadratic flux dependence expected for the $|1_m, 0_s\rangle$ state. Accordingly, it is strongly localized in the $m = 1$ minimum. However, due to the large inter-band coupling for higher-lying levels, this state is already significantly influenced by the nearby metaplasmon state [see the large avoided crossing of the third and fourth excited states near $\Phi_{\text{ext}}/\Phi_0=0.3$ in Fig. 3.2(a)]. As a result, the wavefunction of the fourth excited state slightly spreads out of the $m = 1$ well. For even higher
Figure 3.3. Comparison of numerical results and asymptotic predictions for the charge matrix elements. Solid curves show numerical results for the magnitude of the charge matrix elements, $|\langle 0_l |N|0_{\nu},1_s^\rangle|$, $|\langle 0_l |N|2_l^\rangle|$ and $|\langle 0_l |N|3_l^\rangle|$. Dashed curves show the asymptotic matrix elements between the ground state and the lowest metaplasmon state, namely $|\langle 0_l |N|0_{\nu},1_s^\rangle|$, and between the two low-lying persistent current states, $|\langle 0_{m},0_s^\nu|N|-1_{m},0_s^\nu\rangle|$. Levels, the inter-band coupling becomes stronger and the classification into metaplasmon and persistent-current states ceases to apply.

The situation of half-integer and integer $\Phi_{ext}/\Phi_0$ is special because of the additional parity symmetry of the potential $V(\varphi)$. For $\Phi_{ext}/\Phi_0 = 0.5$, the state $|-1_{m},0_s^\nu\rangle$ becomes degenerate with $|0_m,0_s\rangle$. The ground and first excited states are hence the symmetric and antisymmetric superposition of $|-1_{m},0_s^\nu\rangle$ and $|0_m,0_s\rangle$. For zero external flux, the ground state is $|0_m,0_s\rangle$, while the first and second excited states become the symmetric and antisymmetric superposition of $|-1_{m},0_s^\nu\rangle$ and $|1_{m},0_s^\nu\rangle$.

With the classification of states in hand, we now employ the analytic results from Sec. 3.2 to describe the qualitative behavior and magnitudes of the charge matrix elements. Away from the degeneracies at integer and half-integer $\Phi_{ext}/\Phi_0$, the charge matrix element between the ground and the first excited state is approximated by the matrix element between two different
persistent-current states, namely

\begin{equation}
\langle 0_l | N | 1_l \rangle \approx \langle 0_m, 0_s | N | -1_m, 0_s \rangle.
\end{equation}

Here, \( l \) enumerates the fluxonium eigenstates in the order of their eigenenergies. The magnitude of this matrix element is relatively small because of the suppression enforced by the asymptotic selection rules for two persistent-current states [\( \Delta s = \pm 1 \) and \( \Delta m = 0 \); see Eq. (3.10)]. Figure 3.3 shows that the charge matrix element between ground and first excited state, \( |N_{01}\rangle \), is indeed significantly smaller than the other elements (especially compared to \( |N_{02}\rangle \)) over most of the flux range.

We note this discrepancy in matrix element magnitudes could possibly lead to an interesting potential application: if coupling to the environment via charge dominates the qubit relaxation, then the lowest three fluxonium levels (\( l = 0, 1, 2 \)) could form a \( \Lambda \)-system over a wide flux range, with the state \( |1_l\rangle \) being a relatively long-lived metastable state, as noted previously in Ref. [64]. The origin of the \( \Lambda \)-configuration is intuitive from Fig. 3.2(b): the states \( |0_l\rangle \) and \( |1_l\rangle \) are persistent-current states localized in different minima with only very small wavefunction overlap. The state \( |2_l\rangle \), by contrast, is a metaplasmon state and has a large wavefunction overlap with both persistent-current states, resulting in relatively large matrix elements (and hence transition rates) between these states. As a result, the state \( |1_l\rangle \) may have a significantly longer lifetime than the state \( |2_l\rangle \).

It is instructive to assess the deviation of exact results for the experimental parameters from the asymptotic prediction. For this comparison, we choose two eigenstates which, in a given flux range, can be approximately classified as a metaplasmon state and a persistent-current state, respectively. The approximate metaplasmon state we choose is \( |0_\nu, 1_s\rangle \). Figure 3.2(a)
shows that, in the flux region $0 < \Phi_{\text{ext}}/\Phi_0 < 0.1$, this metaplasmon state approximates the state $|3\rangle$. In the remaining flux region, this metaplasmon state approximates the state $|2\rangle$. The persistent-current state we choose is $|0_m, 0_s\rangle$, which approximates the ground state $|0\rangle$ away from $\Phi_{\text{ext}}/\Phi_0 = 0.5$. We employ Eq. (3.12) to calculate the asymptotic result for the matrix element $|\langle 0_m, 0_s | N | 0_\nu, 1_s \rangle|$, where the input parameter $\epsilon_{1,1}/\hbar = 1.774$ GHz is acquired from the half-width of the $s = 1$ CPB band by diagonalizing $H'$.

The result obtained from Eq. (3.12) is valid only sufficiently away from $\Phi_{\text{ext}}/\Phi_0 = 0.5$. There, the ground state $|0\rangle$ becomes a hybridization of the two states, $|-1_m, 0_s\rangle$ and $|0_m, 0_s\rangle$, which are energy degenerate states in the absence of $\epsilon_{0,1}$. To account for this, we consider the $2 \times 2$ subspace containing both persistent-current states. The Hamiltonian in this subspace is

$$H_{\text{sub}} \approx \begin{pmatrix} 2\pi^2 E_L (\Phi_{\text{ext}}/\Phi_0)^2 + \epsilon_{0,0} & \frac{1}{2} \epsilon_{0,1} \\ \frac{1}{2} \epsilon_{0,1} & 2\pi^2 E_L (\Phi_{\text{ext}}/\Phi_0 - 1)^2 + \epsilon_{0,0} \end{pmatrix},$$

a truncated version of Eq. (3.7). Here, the input parameter $\epsilon_{0,1}/\hbar = 0.187$ GHz is obtained from the half-width of the $s = 0$ CPB band. By diagonalizing this matrix, we obtain an improved approximation for the ground state $|0\rangle$, and for the asymptotic prediction of the matrix element $|\langle 0| N | 0_\nu, 1_s \rangle|$.

The asymptotic prediction (dashed curve in Fig. 3.3) is to be compared with the corresponding solid curves showing the numerically exact results – in particular, the results for $N_{03}$ and $N_{02}$ in the previously mentioned flux ranges. Agreement is qualitative rather than quantitative, as expected. Note that, by accounting for hybridization, the complete suppression of $N_{02}$ at $\Phi_{\text{ext}}/\Phi_0 = 0.5$ enforced by parity symmetry is correctly predicted. Similarly, the asymptotic
prediction for vanishing \( N_{01} \) agrees qualitatively with the significantly smaller values obtained numerically.

### 3.4. Summary

We have derived asymptotic expressions for the charge matrix elements of the fluxonium circuit in the parameter limit \( E_J \gg E_C \gg E_L \), presented in Eqs. (3.10)–(3.12). Our derivation is based on the classification of fluxonium eigenstates into persistent-current and metaplasmon states [53], and produces simple selection rules for the band indices \( s \) and other quantum numbers which can be intuitively understood from the localization properties of the different types of states.

We employ our asymptotic predictions to interpret the numerically calculated matrix elements for the intermediate parameter regime realized in experiments [65]. Even though quantitative agreement cannot be expected in this intermediate regime, we find good qualitative agreement and confirm that the asymptotic selection rules provide a useful predictor for different magnitudes of charge matrix elements. Thus, our results can easily guide the choice of experimental parameters in order to reach the desired tunability of charge matrix elements in future fluxonium devices. The relatively large degree of tunability in fluxonium devices can be harnessed for influencing transition rates (providing a route towards a \( \Lambda \)-system [64]), dispersive shifts [113], as well as the effective qubit-qubit interaction strength when coupling multiple fluxonium devices to a single microwave resonator mode [61], or coupling a single fluxonium to each resonator site in a Jaynes-Cummings lattice as discussed in the next chapter.
CHAPTER 4

Dispersion regime of Jaynes-Cummings and Rabi lattices

In the previous two chapters, we have explored the single-site Jaynes-Cummings/Rabi system, namely a single multi-level qudit, the fluxonium circuit, coupled to a single microwave resonator. In this chapter, we scale up the elementary building blocks to form a full quantum simulator, and hence switch from the study of single-body physics to many-body physics, namely physics of interacting photons and qubits in Jaynes-Cummings and Rabi lattices. In order to highlight the central physics, we limit our consideration here to a two-level qubit in these lattices, instead of the multi-level qudits discussed in the previous chapters.

4.1. Introduction

In the Jaynes-Cummings and Rabi lattices (shown in Fig. 4.1), each lattice site consists of a photon mode interacting locally with a two-level system, and is described by the ordinary Jaynes-Cummings [45] or Rabi model [80]. In addition, photons can hop between nearest-neighbor lattice sites. A key difference between the traditional ultra-cold boson and fermion gases in optical lattices and the less conventional Jaynes-Cummings and Rabi lattice is that the latter provide an interesting additional tunable parameter: the detuning $\Delta$. Its origin lies in the two-component nature of the Jaynes-Cummings and Rabi model, comprising an electromagnetic field component and a matter component. Each component is associated with its own characteristic energy scale. The possible energy mismatch between the two is quantified by the detuning $\Delta$. 
Figure 4.1. [Credit: J. Koch et al. [51]] Circuit-QED realization of Jaynes-Cummings and Rabi lattices. It consists of SC resonators (e.g., coplanar waveguides, schematically shown as rectangular boxes), each of which is coupled to a SC qubit (symbolized as dots centered in the resonators). Microwave photons can hop between nearest-neighbor resonators, with the coupling strength $t$ set by the mutual capacitance between resonator ends. The onsite interaction between the photons and the SC qubits is of Jaynes-Cummings type if the interaction strength $g$ is much smaller than both the photon and qubit frequency, i.e. $g \ll \epsilon, \omega$. On the other hand, the onsite interaction is of Rabi type if the interaction strength $g$ is comparable to either the photon or qubit frequency, i.e. $g \sim \epsilon$ or $\omega$.

By changing the detuning, three qualitatively different regimes of the Jaynes-Cummings lattice and Rabi lattice can be accessed. In the resonant regime, the detuning is small and photons and matter excitations readily hybridize to form polaritons. In the dispersive regime, the magnitude $|\Delta|$ of the detuning between the two-level splitting $\epsilon$ and the photon frequency $\omega$ is large. According to the sign of $\Delta = \epsilon - \omega$, we distinguish between the dispersive regime with negative detuning ($\epsilon < \omega$), where low-energy physics predominantly involves matter excitations, and the dispersive regime with positive detuning ($\omega < \epsilon$), in which photons govern the behavior at low energies. In this chapter, we focus primarily on the two dispersive regimes where all interaction strengths are small compared to $|\Delta|$.
The circuit QED architecture \[7, 91, 105\] constitutes one of the most promising experimental platforms for the realization of dispersive Jaynes-Cummings and Rabi lattice systems \[40, 89\]. In circuit QED lattices (as shown in Fig. 4.1), photons can hop between transmission line resonators (which are coupled capacitively) and locally interact with a superconducting qubit. The qubit energy \(\epsilon\) (and hence the detuning parameter \(\Delta\)) can be tuned in-situ by an externally applied magnetic flux. Recently, the coherent photon exchange via hopping between several coupled resonators has indeed been realized experimentally \[102\].

Theoretically, the dispersive regime for a single Jaynes-Cummings \[7\] or Rabi system \[114\] is well understood. Just as in our study of the for a generalized Jaynes-Cummings/Rabi model for the coupled fluxonium-resonator system in Chapter 2, the usual description of dispersive regime is based on employing a perturbative Schrieffer-Wolff transformation, which eliminates the Jaynes-Cummings or Rabi coupling by switching to an appropriate dressed-state basis.

Here, we extend this procedure to an entire lattice of sites and systematically discuss all contributions in second-order perturbation theory (Sec. 4.2). We find that effective qubit-qubit interactions, qubit-state dependent photon hopping terms and photon pairing terms (squeezing terms) emerge. All inter-site interactions are short-ranged but not limited to nearest-neighbor sites.

We explore the implications of the derived effective Hamiltonian (up to second order) for the low-energy physics of the Jaynes-Cummings lattice in Sec. 4.3. For negative detuning, we show that the system reduces to an effective spin model with XY-type interaction. We also consider the generic structure of the fourth-order effective interactions, and for the case of large positive detuning \((\omega \ll \epsilon)\) we derive the leading-order (in \(t/\Delta\)) effective interaction, which is of Hubbard form. This finding directly connects to Chapter 5, where we will use the
Bose-Hubbard model as an effective description for the interacting photons in the large negative detuning ($\epsilon \ll \omega$) regime.

We study the low-energy physics of the Rabi lattice in Sec. 4.4. For negative detuning, the effective model reduces to a transverse Ising model. For positive detuning, we discuss in detail the one-mode and two-mode vacuum squeezing relevant in the ultra-strong coupling regime as described by the dispersive Rabi model. Due to the ultra-strong coupling, approached indeed in a recent experiment for a single site in circuit-QED architecture [70], the non-trivial nature of the ground state makes the Rabi lattice particularly interesting. In Sec. 4.5, we study the application of the dispersive regime to the Rabi dimer and confirm the validity of the derived effective Hamiltonians by comparison with results from exact diagonalization. Finally, we summarize and give an outlook on questions of future interest in Sec. 4.6.

4.2. Derivation of the effective Hamiltonian in the dispersive regime

The Rabi lattice is described by the model Hamiltonian

\[ H = \omega \sum_j a_j^\dagger a_j + \epsilon \sum_j \sigma_j^+ \sigma_j^- + g \sum_j \left( a_j \sigma_j^+ + a_j^\dagger \sigma_j^- + \text{H.c.} \right) + t \sum_{\langle j,j' \rangle} \left( a_j^\dagger a_{j'} + \text{H.c.} \right). \]

Here, each Rabi site is labeled by an index $j$, and consists of a harmonic mode coupled to a spin-$1/2$. As usual, excitations of the harmonic mode and spin on site $j$ are created by $a_j^\dagger$ and $\sigma_j^+$, and annihilated by their Hermitean-conjugate counterparts. The energy necessary for an excitation of either type is fixed by $\omega$ and $\epsilon$, respectively. The coupling strength is set by the parameter $g$. The strength of $g$ compared to the frequency $\omega$ and $\epsilon$ determines whether the interaction is of Jaynes-Cummings type or Rabi type.
Although the onsite Rabi interaction $V_j = g \left( a^+_j \sigma^+_j + a^+_j \sigma^-_j + \text{H.c.} \right)$ always holds as the correct description, in the parameter regime $g \ll \epsilon, \omega$ one can apply the rotating-wave approximation (RWA) and drop the counter-rotating term $g \left( a^+_j \sigma^+_j + \text{H.c.} \right)$ from the Rabi interaction. For example near the resonant regime ($\epsilon \sim \omega$), the counter-rotating term has much higher frequency $\sim \Sigma = \epsilon + \omega$ in the Heisenberg picture, while the rotating term has much lower frequency $\sim \Delta = \epsilon - \omega$. Therefore, the counter-rotating term is considered as fast-rotating in the Heisenberg picture, and can be dropped if the interaction strength $g$ is much smaller than $\Sigma$. Thus, the interaction can be approximated as $V^{\text{JC}}_j = g \left( a^+_j \sigma^+_j + \text{H.c.} \right)$, which is of Jaynes-Cummings type. However, if the interaction strength is comparable to either the spin or harmonic frequency (so-called ultra-strong coupling regime), i.e. $g \sim \epsilon \text{ or } \omega$, the RWA is not valid and we have to use the full expression of the Rabi interaction. The corresponding two lattice models in these two different situations are called the Jaynes-Cummings lattice and the Rabi lattice, respectively.\(^1\)

From the beginning on, we will include counter-rotating terms characteristic of the Rabi model and the ultra-strong coupling regime, and only drop those terms in our discussion of the Jaynes-Cummings limit where the RWA is applicable (see text below). For the entirety of this chapter, we will focus on the disorder-less case, assuming that all lattice sites have identical parameters. In the following and for the sake of brevity, we simply refer to the spin degree of freedom as “qubit”.

In addition to the onsite Rabi interactions, the last term in Eq. (4.1) introduces coupling between resonators. We consider weak resonator coupling, $|t| \ll \omega, \epsilon$, and treat it within the RWA. As written in Eq. (4.1), the coupling term then allows for photons to hop from one resonator to another.

\(^1\)One can think of the Jaynes-Cummings lattice as a particular limit of the Rabi lattice.
resonator to its nearest neighbors, as indicated by the angular brackets in the summation over resonator pairs. The sign of the hopping amplitude $t$ depends on the specific system realization. In the circuit QED architecture, for example, it depends on the lattice geometry and the specific photon modes used [74, 89].

The Rabi lattice (4.1) enters the dispersive regime when the detuning $|\Delta| = |\epsilon - \omega|$ between qubit and resonator frequency is large compared to the coupling strength $g$. While the sum frequency $\Sigma = \epsilon + \omega \geq |\Delta|$ obeys $\Sigma \gg |\Delta|$ whenever the RWA holds, a hallmark of the dispersive regime of the Rabi model beyond RWA is that detuning and frequency sum may be of the same order, $\Sigma \sim |\Delta|$ [114]. In this case, two sub-regimes are of particular interest: the dispersive Rabi regime with negative detuning, $\epsilon \ll g \ll \omega$, and the dispersive Rabi regime with positive detuning, $\omega \ll g \ll \epsilon$. Both sub-regimes will be investigated in Sec. 4.3.

In any of the mentioned cases, the idea underlying the dispersive regime remains the suppression of interconversion between qubit and photon excitations due to a large energy mismatch which is not overcome by the coupling $g$. Under these conditions, the Rabi interaction terms $\sim g$ can be treated perturbatively.

To obtain a simple effective Hamiltonian describing the dispersive regime, it is convenient to carry out the perturbation theory in the form of a unitary Schrieffer-Wolff transformation, $\tilde{H} = e^{iS}He^{-iS}$ [17, 93]. For the cases of a single Rabi site and multiple qubits strongly coupled to a single resonator, this procedure was previously discussed by Zueco et al. [114]. Here, we extend it to a lattice of coupled Rabi sites. Using the appropriate Hermitian generator $S$, the unitary transformation switches to a dressed-state basis in which the original Rabi interaction is eliminated. Being unitary, the transformation clearly preserves the spectrum of the original Hamiltonian.
In our case, the unperturbed Hamiltonian $H_0$ consists of the terms in Eq. (4.1) with the exception of the Rabi coupling term:

\begin{equation}
H_0 = \omega \sum_j a_j^\dagger a_j + t \sum_{(j,j')} \left( a_{j'}^\dagger a_j + \text{H.c.} \right) + \epsilon \sum_j \sigma_j^+ \sigma_j^-.
\end{equation}

This corresponds to a photonic tight-binding model and uncoupled qubit. To avoid distractions, we limit our discussion to one-dimensional Rabi lattices. The generalization to lattices with more complex structure is straightforward. Thus, considering a one-dimensional photon tight-binding model with Born-von Karmann periodic boundary conditions over a number $N$ of lattice sites, we define the itinerant photon operators by

\begin{equation}
a_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ikj} a_j, \quad k = 0, \frac{2\pi}{N}, \frac{2\pi}{N}, \ldots, (N-1)\frac{2\pi}{N}.
\end{equation}

Here, for a large number of sites ($N \rightarrow \infty$), the quasi-momentum $k$ spans the entire first Brillouin zone, $-\pi < k \leq \pi$. Employing this basis, the unperturbed Hamiltonian can be rewritten in the diagonal form as

\begin{equation}
H_0 = \sum_k \omega_k a_k^\dagger a_k + \epsilon \sum_j \sigma_j^+ \sigma_j^-.
\end{equation}

Here, the dispersion of the itinerant photons for a one-dimensional lattice is simply $\omega_k = \omega + 2t \cos k$.

The perturbation $V$ is the onsite Rabi interaction on each lattice site and can be expressed in terms of the itinerant photon operators as

\begin{equation}
V = g \sqrt{N} \sum_k \sum_j \left( a_k \sigma_j^+ e^{ikj} + a_k^\dagger \sigma_j^- e^{-ikj} + \text{H.c.} \right).
\end{equation}
For itinerant photons, the energy gap towards the qubit energy now depends on the quasi-momentum \( k \). We thus define the \( k \)-dependent detuning parameter \( \Delta_k = \epsilon - \omega_k \) and the frequency sum \( \Sigma_k = \epsilon + \omega_k \). Ensuring that the qubits remain detuned from all itinerant photons, we recognize that

\[
\Delta_{\text{min}} \equiv \min_k |\Delta_k| = \min_k |\epsilon - \omega_k| \gg g,
\]

constitutes a necessary condition for the dispersive regime of the Rabi lattice model. Figure 4.2 illustrates this condition for both positive and negative detuning.

In the perturbative approach, the Schrieffer-Wolff transformation is carried out to a certain order in the interaction strength \( g \). In this section, we present results for the Rabi lattice model to second order in \( g \). The generator necessary to achieve this must be of first order in \( g \) [17],

![Figure 4.2. Dispersive regime of the Rabi lattice: relevant energy scales. The plot shows the itinerant photon dispersion \( \omega_k \) for positive (blue solid) and negative (blue dashed) hopping amplitude. The shaded region indicates the full width \( 4t \) of the photon band, centered at the bare photon frequency \( \omega \). Examples for qubit energies with positive (\( \epsilon \)) and negative (\( \epsilon' \)) detuning are shown in red. Expressed in terms of quasi-momenta, the detuning \( \Delta_k \) becomes \( k \) dependent (see example for \( k = k_1 \), shown for the \( t > 0 \) case).](image-url)
and is given by

\begin{equation}
S_1 = \frac{i}{\sqrt{N}} \sum_k \sum_j \left[ \frac{g}{\Delta_k} a_k^\dagger \sigma_j^- e^{-ikj} + \frac{g}{\sum_k} a_k \sigma_j^- e^{ikj} - H.c. \right].
\end{equation}

We then construct the effective Hamiltonian by expanding the exponentials in $e^{iS_1} H e^{-iS_1}$ and collecting terms up to second order. Due to the form of the interaction $V$, the generator $S_1$ splits into 4 terms, resulting in $4^2 = 16$ second-order terms which contribute to the effective Hamiltonian. (Note that the first-order term vanishes since $[H, S_1] = 0$.) Figure 4.3 visualizes all 16 contributions in the form of ladder diagrams, similar to those previously introduced in Chapter 2.3.

Each diagram can be directly translated into a contribution to the effective Hamiltonian according the following rules:

1. Each ladder step corresponds to one unperturbed eigenstate of $H_0$, with well-defined number of photons and qubit excitations. Virtual intermediate states are marked by dashing.

2. Diagrams are read from right to left. Arrows show virtual transitions produced by a specific operator term from $S_1$ (label on the arrow), e.g., $a_k^\dagger, \sigma_j^-$. The contribution to the effective Hamiltonian contains the same operator combination (including the operator ordering) as shown by the arrow label. For each occurrence of photon operators, traveling-wave factors should be included according to $a_k \rightarrow a_k e^{ikj}$ and $a_k^\dagger \rightarrow a_k^\dagger e^{-ikj}$.

3. Each contributing diagram involves summation over all intermediate labels $j, j', k, k'$ with a $1/N$ prefactor.

\footnote{Recall that $S_2$ does not contribute to the second-order effective Hamiltonian since $[H, S_2] = 0$, see e.g., Ref. [17].}
Figure 4.3. Ladder diagrams used in deriving the effective Hamiltonian. Horizontal ladder steps represent unperturbed eigenstates of $H_0$ and red arrows the virtual transitions between them. Dashing of horizontal steps indicates virtual intermediate states. Each diagram is to be read from left to right. Labels on horizontal steps show the relevant qubit configurations and labels on arrows the operators producing the transition. Diagrams with two paths lead to partial cancellation in the Hamiltonian. The shown ordering of energies (as indicated by the vertical position of steps in each diagram) refers to the positive detuning case, $\omega \ll \epsilon$. Completely analogous diagrams, differing only in the ordering of energies, apply to the negative detuning case, $\omega \gg \epsilon$. The diagrams XIII–XVI vanish when summed over $k,k'$, and hence do not contribute to the effective Hamiltonian.
Figure 4.4. Paths from Fig. 4.3 for the special case of \( j = j' \). As an example, the paths I and II are shown here. In this case, initial and final states differ, no interference occurs and photon operators are not cancelled. Such paths contribute to all those second-order terms in the effective Hamiltonian (4.11) that involve photon operators.

(4) The energy coefficient for each contribution is given by 
\[
\frac{g^2}{2} \left[ \frac{1}{E_R - E_I} + \frac{1}{E_L - E_I} \right],
\]
where \( E_L, E_R \) and \( E_I \) denote the bare energies of the left, right and intermediate state respectively.

As an example, the analytical expressions obtained for the first two diagrams read:

\[
\tilde{H}_I = \frac{1}{N} \sum_{k,k'} \sum_{j,j'} \frac{g^2}{2} \left[ \frac{1}{\Delta_{k'}} + \frac{1}{\Delta_k} \right] e^{i(k'j'-kj)} a_k^\dagger a_k' \sigma_j^- \sigma_{j'}^+, \tag{4.8}
\]

\[
\tilde{H}_{II} = \frac{1}{N} \sum_{k,k'} \sum_{j,j'} \frac{g^2}{2} \left[ \frac{1}{\Delta_{k'}} + \frac{1}{\Delta_k} \right] e^{i(k'j' - kj)} a_k^\dagger a_k' \sigma_j^+ \sigma_{j'}^- . \tag{4.9}
\]

We now turn to the systematic discussion of the contributions obtained from the diagrams shown in figure 4.3. All contributions from the paths XIII–XVI vanish. For each of these paths, summation over \( k \) and \( k' \) leads to complete cancellation due to the opposite signs of the energy denominators involved. Several paths in Fig. 4.3 including paths I and II, are shown as pairs. Each member in such a pair has the same initial and final states but undergoes its two virtual transitions in opposite order, thus leading to interference and partial cancellation. This cancellation originates from the opposite signs of the prefactors, see, e.g., the example in Eqs. (4.8) and (4.9).
We first discuss the case of distinct site indices $j \neq j'$. Since Pauli operators on different sites commute and itinerant photon operators obey the canonical commutation relation $[a_k, a^\dagger_{k'}] = \delta_{kk'}$, we find that all terms in $\tilde{H}^I + \tilde{H}^{II}$ with $k \neq k'$ and $j \neq j'$ exactly cancel. In the remaining ($k = k'$) term, all photon operators are eliminated:

\begin{equation}
(4.10) \quad \tilde{H}^I + \tilde{H}^{II} \bigg|_{j \neq j'} = \frac{1}{N} \sum_k \sum_{j \neq j'} \frac{g^2}{\Delta_k} e^{ik(j' - j)} \sigma^+_j \sigma^-_j.
\end{equation}

Equation (4.10) represents photon-mediated flip-flop (XY) interaction between qubits on different sites. Further contributions of this type are produced by paths $\text{III}$ and $\text{IV}$. By contrast, the paths $\text{IX} - \text{XII}$ produce an effective qubit interaction of the type $\sigma^+_j \sigma^+_j + \sigma^-_j \sigma^-_j$. Finally, the $j \neq j'$ contributions of the paths $\text{V} - \text{VIII}$ exactly vanish.

Next, we consider the onsite case, i.e., the situation of $j = j'$ in each path. By comparing with the expressions in Eqs. (4.8) and (4.9), we note that the initial and final states must differ in this special case. For the example of the paths $\text{I}$ and $\text{II}$, the resulting proper diagrams are shown in Fig. 4.4. They involve a single qubit flip accompanied by the creation and annihilation of one itinerant photon each. The $j = j'$ contributions of the paths $\text{V} - \text{VIII}$ produce photon pair creation and annihilation terms. Finally, the $j = j'$ contributions of the paths $\text{IX} - \text{XII}$ identically vanish due to the occurrence of two Pauli raising or lowering operators on the same site, where $(\sigma^+_j)^2 = (\sigma^-_j)^2 = 0.$
By transforming all itinerant photon operators back into real space, we obtain the effective second-order Hamiltonian for the dispersive Rabi regime:

\[ \tilde{H}_{\text{eff}} = H_0 + \frac{g^2}{2} \sum_j \tilde{C}_j^+ \sigma_j^z + \frac{g^2}{2} \sum_{j \neq j'} \tilde{C}_{j-j'}^\pm \sigma_j^x \sigma_{j'}^x + g^2 \sum_j a_j^\dagger a_j^0 \sigma_j^z + H.c. + \frac{g^2}{2} \sum_{j \neq j'} \tilde{C}_{j-j'}^+ a_j^\dagger a_{j'}^\dagger (\sigma_j^z + \sigma_{j'}^z) + \frac{g^2}{2} \sum_{j<j'} \tilde{C}_{j-j'}^+ (a_j^\dagger a_{j'}^\dagger + a_j a_{j'}) (\sigma_j^z + \sigma_{j'}^z), \]

where a global constant has been dropped. The coupling constants \( \tilde{C}_m^\pm \) depend on the distance \( m \) between lattice sites and are defined as

\[ \tilde{C}_m^\pm = \frac{1}{N} \sum_k \left( \frac{1}{\Delta_k} \pm \frac{1}{\Sigma_k} \right) e^{imk} = \frac{1}{N\Delta} \sum_k \frac{e^{imk}}{1 - \frac{2t}{\Delta} \cos k} \pm \frac{1}{N\Sigma} \sum_k \frac{e^{imk}}{1 - \frac{2t}{\Sigma} \cos k}. \]

Since the condition (4.6) for the dispersive regime of the Rabi lattice also implies that the inequalities \( |2t/\Delta| < 1 \) and \( |2t/\Sigma| < 1 \) must hold, we can ascertain that \( g/\Delta, g/\Sigma, t/\Delta \) and \( t/\Sigma \) are all small parameters. The effective Hamiltonian (4.11) obtained from the perturbative Schrieffer-Wolff transformation is a series expansion in both \( g/\Delta \) and \( g/\Sigma \). Due to exact diagonalization of the photon tight-binding model, the coupling constants \( \tilde{C}_m^\pm \) contain terms to all orders in \( t/\Delta \) and \( t/\Sigma \). We can further elucidate this fact by re-expressing the denominators in Eq. (4.12) in terms of convergent geometrical series, namely

\[ \tilde{C}_m^\pm = \frac{1}{N} \sum_k e^{imk} \sum_{n=0}^{\infty} \left[ \frac{1}{\Delta} \left( \frac{t}{\Delta} \right)^n \pm \frac{1}{\Sigma} \left( \frac{t}{\Sigma} \right)^n \right] (e^{ik} + e^{-ik})^n. \]
Applying the binomial theorem to the last factor, using the relation
\[ N^{-1} \sum_k e^{ikl} = \sum_{z=-\infty}^{\infty} \delta_{l,zN}, \]
and keeping only the leading order terms in \( t/\Delta \) and \( t/\Sigma \), we find the approximation

\[ \tilde{C}_m^{\pm} \approx \frac{1}{\Delta} \left( \frac{t}{\Delta} \right)^m \pm \frac{1}{\Sigma} \left( \frac{-t}{\Sigma} \right)^m \]

for the coupling constants. Equation (4.14) is valid for \( 0 \leq m \leq N/2 \). Whenever \( m \) is outside this range, the exponents in Eq. (4.14) should be replaced by \( |m \mod N| \). Equations (4.11), (4.12) and (4.14) constitute the main results of this first part of this chapter. In the following we will explore the implications of this effective Hamiltonian and discuss the physics of the dispersive regime of the Rabi lattice and the Jaynes-Cummings lattice in the subsequent section.

As expected, the dispersive approximation to the Rabi lattice Hamiltonian involves energy shifts and interaction terms which do not inter-convert between qubit and photon excitations. Based on Eq. (4.11), we now discuss shift and interaction terms one by one. The second term on the right-hand side of Eq. (4.11) captures the Lamb shift for the on-site qubit-resonator system. The shift is identical to the one obtained for a single qubit-resonator system in the dispersive regime \[7\] when using the weak-coupling approximation \( \tilde{C}_0^{+} \approx 1/\Delta - 1/\Sigma \).

The third term in Eq. (4.11) produces photon-mediated qubit-qubit interactions of the transverse-Ising type.\(^3\) The contributions responsible for going beyond the bare flip-flop (XY) interaction are the additional counter-rotating terms \( \sigma_j^x \sigma_j^x \) and \( \sigma_j^y \sigma_j^y \). The strength of this interaction is set by the coupling constant \( \tilde{C}_m^- \) which, according to Eq. (4.14), decays exponentially with increasing distance \( m \) between lattice sites.

The terms 4 – 7 on the right-hand side of Eq. (4.11) all directly involve photons. Term 4 with the form \( a_j^\dagger a_j \sigma_j^z \) produces the well-known AC Stark shift on each lattice site \[7\]. Term 5

\(^3\)Transverse-Ising coupling is also expected for multiple qubits interacting with a single resonator, see Ref. [114].
with the structure $a_j^+ a_j^+ \sigma_j^z$ is an onsite term as well but goes beyond a mere energy shift: here, photon pairs are created or annihilated on a single site. At the same time, the amplitude sign for this process depends on the state of the local qubit. Counter-rotating terms like this one are characteristic of ultra-strong coupling and reflect, naturally, that the total excitation number $N_{\text{tot}} = \sum_j (a_j^+ a_j + \sigma_j^+ \sigma_j^-)$ is not conserved in the case of the Rabi lattice.

The terms 6 and 7 involve two sites and describe conditional photon hopping and two-mode photon pair creation or annihilation. Remarkably, in both cases the amplitude for these processes depends on the two-qubit operator $(\sigma_j^z + \sigma_j^z)$ including the $z$-projections of the qubits on the two sites involved in the hopping or pair creation. Assuming qubit configurations composed of $\sigma^z$ eigenstates, hopping and pair creation can be enhanced or suppressed by choosing qubits on the corresponding sites to be aligned or anti-aligned. Again, overall coupling strengths are fixed by $\tilde{C}_m^+$ which favors hopping and pair creation across small distances $m$.

4.2.1. Reduction to the Jaynes-Cummings limit

When we reduce the strength $g$ of the Rabi coupling sufficiently to reach the limit $g \ll \omega, \epsilon$ typical of the Jaynes-Cummings model, we can apply the RWA and drop counter-rotating terms. It is instructive to consider how, in this case, the effective Hamiltonian (4.11) reduces to the dispersive regime of the Jaynes-Cummings lattice.

Neglecting counter-rotating terms, the onsite interaction simplifies to the Jaynes-Cummings form

\begin{equation}
V = g \sum_j \left( a_j \sigma_j^+ + \text{H.c.} \right).
\end{equation}
Neglecting all counter-rotating terms in an analogous derivation of the dispersive Hamiltonian, we only obtain contributions from paths I and II. Note that, generally, smaller energy differences between the intermediate and initial/final levels in figure 4.3 lead to larger effective coupling. Further, \( \Lambda \) and \( V \)-shaped paths have larger effective coupling due to a constructive sum of the two inverse energy differences. Finally, the energy difference between the initial and final states for each path, when compared to the magnitude of the effective coupling, determines whether or not a path contributes within the RWA.

The resulting effective Hamiltonian (up to second-order) describing the Jaynes-Cummings lattice in the dispersive regime reads

\[
\tilde{H}_{\text{eff}} = H_0 + g^2 \sum_{j \neq j'} C_{j-j'} \sigma^+_j \sigma^-_{j'} + \frac{g^2}{2} \sum_{j \neq j'} C_{j-j'} a_{j'}^\dagger a_j (\sigma^z_j + \sigma^z_{j'}) + \frac{g^2}{2} C_0 \sum_j (2a_{j'}^\dagger a_j + 1) \sigma^z_j
\]

where we have again dropped a global constant. We define and approximate the involved coupling constants \( C_m \) by

\[
C_m = \frac{1}{N} \sum_k \frac{1}{\Delta_k} e^{imk} = \frac{1}{N\Delta} \sum_k \frac{e^{imk}}{1 - \frac{2\pi}{\Delta} \cos k} \approx \frac{1}{\Delta} \left( \frac{t}{\Delta} \right)^m,
\]

where we assume \( 0 \leq m \leq N/2 \). (Outside this range, the same substitution \( m \to |m \mod N| \) applies.) Note that the difference between \( \tilde{C}_m^+ \) and \( \tilde{C}_m^- \) disappears once the counter-rotating term \( \sim 1/\Sigma_k \) is dropped.

The photon-mediated qubit-qubit interaction captured by the second term on the right-hand side of Eq. (4.16) now has the typical flip-flop form reminiscent of the well-known “quantum bus” interaction in the context of multiple qubits in a single resonator [61]. According to the
Figure 4.5. Illustration of the “flip-flop” interaction between qubits separated by several lattice sites in dispersive JC regime. The qubit on the left flips down and creates a virtual photon, which hops $m$ steps and is absorbed by the qubit on the right. The qubit on the right hence flips up. The interaction strength is proportional to $(t/\Delta)^m$.

form of the coupling constants $C_m$, this interaction is again short-ranged and decreases exponentially with the distance between lattice sites. As illustrated in Fig. 4.5, mediation of this interaction requires a virtual photon to hop across $m$ lattice sites, thus explaining the factor $(t/\Delta)^m$ in $C_m$ responsible for the short-range nature. We name such a short-range flip-flop interaction as a “quantum metro”, in the sense that it involves multiple intermediate “stations” (sites). The exponential factor $(t/\Delta)^m$ is also recently observed in the experiment by David Schuster’s group at U Chicago [67].

The third term describes the same conditional photon hopping discussed for the Rabi lattice above. The fourth and final term combines the AC Stark and Lamb shifts of the on-site qubit-photon system, in agreement with the results in Ref. [7] when using the weak-coupling approximation $C_0 \approx 1/\Delta$. 
4.3. Physics of Jaynes-Cummings lattices in the dispersive regime

4.3.1. Effective flip-flop interaction between qubits

In the Jaynes-Cummings regime, the interaction described by Eq. (4.15) only swaps qubit and resonator excitations. As a consequence, the Hamiltonian has a $U(1)$ symmetry and the total number of excitations $N_{\text{tot}} = \sum_j (a_j^\dagger a_j + \sigma_j^+ \sigma_j^-)$ is conserved. In the dispersive Jaynes-Cummings regime, the inter-conversion of qubit and photon excitations is suppressed. By switching to a dressed-state basis, the Schrieffer-Wolff transformation eliminates this interaction term. In that dressed-state basis, the total numbers of photon excitations, $N_{\text{ph}} = \sum_j a_j^\dagger a_j = \sum_k a_k^\dagger a_k$, and of qubit excitations, $N_{\text{qu}} = \sum_j \sigma_j^+ \sigma_j^-$, are conserved separately and the effective Hamiltonian, Eq. (4.16), hence possesses a $U(1) \times U(1)$ symmetry. In other words, the effective Hamiltonian separates into blocks with fixed $N_{\text{ph}}$ and $N_{\text{qu}}$, thus greatly simplifying the numerical diagonalization.

The interaction terms emerging in the second-order treatment of the Jaynes-Cummings lattice are ordinary AC Stark shifts, conditional photon hopping terms, and qubit-qubit interaction of flip-flop (XY) type; see Eq. (4.16). We now focus on the qubit-qubit interaction. As usual, the effective flip-flop interaction can be rewritten as an XY interaction between (pseudo) spins,

\[
\tilde{H}_{\text{qubit-qubit}} = g^2 \sum_{j \neq j'} C_j \sigma_j^+ \sigma_{j'}^- = \sum_{j > j'} J_{j-j'} (\sigma_j^x \sigma_{j'}^x + \sigma_j^y \sigma_{j'}^y),
\]

with an interaction strength given by $J_m$. Keeping the leading order term in $t/\Delta$, we can approximate the interaction strength as

\[
J_m = \frac{g^2}{2} C_m \approx \frac{g^2}{2\Delta} \left( \frac{t}{\Delta} \right)^m.
\]
Table 4.1. Summary of the effective spin-spin interactions in the dispersive Jaynes-Cummings lattice, Eqs. (4.16) and (4.18). Analogous statements hold for the dispersive Rabi lattice, Eqs. (4.11) and (4.27), where $J_m$ should be replaced by $\tilde{J}_m$.

<table>
<thead>
<tr>
<th>detuning</th>
<th>hopping</th>
<th>nearest neighbor</th>
<th>next-nearest neighbor</th>
<th>Frustration?</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta &gt; 0$</td>
<td>$t &gt; 0$</td>
<td>$J_1 &gt; 0$ (AF)</td>
<td>$J_2 &gt; 0$ (AF)</td>
<td>Yes</td>
</tr>
<tr>
<td>$\Delta &gt; 0$</td>
<td>$t &lt; 0$</td>
<td>$J_1 &lt; 0$ (FM)</td>
<td>$J_2 &gt; 0$ (AF)</td>
<td>Yes</td>
</tr>
<tr>
<td>$\Delta &lt; 0$</td>
<td>$t &gt; 0$</td>
<td>$J_1 &gt; 0$ (AF)</td>
<td>$J_2 &lt; 0$ (FM)</td>
<td>No</td>
</tr>
<tr>
<td>$\Delta &lt; 0$</td>
<td>$t &lt; 0$</td>
<td>$J_1 &gt; 0$ (FM)</td>
<td>$J_2 &lt; 0$ (FM)</td>
<td>No</td>
</tr>
</tbody>
</table>

An interesting fact to note is that $J_m$ can be tuned with the detuning $\Delta$ and the photon hopping strength $t$. It is thus conceivable to engineer both “ferromagnetic” (FM) or “antiferromagnetic” (AF) qubit-qubit interactions, including the possibility of terms leading to non-nearest-neighbor frustration. The signs for $J_1$ (nearest-neighbor), $J_2$ (next-nearest-neighbor), and the presence or absence of frustration is summarized in Table 4.1 for the configurations that can occur.

It is well known that the 1D antiferromagnetic $J_1$-$J_2$ XY and Heisenberg models show a phase transition related to frustration and spontaneous dimerization [33, 62, 71, 72, 73]. According to Refs. [72, 73], the critical point for the $J_1$-$J_2$ XY model is given by $J_2/J_1 = 0.32$, which could indeed be accessible with the dispersive Jaynes-Cummings lattice where $J_2/J_1 = t/\Delta$. [We recall that: the necessary condition $|t/\Delta| < 1/2$ mentioned subsequent to Eq. (4.12) is indeed weaker and compatible with this value.] The frustration physics for the Jaynes-Cummings lattice, however, is more intricate: next-nearest neighbor frustration only occurs in the positive-detuning regime where the participation of photons is unavoidable. In order to determine the fate of the phase transition, one thus needs to investigate the relevance of the photon terms in Eq. (4.11) for the infinite chain near criticality, which is beyond the scope of this thesis.
4.3.2. **Effective Hubbard interaction between photons (fourth-order perturbation)**

In the previous section, we have derived the effective Hamiltonian up to second order. However, although the effective interaction between different qubits mediated by virtual photons appears at the second order, the effective interaction between photons mediated by qubits is missing at that order. Here, we consider the fourth-order effective interactions in the Jaynes-Cummings regime. The complete derivation with the Schrieffer-Wolff transformation to fourth-order is in principle possible but very cumbersome. Thus, instead of a complete derivation, we point out the generic form to fourth order, and discuss certain terms in a simplified limit.

The Jaynes-Cummings interaction (treated as perturbation) written with itinerant photon operators can be expressed as follows:

\[
V = \frac{g}{\sqrt{N}} \sum_k \sum_j \left( a_k \sigma_j^+ e^{ikj} + \text{H.c.} \right).
\]

The fourth-order perturbation theory produces terms which are proportional to \( V^4 \). As pointed out in the previous subsection, in the dispersive regime, the total numbers of photons \( N_{\text{ph}} = \sum_j a_j^+ a_j = \sum_k a_k^+ a_k \), and of qubit excitations, \( N_{\text{qu}} = \sum_j \sigma_j^+ \sigma_j^- \) are conserved separately. Thus, besides fourth-order corrections to existing types of terms in second-order effective interactions,
the following new types of effective interaction emerge in fourth order:

\[
\tilde{V}_{4th} = \sum_{\{k_p\},\{j_p\}} \left[ \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^a a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \right.
\]
\[
\left. \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^b a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \sigma_1^+ \sigma_2^- \sigma_3^- \sigma_4^+ e^{-i k_1 j_1} e^{-i k_2 j_2} e^{-i k_3 j_3} e^{i k_4 j_4} \right]
\]
\[
+ \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^c a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} \sigma_1^+ \sigma_2^- \sigma_3^- \sigma_4^+ e^{-i k_1 j_1} e^{-i k_2 j_2} e^{-i k_3 j_3} e^{i k_4 j_4} \right]
\]
\[
+ \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^d a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} \sigma_1^+ \sigma_2^- \sigma_3^- \sigma_4^+ e^{-i k_1 j_1} e^{-i k_2 j_2} e^{i k_3 j_3} e^{-i k_4 j_4} \right]
\]
\[
+ \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^e a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} \sigma_1^+ \sigma_2^- \sigma_3^- \sigma_4^+ e^{-i k_1 j_1} e^{i k_2 j_2} e^{i k_3 j_3} e^{-i k_4 j_4} \right]
\]
\[
+ \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^f a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4} \sigma_1^+ \sigma_2^- \sigma_3^- \sigma_4^+ e^{i k_1 j_1} e^{i k_2 j_2} e^{-i k_3 j_3} e^{-i k_4 j_4} \right].
\]

The coefficients \( \tilde{U}_{k_1,k_2,k_3,k_4,j_1,j_2,j_3,j_4}^{a,b,c,d,e,f} \) must be determined by detailed calculation with the Schrieffer-Wolff transformation. In general, this type of interaction involves four qubits and four photons. An example involving four different sites and the corresponding ladder diagrams are shown in Fig. 4.6.

In the large negative-detuning regime (\( \epsilon \ll \omega \)), the low-energy manifold has zero total photons \( N_{ph} = 0 \). Therefore, we project the effective interaction \( \tilde{V}_{4th} \) into the zero photon subspace, namely \( \tilde{V}_{4th,ph=0} = P_{ph=0} \tilde{V}_{4th} P_{ph=0} \). Here, the projector is defined as \( P_{ph=0} = |0\rangle_{ph} \langle 0| \), where \( |0\rangle_{ph} \) represents the photon vacuum. The projected effective interaction hence contains no photon operator, since these operators are contained in the following matrix element

\[
\langle 0 | a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} | 0 \rangle_{ph}
\]

which becomes as a c-number (to have nonzero contribution, momentum conservation of the created and annihilated photons is required). Thus, the projected effective interaction is a four-spin interaction mediated by virtual photons, namely...
Figure 4.6. (a) Illustration of fourth-order effective interaction involving qubits on four different sites of a plaquette. Two qubits are flipped down accompanied by creation of two itinerant photons, and two qubits are flipped up accompanied by annihilation of two itinerant photons. One should keep in mind that this illustrated effective interaction is accompanied by its Hermite conjugate partner (inverse the flip-flop process mentioned above) to ensure the Hermiticity of the effective Hamiltonian. Note that we have promoted the quasi momentum $k$ into vector $\vec{k}$ to discuss the situation in 2D. (b) The four different virtual paths corresponding to the effective interaction shown in panel (a).

\[ \sum_{\{j_p\}} \tilde{U}_{j_1,j_2,j_3,j_4} \sigma^+_{j_1} \sigma^-_{j_2} \sigma^+_{j_3} \sigma^-_{j_4}. \]  The coefficient $\tilde{U}_{j_1,j_2,j_3,j_4}$ needs to be determined by detailed calculation.

In the large positive-detuning regime ($\epsilon \gg \omega$), the low-energy manifold has zero total qubit excitation $N_{\text{qu}} = 0$. Therefore, we project the effective interaction $\tilde{V}_{\text{4th}}$ into the zero qubit excitation subspace, namely $\tilde{V}_{\text{4th, qu}=0} = P_{\text{qu}=0} \tilde{V}_{\text{4th}} P_{\text{qu}=0}$. Here, the projector is defined
as $P_{\text{qu}=0} = |0\rangle_{\text{qu}} \langle 0 |$, where $|0\rangle_{\text{qu}}$ represents the qubit vacuum (all qubits point down). The
projected effective interaction hence contains no spin operator, since these operators are con-
tained in the following matrix element $\text{qu} \langle 0 | \sigma_{j_1}^- \sigma_{j_1}^+ \sigma_{j_2}^- \sigma_{j_2}^+ | 0 \rangle_{\text{qu}}$ (only involving at most two qubit sites to have nonzero contribution) which becomes a c-number. Thus, the projected effective interaction is a four-photon interaction mediated by the virtual excitations of qubits, namely
$\sum_{\{k_p\}} \tilde{U}_{k_1,k_2,k_3,k_4} a_{k_1}^\dagger a_{k_2} a_{k_3}^\dagger a_{k_4}$. From the gained experience in second-order perturbation theory,
we know that, when we express the itinerant photon operators in terms of onsite photon oper-
ators, a prefactor $\left(\frac{t}{\Delta}\right)^m$ arises, where $m$ depends on the distance between the lattice sites. A
similar prefactor is anticipated to appear at fourth-order, and the leading term in the series of
$\left(\frac{t}{\Delta}\right)^m$ should be $m = 0$, which means the four photon operators are at the same site. In that case,
the effective Hubbard interaction should be independent of the hopping rate $t$ and hence can be
derived from a single-site Jaynes-Cummings model. Thus, we can directly derive the effec-
tive Hubbard interaction from expanding the exact solution of the single-site Jaynes-Cummings
Hamiltonian given in Chapter \[1.2.2\] The exact eigen-energy Eq. (1.4) of the upper and lower
polaritons can be expanded as a series in $g/\Delta$ as:

\[
E_{n\pm} = n\omega + \frac{\Delta}{2} \pm \sqrt{\left(\frac{\Delta}{2}\right)^2 + ng^2} = n\omega + \left(\frac{\Delta}{2} \pm \frac{\Delta}{2}\right) \pm g^2 \frac{\Delta}{\Delta^2 n^2} \pm \frac{1}{4} \frac{g^4}{\Delta^3 n^2} + O(\frac{g}{\Delta})^6).
\]

Here, $n$ represents the number of total excitation. In the large positive-detuning regime, we
assume that the qubit excitation is always being zero. Hence $n$ represents the photon number in
this case. Since the qubit is not excited for the low-lying states, the relevant low energy states
all correspond to the lower-polariton. Thus, we get the low-lying eigen-energy of the single JC
site as:

\[ E_n^- = (\omega - \frac{g^2}{\Delta} + \frac{g^4}{4\Delta^3})n + \frac{1}{4} \frac{g^4}{\Delta^3} n(n-1) + O[(\frac{g}{\Delta})^6]. \]

Thus, to fourth order of \( g/\Delta \), we get an effective repulsive Hubbard interaction (since \( \Delta > 0 \)).

For the JC lattice model, it can be written as

\[ \tilde{V}_{\text{Hubbard}} = \sum_j \frac{1}{4} \frac{g^4}{\Delta^3} a_j^\dagger a_j (a_j^\dagger a_j - 1). \]

In Chapter 4, we will focus on the Jaynes-Cummings lattice model in the positive-detuning regime, and rely on this derivation to assume an effective Bose-Hubbard model for the interacting photons.

### 4.4. Physics of Rabi lattices in the dispersive regime

Now we switch from the physics of Jaynes-Cummings lattices to Rabi lattices when the interaction strength reaches the ultra-strong coupling limit. In particular, we consider physics in two different dispersive regimes, namely when the detuning is negative \( (\Delta = \epsilon - \omega < 0) \) or positive \( (\Delta = \epsilon - \omega > 0) \). The ground states in these two cases are distinct: in the negative detuning regime, the ground state is a ferromagnetic state with photon-dressed qubits; in the positive detuning regime, the ground state has an unusual photon pairing property.

#### 4.4.1. Ferromagnetic ground state of photon-dressed qubits \( (\Delta < 0) \)

In the case of negative detuning, the qubit frequency \( \epsilon \) is small compared to the photon frequency \( \omega \) and we may perform a series expansion in the small parameter \( \epsilon/\omega \ll 1 \). Referring to
Eq. (4.14), we find that the resulting coupling constants scale as

\[ \tilde{C}_m^+ = -\frac{2(m + 1)}{\omega} \frac{\epsilon}{\omega} \left( \frac{-t}{\omega} \right)^m + O(\epsilon^3/\omega^3), \quad \tilde{C}_m^- = -\frac{2}{\omega} \left( \frac{-t}{\omega} \right)^m + O(\epsilon^2/\omega^2), \]

from which we infer that \( \tilde{C}_m^+ \ll \tilde{C}_m^- \) as long as \( m \) is sufficiently small.

By inspection, we note that there are only two terms in the effective Hamiltonian (4.11) – the last two – which do not conserve photon number. These correspond to photon pair creation contributions with individual strengths set by \( g^2 \tilde{C}_m^+ \) with \( m \geq 1 \). For large photon energies \( \omega \gg \epsilon, t, g \), it is clear that the inequality

\[ \omega \gg g^2 \tilde{C}_m^+ \sim \epsilon \left( \frac{g}{\omega} \right)^2 \left( \frac{t}{\omega} \right)^m \]

is satisfied automatically. Consequently, photon pair creation is strongly suppressed. Therefore, the resulting ground state is expected to be essentially free of photons in the dressed-state basis.

These arguments lead us to the following dispersive Rabi model at negative detuning, valid in the \( N_{\text{ph}} = 0 \) manifold:

\[ \tilde{H}_{\text{eff}} \bigg|_{N_{\text{ph}}=0} \approx \frac{\epsilon + \tilde{K}_0}{2} \sum_j \sigma_j^z + \sum_{j>j'} \tilde{J}_{j-j'} \sigma_j^x \sigma_{j'}^x \]

Here, the Ising coupling and Lamb shift parameter are given by

\[ \tilde{J}_m = g^2 \tilde{C}_m^- \approx -\frac{2g^2}{\omega} \left( \frac{-t}{\omega} \right)^m \quad \text{and} \quad \tilde{K}_0 = g^2 \tilde{C}_0^+ \approx -\frac{2g^2 \epsilon}{\omega^2}. \]

As before, the interaction strength \( \tilde{J}_m \) decreases exponentially with the lattice site distance \( m \).

The relevant signs of the coupling parameters can be inferred from Table 4.1 (substituting \( J_m \rightarrow \))
\( \tilde{J}_m \). The renormalized qubit frequency \( \epsilon' = \epsilon + \tilde{K}_0 \) plays the role of the effective “magnetic field” (up to a factor of 2), and tends to align the pseudo spin in the negative \( z \) direction. However, the counter-rotating terms of the \( \sigma^x_j \sigma^x_j' \) interaction compete with this tendency by tilting the pseudo spin towards the \( xy \)-plane.

For nearest-neighbor coupling only (i.e., \( \tilde{J}_m \approx 0 \) for \( m > 1 \)), we obtain a simple transverse-Ising model, which is exactly solvable via the Jordan-Wigner transformation \[84\]. In the thermodynamic limit (infinite chain), one recovers the usual quantum phase transition between a paramagnetic and a ferromagnetic phase. The transition occurs at \( \tilde{J}_1 = \epsilon/2 \), which here implies a critical coupling of \( g^* = \frac{\omega}{2} \sqrt{\frac{t}{T}} \). (Corrections from weak non-nearest-neighbor interaction are expected to slightly shift this transition point.) Below \( g^* \), the system is in the “paramagnetic” (PM) phase – with the ground state approximately given by the trivial vacuum state \( | \tilde{g} \rangle_{PM} \approx |0\rangle_{ph} \otimes |\downarrow\downarrow\cdots\downarrow\rangle \), where \( |0\rangle_{ph} \) denotes the photon vacuum and \( |\downarrow\rangle \) the low-energy \( \sigma^z \) eigenstate of each qubit. Above \( g^* \), the system is in the “ferromagnetic” (FM) phase (assuming \( t > 0 \)). The two symmetry-broken ground-state wavefunctions of the system are approximately given by \( | \tilde{g}_R \rangle_{FM} \approx |0\rangle_{ph} \otimes |\rightarrow\rightarrow\cdots\rightarrow\rangle \) and \( | \tilde{g}_L \rangle_{FM} \approx |0\rangle_{ph} \otimes |\leftarrow\leftarrow\cdots\leftarrow\rangle \), where \( |\rightarrow\rangle \) and \( |\leftarrow\rangle \) are the two \( \sigma^x \) eigenstates.

The latter states, marked with tildes, denote eigenstates of the effective Hamiltonian. To obtain the eigenstates of the original Hamiltonian, we perform the inverse Schrieffer-Wolff transformation \( |g\rangle = e^{-iS_1}|\tilde{g}\rangle \) with the previously used generator from Eq. (4.7). We illustrate the inverse transformation for the weak-hopping limit, \( t \to 0 \). In this case, the generator reduces to

\[
(4.29) \quad S_1 \approx i \sum_j \left[ \frac{g}{\Delta} (a_j^\dagger \sigma^-_j - \text{H.c.}) + \frac{g}{\Sigma} (a_j \sigma^-_j - \text{H.c.}) \right],
\]
and the inverse transformation decouples into mere onsite terms. Further approximating $\Delta \approx -\omega$ and $\Sigma \approx \omega$, we obtain

$$
| g \rangle = e^{-iS_1} | \tilde{g} \rangle \approx \prod_j \exp \left[ -\frac{g}{\omega} (a_j^\dagger - a_j) \sigma_j^x \right] | \tilde{g} \rangle.
$$

(4.30)

For the first of the two “FM” ground states, we evaluate

$$
| g_R \rangle_{FM} \approx \prod_j \exp \left[ -\frac{g}{\omega} (a_j^\dagger - a_j) \sigma_j^x \right] | 0 \rangle_{ph} \otimes | \rightarrow \rightarrow \rightarrow \cdots \rightarrow \rangle.
$$

(4.31)

Since each qubit is in a $\sigma^x$ eigenstate, we recognize the remaining operator acting on the photon vacuum as a displacement operator $D(\mp \frac{g}{\omega})$ [27], producing a coherent photon state on each site:

$$
| g_R \rangle_{FM} \approx \prod_j | \alpha_j = -\frac{g}{\omega} \rangle_j \otimes | \rightarrow \rangle_j \quad \text{and} \quad | g_L \rangle_{FM} \approx \prod_j | \alpha_j = \frac{g}{\omega} \rangle_j \otimes | \leftarrow \rangle_j.
$$

(4.32)

In a similar way, we find

$$
| g \rangle_{PM} \approx \prod_j \left[ | \alpha_j = -\frac{g}{\omega} \rangle_j \otimes | \rightarrow \rangle_j - | \alpha_j = \frac{g}{\omega} \rangle_j \otimes | \leftarrow \rangle_j \right].
$$

(4.33)

for the paramagnetic ground state in the $t \rightarrow 0$ limit. We note that these results are consistent with those obtained by a different method in Ref. [43]. In the general case, and particularly for quantitative comparison, the inverse transformation must be carried out for arbitrary hopping strength $t$, leading to further corrections to Eqs. (4.32) and (4.33). We will properly account for this in our discussion in Sec. 4.4.

Finally, we note that for the $N_{ph} > 0$ manifolds, the situation is slightly more complicated. According to Eq. (4.25), when keeping terms with coefficient $\tilde{C}_1^-$, we can ignore all terms
with coefficients $\tilde{C}_m^\pm$ except for those with $\tilde{C}_0^+$, which give rise to the Lamb shifts and the AC Stark shifts. Thus, our effective Hamiltonian turns into a transverse-Ising model and a photon tight-binding model, with the only coupling between the two being the AC Stark shifts term, namely

$$\tilde{H}_{\text{eff}} \approx \frac{\tilde{K}_0}{2} \sum_j \sigma_j^z + \sum_j \tilde{J}_1 \sigma_j^x \sigma_{j+1}^x + \omega \sum_j a_j^\dagger a_j + t \sum_{j,j'} \left( a_j^\dagger a_{j'} + \text{H.c.} \right)$$

$$+ g^2 \tilde{C}_0^+ \sum_j a_j^\dagger a_j \sigma_j^z. \quad (4.34)$$

4.4.2. Photon pairing ($\Delta > 0$)

In the dispersive Rabi regime with positive detuning, the photon frequency $\omega$ is small compared to the qubit frequency $\epsilon$. Thus, we may Taylor-expand in $\omega/\epsilon$ and find that the coupling constants $\tilde{C}_m^\pm$ now depend on whether $m$ is even or odd in the following way:

$$\text{odd } m : \quad \tilde{C}_m^+ = \frac{2(m+1)}{\epsilon} \frac{\omega}{\epsilon} \left( \frac{t}{\epsilon} \right)^m + O(\omega^3/\epsilon^3), \quad (4.35)$$

$$\text{even } m : \quad \tilde{C}_m^+ = \frac{2}{\epsilon} \left( \frac{t}{\epsilon} \right)^m + O(\omega^2/\epsilon^2). \quad (4.36)$$

For $\tilde{C}_m^-$ exactly the same expressions apply, except for an interchange of the roles of ‘even’ vs. ‘odd’. Thus, in addition to the overall decrease in coupling with increasing lattice site distance $m$, we see that $\tilde{C}_m^+$ is further suppressed for odd $m$, whereas $\tilde{C}_m^-$ is further suppressed for even $m$.

Following a line of argument analogous to the one we employed for negative detuning, we note that now the effective Ising coupling is small compared to the qubit frequency, $\tilde{J}_m \ll \epsilon$. As a result, we may neglect the counter-rotating terms $\sigma_j^+ \sigma_j^+ + \sigma_j^- \sigma_j^-$ of the Ising interaction. The
remaining qubit-qubit interaction is then of XY-type, and conserves the total number of qubit
excitations \( N_{\text{qu}} \). Since we are here interested in the ground state and low-lying states only, we
can restrict our discussion to the \( N_{\text{qu}} = 0 \) subspace. In this subspace, the effective dispersive
Hamiltonian consequently takes the form

\[
\hat{H}_{\text{eff}} \big|_{N_{\text{qu}} = 0} \approx \omega \sum_j a_j^\dagger a_j + t \sum_j \left( a_j^\dagger a_{j+1} + \text{H.c.} \right) \\
- \frac{g^2}{2} \sum_{j,j'} \tilde{C}^{+}_{j-j'} (a_j^\dagger a_{j'} + a_{j'}^\dagger a_j^\dagger + \text{H.c.}).
\]

This corresponds to a photon tight-binding model with additional on-site and off-site photon
pair creation/annihilation as well as additional, second-order photon hopping terms. Compari-
on with the expressions for \( \tilde{C}^+_{m} \) in Eqs. (4.35) and (4.36) shows that onsite terms dominate the
second-order contributions. Nearest neighbor and next-nearest neighbor terms are suppressed
by factors of \( \omega t/\epsilon^2 \) and \( t^2/\epsilon^2 \), respectively.

By rewriting the effective Hamiltonian (4.37) in \( k \) space, we obtain

\[
\hat{H}_{\text{eff}} \big|_{N_{\text{qu}} = 0} = \sum_k \left[ \omega_k a_k^\dagger a_k + \frac{1}{2} \delta_k (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger) \right].
\]

The photon dispersion \( \omega_k \) and photon pairing amplitude \( \delta_k \) can be expressed as a Fourier series
with coefficients determined by \( \tilde{C}^{+}_{m} \). We approximate them by truncating the series at \( \tilde{C}^{+}_{0} \) and
neglecting higher-order hopping and pairing. That way, we find

\[
\omega_k \approx \omega + 2t \cos k - 2g^2/\epsilon, \quad \delta_k \approx -2g^2/\epsilon.
\]
Here, the pairing amplitude has become $k$-independent since only on-site pairing is taken into account.

We solve this Hamiltonian by performing the Bogoliubov transformation

\begin{equation}
  b_k = u_k a_k + v_k a^\dagger_{-k}, \quad b^\dagger_{-k} = v_k a_k + u_k a^\dagger_{-k},
\end{equation}

where the coefficients $u_k$ and $v_k$ can be chosen real-valued and must satisfy $u_k = u_{-k}, v_k = v_{-k}$ and $u_k^2 - v_k^2 = 1$, such that canonical bosonic commutation relations hold for the new operators. As usual, we ensure these conditions by expressing the coefficients in the form $u_k = \cosh r_k$, $v_k = \sinh r_k$. Defining the remaining $r_k$ parameter via $\tanh (2 r_k) = \frac{\delta_k}{\omega_k}$, the effective Hamiltonian is rendered diagonal, i.e., $\tilde{H}_{\text{eff}} \bigg|_{N_{\text{qu}}=0} = \sum_k E_k b_k^\dagger b_k$, and the spectrum is given by

\begin{equation}
  E_k = \sqrt{\omega_k^2 - \delta_k^2} \approx \sqrt{\left(\omega + 2t \cos k - 2g^2 / \epsilon\right)^2 - 4g^4 / \epsilon^2}.
\end{equation}

Next, we show that the ground state (i.e., the ‘vacuum’ of Bogoliubov excitations) corresponds to a squeezed vacuum state of photons. The two-mode squeezing operator is $S_2(\xi_k) = \exp[\xi_k^* a_k a_{-k} - \xi_k a^\dagger_k a^\dagger_{-k}]$ where $\xi_k = r_k e^{i \varphi k}$ is the squeezing parameter [27]. The Bogoliubov transformation is then equivalent to a two-mode squeezing transformation according to

\begin{equation}
  b_k = S_2(\xi_k) a_k S_2^\dagger(\xi_k) = a_k \cosh r_k + e^{i \varphi k} a^\dagger_{-k} \sinh r_k,
\end{equation}

\begin{equation}
  b_{-k} = S_2(\xi_k) a_{-k} S_2^\dagger(\xi_k) = a_{-k} \cosh r_k + e^{i \varphi k} a^\dagger_k \sinh r_k.
\end{equation}
Comparing with the results from the Bogoliubov transformation above, we find that the squeezing parameters are given by $\phi_k = 0$ and

$$r_k = \frac{1}{2} \tanh^{-1}(\delta_k/\omega_k) \approx \frac{1}{2} \tanh^{-1}\left(-\frac{2g^2/\epsilon}{\omega + 2t \cos k - 2g^2/\epsilon}\right).$$

For the two special cases of $k = 0$ or $k = \pi$ (center and edge of the first Brillouin zone), one obtains one-mode squeezing instead of two-mode squeezing. The ground state of the Rabi lattice in this regime can hence be expressed as a squeezed vacuum state,

$$|\tilde{g}\rangle = \prod_{k \geq 0} S_2(r_k) |0\rangle = \prod_{k \geq 0} \exp \left[ r_k a_k a_{-k} - r_k a_k^\dagger a_{-k}^\dagger \right] |0\rangle.$$  

involving entangled dressed photon pairs with opposite quasi-momenta.

It is useful to point out that Eqs. (4.41) and (4.44) also reveal the necessary breakdown of perturbation theory when $g$ exceeds a critical value $g_c$. Specifically, when $|\delta_k| > \omega_k$, the squeezing parameter is ill-defined and $E_k$ becomes imaginary. The resulting critical value

$$g_c = \frac{1}{2} \min_k \sqrt{\epsilon(\omega - 2t \cos k)} = \frac{1}{2} \sqrt{\epsilon(\omega - 2|t|)}$$

thus marks the maximum possible value for the convergence radius of the perturbative expansion. In the context of a single Rabi site, the critical coupling strength $g_c = \frac{1}{2} \sqrt{\epsilon \omega}$ has previously been derived in Ref. [2]. We note that for positive detuning, $g \ll g_c$ is a more restrictive condition than the condition $g \ll \Delta_{\text{min}}$. The inequality $g \ll g_c$ thus replaces Eq. (4.6) as the necessary condition for the dispersive regime at positive detuning. As $g$ is increased beyond $g_c$, perturbation theory is no longer valid. Entering this quasi-resonant regime of the Rabi lattice,
it is plausible that the system will undergo the same type of phase transition with $Z_2$ symmetry breaking that was studied by Schiro et al. [86] for the case of exact resonance, $\epsilon = \omega$.

We illustrate the dressed-photon ground state by calculating several observables related to photon numbers and pairing amplitudes. The ground state expectation value for the photon number in mode $k$ is given by

$$\langle \tilde{g} | a_k^\dagger a_k | \tilde{g} \rangle = \langle 0 | S_2^\dagger(r_k) a_k^\dagger S_2(r_k) a_k S_2(r_k) | 0 \rangle = \sinh^2(r_k) .$$

Similarly, we find that the pair amplitude for dressed photons of opposite quasi-momenta is

$$\langle \tilde{g} | a_k a_{-k} | \tilde{g} \rangle = \langle \tilde{g} | a_k^\dagger a_{-k}^\dagger | \tilde{g} \rangle = - \sinh r_k \cosh r_k .$$

No such pairing occurs for photons with identical quasi-momenta:

$$\langle \tilde{g} | a_k a_k | \tilde{g} \rangle = \langle \tilde{g} | a_k^\dagger a_k^\dagger | \tilde{g} \rangle = 0 ,$$

as long as the quasi-momenta $k$ and $-k$ are distinct (i.e., $k = 0$ and $k = \pi$ are excluded). All these are the usual properties of two-mode squeezed states [27].

4.5. Application to the Rabi dimer and comparison with the results from exact diagonalization

In order to illustrate the utility of the effective dispersive Hamiltonian, and to demonstrate its validity by comparison with results from exact numerical diagonalization, we now turn to the specific example of the Rabi dimer, i.e., two coupled Rabi sites. We choose this example to make exact diagonalization of the full Rabi lattice Hamiltonian (4.1) as tractable as possible, and emphasize that results obtained from the effective Hamiltonian easily carry over to larger
lattices, as evident from our Eq. (4.11). For verification of our approximations, we select representative observables, and calculate their expectation values by exact diagonalization of the original Rabi lattice Hamiltonian (4.1). We then compare these results with those obtained from our effective Hamiltonians (4.34) and (4.37), which are simplified approximations to Hamiltonian (4.11) in the negative- and positive-detuning regimes respectively using the full expressions for the coupling constants $\tilde{C}_m^\pm$ from Eq. (4.12).5

### 4.5.1. The dispersive regime with negative detuning

Figure 4.7 shows the comparison for the dispersive regime with negative detuning, where example parameters have been chosen as $\omega = 5\epsilon$ and $t = \epsilon$. With this choice of $t$, the inequality $|t/\Delta| < 1$ holds and the dispersive condition (4.6) can be satisfied. For the Rabi dimer with positive $t$, Eq. (4.6) takes the simple form $\Delta_{\text{min}} = \omega - |t| - \epsilon \gg g$, where $\Delta_{\text{min}}$ corresponds to the detuning of the antisymmetric photon mode. Perturbation theory and the effective Hamiltonian are expected to work reasonably well as long as $g/\Delta_{\text{min}}$ is sufficiently small. This is indeed confirmed by figure 4.7. The individual results from the four panels are as follows.

Panel (a) shows the lowest seven excitation gaps $E_j - E_0$ ($E_0$ being the ground-state energy and $E_j$ the $j$-th excited-state energy) as a function of the Rabi coupling strength $g$. The lower three gaps correspond to states in the $N_{\text{ph}} = 0$ manifold, the remaining four to the $N_{\text{ph}} = 1$ manifold. The different curves correspond to exact numerical diagonalization on one hand, and results using the effective Hamiltonian (4.34) on the other hand. We find very good agreement between approximate and exact results, up to values as high as $g/\Delta_{\text{min}} \simeq 0.8$. As expected, the lower gaps in the manifold with lower photon number match comparatively better. Perturbation

---

5An additional replacement $t \rightarrow t/2$ is performed to account for the fact that a two-site Rabi ring is equivalent to a dimer except for a factor of 2 in the hopping amplitude.
Figure 4.7. Rabi dimer in the dispersive regime with negative detuning: comparison of representative observables between exact diagonalization and effective Hamiltonian. All panels show observables as a function of the Rabi coupling $g$. (a) Lowest excitation gaps $E_j - E_0$ between level $j$ and the ground state. Solid curves show results from exact numerical diagonalization, circles mark results obtained from the effective Hamiltonian [4.34]. (b) Fidelity of the ground state wavefunction with respect to the exact result. Green circles (full inverse SW transformation) and the red dashed curve (truncated inverse SW transformation) depict results from the effective Hamiltonian, differing only in the order of the inverse Schrieffer-Wolff transform (see main text). Blue dotted line: fidelity of the vacuum state for comparison. (c) and (d) Ground-state expectation values for number of qubit and photon excitations on the left Rabi site. The comparison shows exact results (blue solid curve), and results from the effective Hamiltonian with two different inverse transformation schemes (green circles and red dashed curve). Over a wide range of $g$, the results from the effective Hamiltonian agree well with the exact results until $g$ approaches $\Delta_{\text{min}}$, where the perturbation is known to break down. (Parameters used: $\omega = 5\epsilon$, $t = \epsilon$; photon cutoff per site: $n_c = 12$.)

theory must break down for $g/\Delta_{\text{min}} \geq 1$, as the qubit reaches quasi-resonance with the antisymmetric photon mode at this point. Note that for small $g/\Delta_{\text{min}}$ the 5th to 7th excitation gap differs from the 1st to 3rd excitation gap by a frequency $4\epsilon$, which corresponds to the photon
frequency of the antisymmetric mode. This recurrence illustrates the approximate decoupling of the transverse Ising and tight-binding model in the effective Hamiltonian (4.34).

Panel (b) shows the fidelity of the approximate ground-state wavefunctions, as obtained from the effective Hamiltonian (4.34) [or, for the ground state, equivalently to the transverse-Ising model, Eq. (4.27)] and subsequent inverse Schrieffer-Wolff (SW) transformation \( |g\rangle = e^{-iS_1} |\tilde{g}\rangle \). The generator \( S_1 \) we choose here is the exact expression from Eq. (4.7) and we do not take the weak hopping \( (t \to 0) \) limit. For careful comparison, we perform the inverse transformation with two different schemes: (1) we apply the transformation directly in its full exponential form \( e^{-iS_1} \) (full inverse SW transformation), and (2) we apply the transformation but keep only terms up to second order in \( g \), namely \( e^{-iS_1} = 1 - iS_1 + \frac{1}{2}(-iS_1)^2 + O(g^3) \) (truncated inverse SW transformation). (This truncation would be used for consistently keeping only terms up to second order.) For comparison, we also show the fidelity of the trivial vacuum state \( |0\rangle_{ph} \otimes |\downarrow\downarrow\downarrow\cdots\downarrow\rangle \). We observe that in the \( g/\Delta_{\text{min}} \to 0 \) limit, all three fidelities are similar and are very close to a 100% value. For large \( g \), the vacuum fidelity decreases significantly, as expected in the ultra-strong coupling regime. Using the full inverse SW transform, the fidelity of the approximate state is very good, exceeding a 99% value over the full range shown and gives better results than those obtained with the truncated transform.

In panels (c) and (d) we show plots for the ground-state expectation values of the qubit excitation \( \langle \sigma^+_L \sigma^-_L \rangle \) and the photon number \( \langle a_L^\dagger a_L \rangle \) (both measured on one of the two Rabi sites). The agreement between exact and approximate results is excellent over the entire range of \( g \) in the plot. As before, results are slightly better when using the full inverse SW transform instead of the truncated version. It is interesting to note that the number of qubit excitations on each site rises to about 0.25 around \( g/\epsilon = 2.5 \), indicating that the spins (qubits) are tilting up
towards the $xy$-plane. The tilting is mainly induced by the transverse Ising interaction between qubits, namely the $\sigma_L^x \sigma_R^x$ term. We have confirmed numerically that this tilting is negligible for a single-site Rabi system, in which no transverse Ising interaction is present.

Although the effective Hamiltonian (4.27) produces a ground state with zero dressed photons in the negative detuning regime, the undressing from the inverse Schrieffer-Wolff transformation induces small corrections. This effect can be motivated from Eqs. (4.30)–(4.32), which indicate that the $\sigma^x$ qubit eigenstate is always accompanied by a photon coherent state on the same site, namely $\ket{\alpha_j} = -\frac{g}{\omega} \ket{j} \otimes \ket{\rightarrow}_j$. For the finite-size Rabi dimer, the transverse-Ising interaction cannot give rise to an actual phase transition to an ordered spin state. Such a phase transition may, however, appear in the thermodynamic limit (infinite lattice size) but is beyond the scope of this thesis.

4.5.2. The dispersive regime with positive detuning

We next turn to the dispersive regime of the Rabi dimer with positive detuning. Figure 4.8 shows a comparison analogous to that presented in figure 4.7 now with model parameters fixed to $\epsilon = 10\omega$ and $t = 0.3\omega$. Here, we compare the original Rabi-lattice Hamiltonian (4.1) to the effective Hamiltonian in the $N_{\text{qum}} = 0$ manifold, namely Eq. (4.37). We investigate the same set of observables as in the previous subsection and plot them as a function of $g$, here in units of the critical coupling strength $g_c = \frac{1}{2} \sqrt{\epsilon (\omega - |t|)}$ [we have already carried out the $t \rightarrow t/2$ replacement relative to Eq. (4.46)] which is the relevant quantity marking the breakdown of perturbation theory for positive detuning. The critical interaction strength for our choice of parameters is given by $g_c = 1.32\omega$. 
Figure 4.8. Rabi dimer in the dispersive regime with positive detuning: comparison of representative observables between exact diagonalization and effective Hamiltonian (4.37). All panels show observables as a function of the Rabi coupling $g$, and are arranged analogous to figure 4.7: (a) Lowest excitation gaps $E_j - E_0$ between level $j$. (b) Fidelity of the ground state wavefunction with respect to the exact result. The inset depicts the same fidelity plot but close to the critical coupling $g/g_c = 1$. (c) and (d) show the ground-state expectation values for number of qubit and photon excitations on the left Rabi site. The legend follows figure 4.7, i.e., exact diagonalization results: solid curves; results from effective Hamiltonian: circles (no truncation) and dashed curves (with truncation); fidelity of pure vacuum state: blue dotted curve; additional dot-dashed curves in panel (a): analytical expressions of quasiparticle energies from Eq. (4.41). Over a wide range of $g$, the results from the effective Hamiltonian agree well with the exact results until $g$ approaches the critical value $g_c$. (Parameters: $\epsilon = 10\omega$, $t = 0.3\omega$; resulting critical coupling: $g_c = 1.32\omega$; photon cutoff per site: $n_c = 12$.)

The lowest five excitation gaps plotted in panel 4.8(a) show very good agreement between exact and approximate results using the effective Hamiltonian over a wide coupling range, with best agreement for the lowest gap. Here, solid lines and circles represent results from exact diagonalization and diagonalizing the low-lying effective Hamiltonian (4.37) respectively, while
the dot-dashed lines represent results using the analytical expression Eq. (4.41) for the quasiparticle energies (the quasimomentum $k = 0$ and $k = \pi$ correspond to the symmetric and anti-symmetric photon mode respectively). In the $g = 0$ limit, original and Bogoliubov operators coincide, $b_k = a_k$, and excitations correspond to photon Fock states in the two modes. Specifically, for our parameters the 1st, 3rd and 5th excitation gaps correspond to creation of 1, 2 and 3 photons in the anti-symmetric mode with frequency $\omega - t = 0.7\epsilon$. The 2nd excitation gap corresponds to creation of 1 photon in the symmetric mode, which here has frequency $\omega + t = 1.3\epsilon$ etc.. For $g > 0$, the Bogoliubov operators $b_k$ involve both photon annihilation ($a_k$) and creation ($a_k^\dagger$) operators. The eigenstates are no longer pure Fock states and the excitation energies decrease as a function of $g$, as expected from Eq. (4.41).

Panel 4.8(b) shows the ground-state fidelities for our perturbative approximations as well as the trivial vacuum state. For $g$ near 0, the ground state remains quite close to the trivial vacuum state. However, as $g$ is further increased, the expected squeezing of the ground state becomes more significant and the fidelity of the vacuum state drops significantly below the fidelities of our perturbative approximations, which remain very close to 1 until $g$ approaches the critical value $g_c$. The expected breakdown of the perturbative treatment close to $g = g_c$ is shown in the inset of panel (b).

Panels 4.8(c) and (d) show the expected photon number and qubit excitation on one of the two Rabi sites for the Rabi dimer ground state. The exact-diagonalization results based on Eq. (4.1) and our perturbative results based on the effective Hamiltonian (4.37) show good agreement in the relevant range of coupling strengths. Note that, by contrast to the situation of negative detuning, the photon number here exceeds the expected value $\langle \sigma_L^+ \sigma_L^- \rangle$ of qubit
Figure 4.9. Rabi dimer in the dispersive regime with positive detuning: joint-probability distribution $P_{n_L, n_R}$ of the ground state in the dimer Fock basis ($n_L, n_R$: photon number on the left/right site). The results are obtained from exact diagonalization of the full Rabi-lattice Hamiltonian (4.1) with a photon cutoff $n_c = 16$ on each site. The two panels show the distributions for two different parameter sets, as specified in the figure. Note that the distribution $P_{n_L, n_R}$ for even-number Fock states, $n_L + n_R = 2N$, is much larger than their neighboring odd-number Fock states, $n_L + n_R = 2N \pm 1$, which evidently serves as a signature of photon pairing. This pairing signature for parameter set (a) is more significant than the one for set (b), due to the larger detuning of set (a) and hence smaller dressing effect which breaks photon parity.

excitation. Since the ground state is in the $N_{qu} = 0$ manifold, the creation of qubit excitations is merely due to the qubit-photon dressing and is recovered as a correction from the inverse Schrieffer-Wolff transformation. We note that due to the qubit-photon dressing, an additional increase in the photon number arises from the qubit excitation, as dictated by the inverse Schrieffer-Wolff transformation.
4.5.2.1. Visualization of squeezing and photon pairing in the Rabi dimer. In order to elucidate the effect of the photon pairing or squeezing terms in (4.37), we briefly discuss results for the Fock-state probability distribution and the Wigner function describing the Rabi dimer.

Figure 4.9 shows the Fock-state probability distribution of the Rabi dimer ground state,

\[ P_{n_L,n_R} = |\text{tr}_{\sigma_L,\sigma_R}\langle n_L,\sigma_L; n_R,\sigma_R|g\rangle|^2, \]

where \( n_L, n_R \) denote the photon numbers on each Rabi site and we have traced out the qubit degrees of freedom. The distribution confirms that the pure vacuum state, even though dominant in the distribution, is not the true ground state, as expected for ultra-strong coupling. Expressed in terms of dressed photon states, Eq. (4.45) predicts that the ground state should only involve even-number Fock states, \( n_L + n_R = 2N \), while the probability for odd-number Fock states should vanish. Due to the undressing by the inverse Schrieffer-Wolff transform, corrections to this simple picture emerge. As seen in the comparison of panels (a) and (b), these corrections become more significant as the detuning is decreased. In both cases, however, we clearly observe the fingerprint of photon pairing: even-number Fock states with \( n_L + n_R = 2N \), have higher probability than their neighboring odd-number Fock states with \( n_L + n_R = 2N \pm 1 \). By comparing \( P_{2,0} \) and \( P_{1,1} \), we also observe that onsite pair creation is more significant than offsite pair creation. This agrees well with the fact that \( \tilde{C}_0^+ \) is larger than \( \tilde{C}_1^+ \), as we demonstrated in Eq. (4.35).

An alternative way of visualizing the squeezing predicted by Eqs. (4.37) and (4.38) is to calculate and plot the Wigner function for the reduced density matrix representing the photon state on one of the two Rabi sites. Given the Hilbert space structure of the dimer, \( \mathcal{H}_{\text{dimer}} = \mathcal{H}_{\text{ph}}^L \otimes \mathcal{H}_{\text{qu}}^L \otimes \mathcal{H}_{\text{ph}}^R \otimes \mathcal{H}_{\text{qu}}^R \), we can obtain the desired reduced density matrix directly from the
calculated ground state,

\[ \rho = \text{tr}_{n_R} \text{tr}_{\sigma_L} \text{tr}_{\sigma_R} |g\rangle \langle g|. \]

Therefore, we perform a partial trace of the ground state density matrix over the Hilbert space except for the subspace \( \mathcal{H}_{L}^{\text{ph}} \), namely the photon Fock space on the left site. The Wigner function...
is then obtained via $W(x, p) = 2\pi^{-1} \text{tr} [D(-\alpha)\rho D(\alpha) \mathcal{P}]$, where $D(\alpha)$ is the usual displacement operator, $\alpha = x + ip$ and $\mathcal{P} = \exp[i\pi a^\dagger a]$ is the photon number parity operator $[34]$.

The resulting Wigner function $W(x, p)$ is plotted in Fig. 4.10 for several values of $g/\omega$, with the first row showing the result obtained from the full Rabi lattice Hamiltonian (4.1) and the second row the corresponding result calculated from the dispersive Hamiltonian (4.11). Note that for an unsqueezed situation, the contours of $W(x, p)$ would be circles. Hence, the elliptical feature of the contour lines in Fig. 4.10 suggests squeezing. For $g = \omega (g/g_c = 0.76)$, the exact and approximate Wigner functions are in good agreement and show the expected squeezing. Increasing the coupling further to $g = 1.3\omega (g/g_c = 0.98)$, squeezing becomes more significant and deviations between approximate and exact result are visible as the breakdown point $g/g_c = 1$ is approached. For $g = 1.4\omega (g/g_c = 1.06)$, we exceed the critical coupling and the Wigner functions differ significantly, signaling the breakdown of perturbation theory.

Overall, our comparison between exact and approximate results for the Rabi dimer in the last two subsections nicely confirm the validity of the perturbative approach in the expected parameter regimes.

4.6. Summary

In summary, we have derived the effective Hamiltonian for the dispersive regime of the Rabi lattice by employing a Schrieffer-Wolff transformation to second order in the Rabi interaction $\sim g$. Our results generalize the well-established treatment of the dispersive limit for a single Rabi site to the case of the Rabi lattice, which has enjoyed substantial recent interest in the context of photon-based quantum simulation. The effective interaction terms emerging from our treatment include transverse-Ising interaction between qubits (XY interaction in the
Jaynes-Cummings limit), photon pairing terms and conditional photon hopping terms. We have presented analytical expressions for the resulting coupling constants and demonstrated that they are short-range but not restricted to nearest-neighbor sites.

At the Jaynes-Cummings limit ($g \ll \omega, \epsilon$), we also discuss the general structure of the fourth-order effective interaction, and at the large positive-detuning regime ($\Delta \equiv \epsilon - \omega \gg g$, “heavy” qubit and “light” photon), give the expression of the $0^{th}$ order (of $t/\Delta$) contribution which is an onsite Hubbard interaction. Such an effective Hubbard interaction is crucial for Chapter 4 where we use the Bose-Hubbard model to study interacting photons in the large positive-detuning regime.

As necessary conditions for the validity of the dispersive regime of the Rabi lattice (ultra-strong coupling $g \sim \omega$ or $g \sim \epsilon$), we identified the inequalities

$$g \ll \min_k |\epsilon - \omega_k| = \omega - 2|t| - \epsilon \quad \text{(negative detuning)}$$

and

$$g \ll \min_k \sqrt{\epsilon \omega_k}/2 = \sqrt{\epsilon(\omega - 2|t|)}/2 \quad \text{(positive detuning)}.$$

For negative detuning, we found that the effective spin physics is given by a transverse-Ising model which includes interaction terms beyond nearest-neighbor spins. We showed how to recover the dressing of these spin states by photon coherent states via the inverse Schrieffer-Wolff transformation. For positive detuning, we studied the manifold of states without qubit excitations and discussed the effects of one-mode and two mode squeezing.

We confirmed the validity of our effective model numerically and discussed in detail the Rabi dimer as the simplest non-trivial example of a Rabi lattice model.
Interesting future work should include extending the perturbative treatment to fourth order, where additional photon-photon interaction is expected due to self-Kerr and cross-Kerr terms. An interesting open question is whether the phase transition discussed in Ref. [86] can be accessed from within the dispersive Rabi regime with positive detuning when including such higher-order terms. Another interesting question concerns the fate of frustration induced phase transitions in the presence of spin-photon dressing. Finally, consideration of the open-system aspect including dissipation and external driving forms an important theoretical challenge in the near future.
CHAPTER 5

Theory of interacting photons in frustrated Kagome lattices

In this chapter, we study interacting photons in a 2D circuit-QED lattice with a specific geometry, i.e. the Kagome lattice. We here focus on the dispersive regime where high-frequency qubit degrees of freedom can be integrated out (as shown in Sec. 4.3.2). This leads to an effective Bose-Hubbard model. Hence, the topic of this chapter is not concerned with details of the light-matter interaction, which has been explored in Chapter 4 but rather focus on novel phases arising from this special geometry of the Kagome lattice.

5.1. Introduction

The Kagome lattice is interesting in two different regards. First, as discussed in Sec. 1.3 and shown in Fig. 1.5 it is the easiest lattice model which can be realized with circuit-QED elements. This is because, the actual superconducting resonator array is the dual of the Kagome photon lattice, i.e. the honeycomb array. Such an array has uniform capacitive coupling between all the neighboring resonators. Second, the Kagome lattice can be frustrated by tuning the sign or the complex phase of the hopping amplitudes, which can also be achieved within the circuit-QED architecture (as shown in Fig. 1.6). In that case, the lowest band becomes flat.

The problem of interacting bosons in frustrated lattices with a flat band has been a subject of significant theoretical interest [6, 41, 96, 106, 107, 108, 110]. Due to the exact degeneracy in the single-particle spectrum, there is no preferred momentum state for the Bose condensation.

\[ A \text{tight-binding lattice model is frustrated if the } \mathbf{k} = \mathbf{0} \text{ mode is not the lowest energy mode and no gauge transformation can make the } \mathbf{k} = \mathbf{0} \text{ mode to be the lowest energy mode.} \]
to occur and, hence, novel phases are expected to emerge. With the single-particle kinetic energy quenched, interaction determines how the massive band degeneracy is resolved. This is reminiscent of the physics of the fractional quantum Hall effect, where Coulomb interaction lifts the degeneracy of a partially filled Landau level. Depending on the specific model and parameter regime, bosonic ground states in such frustrated lattices can belong to topological phases and include composite-fermion states of hard-core bosons \[57, 96, 109\], fractional Chern insulators \[106, 107\], and other exotic broken symmetry states \[6, 41, 42, 68, 108, 110\].

With the rapid advance of artificial condensed matter systems such as cold atoms in optical lattices and interacting photons in circuit-QED lattices, it has become possible not only to realize geometrically frustrated lattices but also lattices subject to synthetic gauge fields \[1, 18, 26, 28, 31, 32, 44, 46, 51, 60, 74\]. Thus, a variety of flat-band interacting boson models can already be engineered with current experimental techniques.

Here we focus on one of the paradigmatic examples of a frustrated lattice – the Kagome lattice \[3, 13, 41, 42, 57, 79, 83, 94, 109, 110\]. In the context of the Bose-Hubbard model, previous studies have considered this lattice with positive hopping, \(|t|\), which produces a flat lowest band, as shown in Fig. 5.1. This flat band is, however, gapless since it is touched by another band at the \(\Gamma\) point \[6, 41, 110\]. That makes analysis of interacting problem quite subtle due to the ability of particles to leak easily into the higher band. However, the flat band can be gapped off by inserting an additional gauge flux into each hexagon of the Kagome lattice \[48\]. We show that the single-particle eigenstates composing the gapped flat band can be chosen as localized loop states, which typically break the rotational \(C_6\) symmetry.
Figure 5.1. Band structure of the positive-hopping Kagome lattice tight-binding model. The lowest flat band is touched with one of the two dispersive bands at the $\Gamma$ point ($k_x = 0, k_y = 0$).

The introduced gap enables a well-controlled projection onto the flat band subspace [41, 98, 100, 111, 112] in the weak-interaction regime $U \ll |t|$, and yields an effective low-energy Hamiltonian. This is analogous to the lowest-Landau level projection employed in the fractional quantum Hall effect. Depending on the filling fraction of the lattice, we find three types of exotic nematic phases. At close packing of maximally compact loop states, a nematic Wigner crystal forms the exact ground state of the system. In the specific case of $\pi$-flux and higher filling fraction, our mean-field treatment predicts transitions to a nematic supersolid followed by a nematic superfluid phase.

The possibility of microscopic liquid crystalline phases has been pointed out previously in the context of strongly correlated electronic materials [23, 50]. In this chapter, we propose the possible existence of quantum liquid crystal phases of interacting bosons. Such a study could be viewed as bridging the areas of hard condensed matter and soft matter physics.

\footnote{In this case, all the particles will stay in the manifold spanned by flat-band states}
The structure of this chapter is as follows. In Sec. 5.2 we provide the model Hamiltonian and its single-particle spectrum. In Sec. 5.3 we discuss a circuit-QED realization of the model in the \( \pi \)-flux case. In Sec. 5.4 we discuss the properties of the single-particle loop states which compose the entire flat band. In Sec. 5.5 we give the exact analytical expression for the ground states of a nematic Wigner crystal at close packing filling and hard-core loop gas below that filling. In Sec. 5.6 we project the Hamiltonian onto the flat-band manifold and express the effective Hamiltonian with Wannier states (orthogonalized loop states). In Sec. 5.7 we set up the mean-field theory to study the ground states of the effective Hamiltonian, with the discoveries of a nematic supersolid phase and a nematic superfluid phase above the close-packing filling. In Sec. 5.8 we clarify the nature of the nematic superfluidity through the calculation of the superfluid stiffness tensor and its anisotropy.

5.2. Gapped flat band of Kagome lattices in the presence of gauge fields

5.2.1. Model

The Bose-Hubbard model on the Kagome lattice subject to gauge flux [Fig. 5.2(a)] is described by the Hamiltonian

\[
H = \sum_{\langle r, r' \rangle} \left( |t| e^{iA_{rr'}} b_{r'}^\dagger b_r + \text{h.c.} \right) + U \sum_r b_r^\dagger b_r^\dagger b_r b_r,
\]

where \( b_r^\dagger \) creates a single boson on the site labeled \( r \). The first term is the tight-binding Hamiltonian \( H_{\text{tb}} \) determining the band structure of the non-interacting bosons. We denote the hopping amplitude by \( |t| \) to stress that it is positive (frustrated). The gauge potential \( A_{rr'} \) is defined on

\footnote{In ultracold-atom experiments, the natural negative hopping can be turned positive by threading triangles of the Kagome lattice with a \( \pi \)-flux. For circuit-QED lattices, such positive hopping arises naturally as will be discussed in Sec. 5.3.}
each nearest-neighbor bond \( \langle r, r' \rangle \), and it determines the flux \( \phi = \sum_{\langle r, r' \rangle} A_{rr'} \) threading each plaquette in the lattice. The second term in \( H \) captures the repulsive Hubbard interaction on each site with strength \( U > 0 \).

5.2.2. Gapped flat band in the presence of flux.

We first discuss the tight-binding band structure for \( U = 0 \). Once flux \( \phi \) is inserted into each hexagon of the Kagome lattice, the single-particle spectrum \( E(\phi) \) takes the typical Hofstadter butterfly form [Fig. 5.2]. For non-integer \( \phi/2\pi \), the lowest band\(^4\) remains flat but acquires a gap that reaches its maximum size of \( \Delta \approx 0.55 |t| \) at \( \pi \)-flux (see Fig. 5.3). At this flux value, time-reversal (TR) symmetry is intact and the model can be realized in a lattice with both types (positive and negative) of real-valued hopping bonds. Energy and degeneracy of the flat band are independent of flux. The latter is given by the number of hexagons in the lattice, \( N_{\text{site}}/3 \) (\( N_{\text{site}} \) denoting the total number of sites).

5.3. Realization of \( \pi \)-flux model with a circuit-QED lattice

Although, in principle, one can introduce synthetic gauge fluxes to realize any gapped flat-band with a varied version of the scheme introduced in Fig. 1.6, it is worthwhile to point out that one can realize the \( \pi \)-flux model (the focus of this chapter) simply with both positive and negative hopping bonds, and without the requirement of an actual gauge field. For photon lattices, different hopping signs can be easily achieved by cleverly choosing proper resonator modes.

\(^4\)The term “band” is applied loosely here. For rational flux, the unit cell is enlarged and the flat band decomposes into multiple ones. No such simple picture applies to irrational flux.
Figure 5.2. (a) Kagome lattice with positive hopping and flux $\phi$ penetrating each hexagon. (b) Tight-binding energies as a function of $\phi$ (Hofstadter butterfly). The lowest flat band is gapped for non-integer $\phi/2\pi$ and reaches its maximum gap size at $\pi$-flux.

Figure 5.3. Band structure of the $\pi$-flux Kagome lattice tight-binding model. (a) The total six bands in this model, corresponding to its six-site unit cell. Note that the lowest flat band(s) are doubly degenerate. (b) Zoom of the low-lying band structure. The lowest flat band(s) are gapped, with the minimum gap $\Delta \sim 0.55t$. 
Specifically, photon lattices based on circuit-QED elements have been realized in recent experiments \cite{40, 81, 90, 102}. The photon lattices are formed by superconducting resonators (labeled by $j$) with frequency $\omega$, coupled capacitively to each other with the mathematical expression being $(\pm)_{jj'}C_cV_jV_{j'}$. Here, $C_c>0$ is the coupling capacitance and $V_j$ and $V_{j'}$ denote the voltages of the two adjacent resonators on the ends where they contact each other. The sign $(\pm)_{jj'}$, being either positive or negative, is equal to the product of the signs of the mode functions on each end, i.e. $(\pm)_{jj'} = \text{sgn}[\phi_j(x)\phi_{j'}(x')]|_{\text{ends}}$ \cite{21}. The possible gauge-equivalent configurations depend on the mode choice of the resonators. As an example, for the $\lambda$-mode which has the same signs on the two ends, one can easily choose positive signs for both ends, and make all hopping signs positive $(\pm)_{jj'} \rightarrow +$. Canonical quantization of the voltage leads to the definition of the photon operator $b_j$ for the chosen mode of the resonator at site $j$ through $V_j = V_0(b_j + b_j^\dagger)$, where $V_0$ has the dimensions of voltage and is determined by the capacitance and mode structure of the resonators. A superconducting qubit with frequency $\epsilon$ is placed in each resonator and interacts with the resonator through a Jaynes-Cummings interaction $g(b_j^\dagger\sigma_j^- + b_j\sigma_j^+)$ \cite{40, 90}. In the dispersive regime ($g \ll \epsilon - \omega$), the qubit can be integrated out via the Schriffer-Wolff transformation (see Section 4.3.2) which yields an effective Hubbard interaction $U b_j^\dagger b_j b_j b_j$. This effective interaction leads to the dispersive photon blockade and has been experimentally observed \cite{38}. One can also think of qubit as a nonlinear medium which effectively introduces Kerr nonlinearity to the resonators. Hence, the entire Hamiltonian which describes the photon lattice is as follows:

\begin{equation}
H = \omega \sum_j b_j^\dagger b_j + |t| \sum_{j,j'}(\pm)_{jj'}[b_j^\dagger b_{j'} + \text{H.c.}] + \sum_j U b_j^\dagger b_j b_j b_j,
\end{equation}
which is nothing but the Bose-Hubbard Hamiltonian. The first term is just a constant shift of energy and can be absorbed into the definition of chemical potential. The hopping strength $|t|$ is proportional to the coupling capacitance $C_c$. The possible gauge-equivalent sign configurations $(\pm)_{jj'}$ are determined by the choice of modes.

As shown in Fig. 5.4, the two-end resonators (black lines) are coupled equally to their neighboring two by the three-way capacitors and form a Honeycomb array. As mentioned before, the actual photon lattice is its graphic dual: the Kagome lattice (shown by red dashed lines), where the lattice sites (yellow dots) reside effectively in the center of the two-end resonators. A single qubit is located in each lattice site in order to introduce nonlinearity to the resonators and create an effective Hubbard interaction.

We first consider the $\lambda/2$ mode for each resonator, which has the lowest frequency and hence is relevant for the ground/low-lying states. As shown in Fig. 5.4(a), one can choose a particular gauge configuration, in which all the mode functions have the same signs (either positive or negative) at any three-way junction. Thus, the photon hoppings across the bonds (represent by dashed lines) in this gauge are made all positive throughout the whole lattice, which means there is a lowest flat-band for the photon tight-binding model. However, in this case, the flat band has band touching with the higher dispersive band at the $\Gamma$ point.

To open a gap above the flat band, we need to introduce gauge flux into the hexagons as discussed in the previous section. The $\pi$-flux model can be simply realized by making a lattice with both $\lambda/2$- and $\lambda$-mode resonators as shown in Fig. 5.4(b), where the wiggling lines represent resonators with twice the length of the straight resonators in the manner of actual experimental implementation [40]. The ground/low-lyings states will only involve the $\lambda/2$ mode
Figure 5.4. Circuit-QED realization of frustrated Kagome lattices. (a) Realization of positive-hopping model with 0-flux. The two-ended resonators (black lines) form a honeycomb array, of which the dual lattice is the actual Kagome photon lattice. The Kagome lattice sites are represented by yellow circles and the bonds by red dashed lines. The mode functions are illustrated with blue shades, where the signs on the ends are shown. The photon hopping amplitudes are shown on the bonds and are all positive in the $\lambda/2$-mode case, since the signs of the mode functions can be chosen the same at each three-way junction. (b) Realization of the $\pi$-flux model. Certain resonators are replaced by “wiggling” resonators with twice the original length, hence corresponding to the $\lambda$ mode. For a particular gauge choice, all signs of the mode functions are shown. All bonds represented by dashed lines still have positive hopping ($|t|$), while decorated bonds have negative hopping ($-|t|$).

in the straight resonators and the $\lambda$ mode in the wiggling resonators. A particular gauge configuration for the mode function is shown in Fig. 5.4b). This leads to the following hopping configurations: all the bonds (red dashed lines) correspond to positive hopping ($|t|$), and all the decorated bonds (red ellipses) have an additional gauge potential with value $\pi$ and hence are equivalent to negative hopping ($-|t|$). This achieves exactly the same gauge for $\pi$-flux model as we mentioned in the previous section.
5.4. Localized single-particle loop eigenstates

The presence of the flat band is directly linked to the existence of degenerate eigenstates that form localized loops. The localization mechanism, called caging [37, 104], is due to destructive interference of the wavefunction amplitude anywhere outside the loop [6]. In the Kagome lattice with positive hopping, the flat band and localization persist as long as there is no flux through triangles.

Previous studies [6, 41, 111, 112] have focused on the zero-flux case and identified the state with amplitudes of equal magnitude but alternating signs on the hexagon loop as maximally compact eigenstates [see Fig. 5.5(a)]. While the existence of flat band and localized eigenstates remains unharmed by the flux through hexagons, we find that the shapes of loop states must change. Specifically, in the spirit of a flux-quantization condition, every loop must enclose an integer number of flux quanta, \( \phi_L = \sum_{\text{loop}} A_{rr'} = \sum_{\text{loop}} \phi \in 2\pi N \). For \( \phi = \pi \) and \( \pi/2 \), we show maximally compact loop eigenstates encircling two and four hexagons in Fig. 5.5(b) and (c), respectively. Note that orientation and shape of maximally compact loop states are not generally unique for \( \phi \neq 0 \).

To be systematic, we list three important properties of the single particle eigenstates in the flat band of the tight-binding Kagome Hamiltonian:

1. The energy of the single particle eigenstate is exactly \(-2|t|\) [can be directly observed from the butterfly spectrum Fig. 5.2(b)]

2. The elementary flat-band eigenstates are single-particle loop states which have equal probability on each involved site. The amplitudes on the adjacent sites outside the loop (on the outward and inward triangles) cancel due to destructive interference (“caging”). Any other flat band state can be composed as a linear superposition of loop states.
(3) “Flux quantization”: a loop eigenstate encloses an integer number of flux quanta
\((2\pi n, n \in \mathbb{N})\).

Property 3 can be derived from properties 1 and 2 as follows. The positive-hopping tight-binding lattice Hamiltonian in the presence of additional gauge field \(A\) has the form:

\[
H_{tb} = \sum_{\langle r, r' \rangle} |t| e^{iA_{rr'}} b^\dagger_r b_r + \text{H.c.} \equiv \sum_{\langle r, r' \rangle} T_{rr'},
\]

where \(T_{rr'}\) is the hopping operator on the nearest-neighbor bond \(\langle r, r' \rangle\). Assuming that there exist single-particle wavefunctions of the loop eigenstate type, they can be expressed as

\[
|\psi_L\rangle = \sum_{r \in L} \psi_r b^\dagger_r |0\rangle,
\]

where the summation index \(r\) runs over all sites on the loop \(L\). When acting with the Hamiltonian \(H_{tb}\) on the loop eigenstates, we can split the expressions into two parts, namely

\[
H_{tb} |\psi_L\rangle = \sum_{\langle r, r' \rangle \in L} T_{rr'} |\psi_L\rangle + \sum_{\langle r, r' \rangle \in L: \langle l, L \rangle} [T_{rl} + T_{r'l}] |\psi_L\rangle.
\]

The first sum includes hopping along the bonds \(\langle r, r' \rangle\) on the loop \(L\), while the second sum corresponds to hopping from the bonds \(\langle r, r' \rangle\) on the loop to the adjacent sites \(l\) on the outward/inward triangles, as illustrated in Fig. 5.6. The cancellation of the probability amplitude outside the loop (caging, property 2) requires the second sum to be zero, while the requirement
of eigenenergy being $-2 |t|$ (property 1) implies that:

\begin{equation}
\sum_{\langle r,r' \rangle \in L} T_{rr'} |\psi_L \rangle \equiv \sum_{\langle r,r' \rangle \in L} |t| \left[ e^{iA_{rr'}} \psi_r b_{r'}^\dagger + e^{-iA_{rr'}} \psi_{r'} b_r^\dagger \right] |0 \rangle = -2 |t| |\psi_L \rangle \equiv \sum_{\langle r,r' \rangle \in L} -|t| \left[ \psi_r b_{r'}^\dagger + \psi_{r'} b_r^\dagger \right] |0 \rangle.
\end{equation}

The above equation leads to a “chain rule” of the single particle wavefunction,

\begin{equation}
\psi_{r'} = -\psi_r e^{iA_{rr'}}.
\end{equation}

That is, the wavefunction has equal probability on every site along the loop, and the adjacent sites differ by a minus sign and an additional phase shift due to the gauge potential $A_{rr'}$ on the bond $\langle r, r' \rangle$. When applying the “chain rule” [Eq. \ref{eq:chain_rule}] around the loop and requiring the probability amplitude $\psi_r$ to be single-valued, we derive the “flux quantization” condition of a loop eigenstate (property 3), namely

\begin{equation}
\phi_L = \sum_{\langle r,r' \rangle} A_{rr'} = 2\pi n, \ n \in \mathbb{N}.
\end{equation}

Here, the direction of the gauge potentials $A_{rr'}$ is chosen to be counterclockwise (\textcircled{C}) around the loop $L$.

Now we consider the cancellation of the second sum in Eq. \ref{eq:sum_trace} which leads to “caging”, and get

\begin{equation}
[T_{rl} + T_{r'l}] |\psi_L \rangle = |t| \left[ e^{iA_{rl}} \psi_r b_l^\dagger + e^{-iA_{r'l}} \psi_{r'} b_l^\dagger + \text{H.c.} \right] |0 \rangle = 0,
\end{equation}
which leads to $\psi_{r'} = -\psi_r e^{i(A_{rl} + A_{tr'})}$. Combined with Eq. (5.7), we get

\begin{equation}
\phi_{\Delta} = A_{rl} + A_{tr'} + A_{r'r} = 0.
\end{equation}

Thus, we have just shown the necessary condition for the existence of lowest flat band with energy $-2|t|$, which is our starting argument that the flux threading all the outward/inward triangles must be zero (gauge-equivalent to $\pi$-flux in the negative hopping model).

To understand one additional feature of the loop state, now we consider the gauge-invariant current operator on the bond $\langle r, r' \rangle$ (from site $r$ to site $r'$), namely,

\begin{equation}
J_{rr'} = 2|t|i [\psi^*_{r'} \psi_r e^{iA_{rr'}} - \text{H.c.}].
\end{equation}

Its expectation value is given by

\begin{equation}
\langle \psi_L | J_{rr'} | \psi_L \rangle = 2|t|i [\psi^*_{r'} \psi_r e^{iA_{rr'}} - \text{H.c.}],
\end{equation}

which equals zero after applying the “chain rule” [Eq. (5.7)]. Therefore, for any flux value $\phi$, the loop states in the flat band carry no current, and thus do not break time-reversal (TR) symmetry, even though the Hamiltonian itself breaks TR except at $\phi = 0, \pi$. From the butterfly spectrum, we observe that the lowest flat band does not change as a function of $\phi$, which leads to zero current due to the linear response formula of the current $J = \frac{\partial E}{\partial \phi} = 0$. The fact that there is no current can also be understood in another way, i.e. the Chern number for the lowest flat band is always zero. This is in contrast to the higher bands near $\phi = 0$ [Fig. 5.2(b)], which are essentially Landau levels with nonzero Chern numbers $C = 1, 2, 3$, etc..
The main focus of this chapter is the case of flux $\phi = \pi$ where TR symmetry is intact and maximally compact loop states are dimers encircling two hexagons. By a convenient gauge choice $A_{rr'} = \pi$ on decorated bonds [Fig. 5.2(b)], all hopping elements are real and given by $|t|$ on regular and $-|t|$ on decorated bonds. In this gauge, amplitudes of loop eigenstates simply alternate in sign across positive-hopping bonds and are identical across decorated negative-hopping bonds. In the following, we consider occupation of these states by multiple bosons and refer to the maximally compact loop states as Loop Orbitals (LOs).

As shown in Sec. 5.3, Circuit QED lattices including both positive and negative hopping can be realized by a clever choice of resonator modes.
5.5. Exact ground states: Nematic Wigner crystal and hard-core loop gas

We next turn to the interacting case, accounting for on-site boson repulsion due to the Hubbard term $U \sum_r b_r^\dagger b_r^\dagger b_r b_r$. Since the interaction is local, we note that any many-body state of the form $\prod_{m \in A} L_m^\dagger |0\rangle$ with single-particle occupation of a set $A$ of non-overlapping LOs is an exact ground state of the interacting system for filling $\nu = |A|/N_{\text{site}}$. Here, the operator $L_m^\dagger$ creates a single particle occupying the LO labeled by $m$. Indeed, the above product state is an eigenstate with eigenenergy $-2|t|$ per particle and interaction does not contribute since double occupancy of sites is avoided.

5.5.1. Nematic Wigner crystal ground state

Once the filling reaches close packing, the ground state becomes an incompressible Wigner crystal [108], i.e. $\frac{\partial F}{\partial \mu} = 0$. No additional particle can be placed on the lattice without incurring an interaction-induced energy increase due to unavoidable overlap. At the critical filling $\nu_c$ of close packing, bosons occupy maximally compact LOs while avoiding double occupation. As discussed above, maximally compact LOs may break the lattice rotational symmetry (here, $C_6$), which directly leads to ground states with spontaneously broken lattice symmetry.

In general, the filling fraction $\nu_c$ for close packing depends on flux. In the $\pi$-flux case, maximally compact LOs are dimers and close packing occurs at $\nu_c = 1/15$. Due to the three possible orientations of a dimer [Fig. 5.2(b)] and the freedom to use one Wigner crystal representative [Fig. 5.2(d)] to produce four other inequivalent ones by translations to four neighboring hexagons, we predict that the ground state is overall 15-fold degenerate. These ground states

\footnote{Note: for filling below close packing, there will generally be a large number of degenerate ground states.}

\footnote{Here, $F = E - N\mu$ is the Gibbs free energy (grand canonical ensemble), where $E$ is the ground state energy, $N$ the total particle number, and $\mu$ the chemical potential.}
are nematic Wigner crystals. Here, nematicity refers to the emergence of dimers that break the lattice rotation symmetry. In this aspect, the $\pi$-flux case is dramatically different from the $0$-flux case studied before where the $\nu = 1/9$ Wigner crystal [41] ground states do not exhibit any nematicity.

### 5.5.2. Hard-core loop gas

We note that for $\phi = \pi$ and filling below $\nu_c$, bosons form an infinitely compressible ($\frac{\partial F}{\partial \mu} = \infty$) hard-core loop gas with macroscopic degeneracy determined by all possible configurations of non-overlapping loops [111][112]. One such configuration is depicted in Fig. 5.7(b).

As one can see, the configuration shown in Fig. 5.7(b) can be connected to another configuration by a local operation, e.g. $|C_2\rangle = L_j^\dagger L_i |C_1\rangle$, namely moving one loop state to another.
nearby place. This means a local external force/perturbation can change it from one degenerate ground state to another degenerate ground state. This is in sharp contrast with the incompressible Wigner crystal state, where only a global perturbation (rotate all the dimers simultaneously) can change it from one symmetry-breaking state to another one.

Another important feature to mention is that slightly below the close-packing filling \( \nu_c \), the loop gas is still nematic, since for any of the degenerate ground state, the majority of the loops orient in the same direction. Only below a certain filling factor, the loop gas becomes isotropic. The isotropic-nematic phase transition warrants systematic study in future.

5.6. Flat band projection in weak-interaction regime and Wannier orbital construction

In the following, we exclusively focus on the \( \pi \)-flux case. To treat filling above close packing, we derive a low-energy effective Hamiltonian by adapting the approach by Huber and Altman \[41\], consisting of a projection onto the subspace spanned by flat-band eigenstates. In our case of nonzero flux, however, we forego the more subtle situation of an ungapped band encountered in \[41\]. In the presence of a gap and in the weak-interaction limit, boson occupation is to a good approximation limited to the flat band and the projection is appropriate unless the filling fraction becomes too large (details depend on the ratio \( U/|t| \)).

To facilitate the projection, we construct an orthonormal basis for the flat band subspace. For \( \pi \)-flux, the unit cell is doubled and contains a left and right hexagon, \( L \) and \( R \), which differ by the relative positions of negative-hopping bonds [Fig. 5.8(a)]. Due to the unit-cell doubling there are, strictly speaking, two degenerate flat bands. Accordingly, we choose two sets of maximally compact dimer LOs aligned in the \( e_3 \) direction [Fig. 5.8(a)] as our basis for the two
degenerate flat bands. We distinguish left-dimer states only containing $L$ hexagons from right-dimer states only containing $R$ hexagons. Although these sets of LOs together form a basis of the two degenerate flat bands, not all basis states are mutually orthogonal. We thus need to determine appropriate superpositions of the dimer LOs to form a set of mutually-orthogonal Wannier orbitals (WOs). As usual, there is not a unique set of WOs, and different choices can vary significantly in their real-space localization. Since we will ultimately employ local-decoupling mean-field theory, it is particularly important to obtain well-localized WOs.

Our construction scheme for suitable WOs involves an important step of orthogonalizing the sets of left and right LOs by means of a symmetrized version of the Gram-Schmidt procedure (see Appendix D for details). The results for two adjacent WOs are depicted in Fig. 5.8(a). The major part of the real-valued WO amplitude is essentially concentrated on each original dimer [Fig. 5.8(a)]. From there, the amplitudes decrease rapidly (asymptotically in an exponential fashion). This is in contrast to the slower power-law decay of WO amplitudes in the 0-flux case which is caused by the touching of bands [41]. The WOs we obtain respect translational symmetry (in terms of probability), TR symmetry, and preserve the mirror symmetry along their major axes, just as the original dimer LOs. They weakly break mirror symmetry along their minor axes.

We define the creation operator for occupation of these Wannier orbitals by $w^\dagger_j \equiv \sum_r w_j(r)b_r^\dagger$, where the Wannier function $w_j(r)$ gives the amplitudes of the dimer-type WO centered at position $j$ of the effective triangular lattice [Fig. 5.8(a)] on each site $r$ of the underlying Kagome

Note: it is possible to construct $C_6$ symmetric but less compact localized orbitals as our flat-band basis. However, the mean-field ansatz with such orbitals has much larger interaction energy cost due to larger overlap and hence is not energetically favorable (see Appendix E for details).
lattice. Upon projection and switching to the grand-canonical ensemble, the effective Hamiltonian takes the form

\[ H_{\text{eff}} = \sum_{j} (-2\,|t| - \mu)w_{j}^{\dagger}w_{j} + \sum_{ijkl} I_{ijkl}w_{i}^{\dagger}w_{j}^{\dagger}w_{k}w_{l}, \]

where \( \mu \) is the chemical potential. For convenience, we define the shifted chemical potential \( \mu' = \mu + 2\,|t| \) which absorbs the energy constant of the flat band. The coefficients \( I_{ijkl} \equiv \)

---

**Figure 5.8.** (a) The two types of dimer LOs used to construct the Wannier basis. Disks in orange/blue represent positive/negative amplitudes of the LO. The shaded area on top shows a single unit cell, containing two hexagons, \( L \) and \( R \). The centers of LOs form a triangular lattice (bottom). (b) Two neighboring orthogonal Wannier orbitals. The area of each disk is proportional to the amplitude of the wavefunction on that site. Bottom panels show four types of effective interactions: (c) on-site repulsion, (d) density-density repulsion, (e) assisted-hopping, and (f) ring-exchange.
$U \sum_r w_i^r(r) w_j^r(r) w_k^r(r) w_l^r(r)$ determine the strength of the effective interaction terms and involve overlaps of four Wannier functions centered on specific sites $i$, $j$, $k$, and $l$ of the triangular lattice. Due to the localization of WOs, the interaction is short range and falls off rapidly with growing spatial distance between the four sites. We note that $I_{ijkl}$ is translationally invariant and real-valued (since the constructed Wannier functions are real-valued themselves).

The distinct spatial configurations of the four dimer WOs labeled $i$ through $l$ give rise to different types of interaction terms. A detailed summary of these types can be found in Appendix F. Whenever all four indices coincide, the contribution corresponds to an effective onsite repulsion $\sum_j U'_w w_j^\dagger w_j w_j$ with strength $U' = I_{jjjj} = 0.11U$. Among the set of all effective interaction terms, this on-site repulsion term has the largest strength. The next sub-leading terms come from two other types of effective interaction, namely density-density repulsion $V_{DD} = \sum_{i,j} I_{ij} n_i n_j$ [Fig. 5.8(d)], and assisted hopping $V_{AH} = \sum_{i,j} \sum_k I_{ijk} w_i^\dagger w_j w_j w_k$ [Fig. 5.8(e)]. Here, $n_j \equiv w_j^\dagger w_j$ denotes the Wannier number operator, and the primes on sums signal that those terms with coinciding summation indices are to be omitted. The strengths of density-density interaction and assisted hopping depend on the specific arrangement of the involved WO dimers. The largest contributing terms are $I_{d0,e_{-1}} = 0.0483U$ and $I_{ah0,e_{-1},-e_{-1}} = -0.055U$, and are thus significantly smaller than the on-site repulsion strength $U'$. Within the low-density regime $\nu < 1/3$ (i.e., $\nu_{\text{eff}} < 1$ in the effective triangular lattice), we therefore employ a hard-core approximation which forbids double occupation of WOs [41]. Within this approximation, interaction terms with repeated Wannier operators on the same site, $w_j^\dagger w_j^\dagger$ or $w_j w_j$, drop out. This includes effective onsite interaction as well as pair hopping $\sum_{i,j} I_{iijj} w_i^\dagger w_i w_j^\dagger w_j$. Besides density-density repulsion and assisted hopping, the only remaining interaction type is ring-exchange [Fig. 5.8(f)], in which the Wannier functions are centered
on four different sites on the triangular lattice. We find that the maximum strength of ring exchange is $0.00814U$ which is significantly weaker than both density-density repulsion and assisted hopping.

5.7. Mean-field theory

While density-density repulsion favors density-wave order and formation of a Wigner crystal, assisted hopping may lead to melting and formation of a superfluid. In addition, this competition also allows for an intermediate supersolid phase in which both types of order are present. Here, we study competition between different types of orders within mean-field theory (MFT). We adopt the Gutzwiller approach [82] and employ a product ansatz consistent with the hardcore constraint

(5.14) \[ |\psi_{\text{MF}}\rangle = \prod_j (f_{j,0} + f_{j,1}w_j^\dagger) |0\rangle, \]

which decouples sites on the effective triangular lattice of WOs. The mean-field ansatz naturally captures the nematic Wigner crystal phase since it is a product of single-particle states with occupation of non-overlapping LOs (in this case approximated by WOs). Above close packing, mean-field solutions continue to break the $C_6$ symmetry due to the anisotropic nature of the Wannier orbitals.

To describe states with density-wave order such as the nematic Wigner crystal, we must allow for the dependence of the mean-field amplitudes $f_{j,n}$ on the spatial index $j$. To obtain mean-field solutions, we decouple the effective Hamiltonian, replacing density-density interaction and assisted-hopping terms by $V_{\text{DD}} \rightarrow \sum_{i,j}2I_{ij}^d n_i \langle n_j \rangle$ and $V_{\text{AH}} \rightarrow \sum_{i,j} \sum_k I_{ijk}^a \langle w_i^\dagger \rangle \langle w_j \rangle n_k + \sum_{i,j} \sum_k I_{ijk}^a (w_i^\dagger \langle w_j \rangle + \text{h.c.}) \langle n_k \rangle$. (We have verified that inclusion of ring-exchange does not
lead to significant changes.) With this, we obtain a mean-field Hamiltonian \( \sum_i h_i(\{\psi_j\}, \{n_j\}) \) where \( h_i \) depends on the mean-field order parameters \( \psi_j = \langle w_j \rangle \) and \( n_j = \langle n_j \rangle \) on each site of the triangular lattice. Starting from a random initial set of order parameters on a lattice of 200 sites with periodic boundary conditions, we repeatedly solve for the eigenstates and re-calculate order parameters until reaching self-consistency (see Appendix G for details).

For a range of chemical potentials, we calculate results for the mean filling \( \langle \nu \rangle \equiv \sum_i n_i / N_{\text{site}} \), density-wave order parameter \( \langle \chi_{\text{dw}} \rangle \) defined as the difference between maximum and average density taking into account the six surrounding sites, and the mean superfluid order parameter \( \langle \psi_{\text{sf}} \rangle \equiv \sum_i \psi_i / N_{\text{site}} \). The key results from this calculation are presented in Figure 5.9. MFT reproduces the exact nematic Wigner crystal [Fig. 5.9(b)] for \( \mu^{' \mu} \simeq 0.05U \) at close packing \( \langle \nu \rangle = 1/15 \), showing maximum density-wave order \( \langle \chi_{\text{dw}} \rangle = 1 \) and vanishing superfluidity \( \langle \psi_{\text{sf}} \rangle = 0 \). Below close packing, MFT produces a gradual change of average filling and superfluid order, which differs from the known exact solution based on LOs. The exact solution exhibits a density plateau at \( \nu_c \) containing the entire nematic Wigner crystal phase, and a vertical jump corresponding to the hard-core loop gas phase which is more appropriately represented in the canonical ensemble.

Above \( \mu_c \), superfluid order sets in and \( \langle \psi_{\text{sf}} \rangle \) grows gradually while, at the same time, the density-wave order parameter \( \langle \chi_{\text{dw}} \rangle \) remains nonzero and decays slowly, overall suggesting a second-order transition to a nematic supersolid [Fig. 5.9(c)] in which a fraction of the bosons condense on interstitial sites between the Wigner-crystal structure. Further on at \( \mu_{c2} \simeq 0.18U \), the density-wave order \( \langle \chi_{\text{dw}} \rangle \) abruptly drops to zero, accompanied by a sudden increase in the superfluid order \( \langle \psi_{\text{sf}} \rangle \). This indicates a sudden melting of the Wigner-crystal structure and a first-order transition into a superfluid phase [Fig. 5.9(d)].
Figure 5.9. (a) Mean-field phase diagram and plot of average density $\langle \nu \rangle$, $\langle \nu_{\text{eff}} \rangle$ on the effective triangular lattice, average density-wave order $\langle \chi_{\text{dw}} \rangle$ (blue dots) and average superfluid order $\langle \psi_{sf} \rangle$ (red squares) versus chemical potential. Dashed lines show the exact solution with LOs. (b-d) Results from MFT for ground states in the three phases. The area of depicted dimers is proportional to the local occupation number $n_i$, arrows show the phase angle $\theta_i$. Results are obtained for a lattice of 200 sites using a self-consistency calculation.

Based on our MFT, we predict that the superfluid phase is nematic since condensation of bosons is based on hopping among anisotropic dimer WOs. Within the superfluid phase, phase
angles $\theta_i = \text{Arg}[\psi_i]$ form stripes in which neighboring stripes differ by a $\pi$-phase difference. The nematicity is not only encoded in the microscopic wavefunction, but can also be identified through a macroscopic quantity, the superfluid stiffness tensor: $\rho_{IJ} = \frac{\partial^2 E}{\partial \Delta \theta_I \partial \Delta \theta_J} \big|_{\Delta \theta_{I,J}=0}$. Here, $\Delta \theta_I$ and $\Delta \theta_J$ represent the phase difference applied to the sample boundary along directions $I$ and $J$ (e.g. $e_1$ and $e_3$ directions). In this case, $\rho_{II}$ differs from $\rho_{JJ}$, which implies anisotropic superflow and hence breaking of discrete rotational symmetry (see next section for details). The nematic supersolid has similar phase stripes, the only difference being that sites with maximum density have an additional $\pi$-phase flip. Finally, we find a narrow region in which non-monotonic dependence of the density on chemical potential suggests phase coexistence between the superfluid and supersolid.

5.8. Nematic superfluidity

Although the superfluid phase predicted by us is a uniform phase, the wavefunction, with the form $|\psi_{\text{MF}}\rangle = \prod_j (f_{j,0} + f_{j,1} w_j^\dagger) |0\rangle$, has internal structure (nematicity). The internal structure is encoded in the Wannier wavefunction $w_j(r)$, as shown in Fig. 5.8(b), which breaks the $C_6$ rotational symmetry. This nematic internal structure can be revealed microscopically through the real-space correlation function, i.e. $\langle b_{r_1}^\dagger b_{r_2} \rangle$.

Now we consider the superfluid stiffness tensor $\rho_{IJ} = \frac{\partial^2 E}{\partial \Delta \theta_I \partial \Delta \theta_J} \big|_{\Delta \theta_{I,J}=0}$, where $I, J = 1, 3$ refer to the directions along $e_1$ and $e_3$. Note that the $e_3$ direction is special because it aligns with the major axis of the dimers. To study $\rho_{IJ}$, we apply phase differences $\Delta \theta_1$ and $\Delta \theta_3$ across the boundaries of the finite sample ($16 \times 16$), as shown in Fig. 5.10(a).

The phase differences across the boundaries induce superflow in the corresponding directions and hence increase the kinetic energy. The contour plot in panel (b) shows the mean-field
energy as a function of the phase differences, namely $E(\Delta \theta_1, \Delta \theta_3)$. The superfluid stiffness tensor corresponds to the curvature of the energy profile in the vicinity of the origin. The anisotropy of the energy contours suggests that the superfluid stiffness is also anisotropic. To see this more clearly, we show cuts of the energy profile along the x- and y-axis (blue solid and red dashed line), namely $E(\Delta \theta_1, 0)$ and $E(0, \Delta \theta_3)$, in panel (c). It is obvious that, in the vicinity of the origin, the curvature of the blue solid line is larger than that of the red dashed line, which means that $\rho_{11} = \frac{\partial^2 E}{\partial \Delta \theta_1^2} |_{\Delta \theta_1=0}$ is larger than $\rho_{33} = \frac{\partial^2 E}{\partial \Delta \theta_3^2} |_{\Delta \theta_3=0}$. Therefore, the superfluid stiffness along the two directions is different. Now we consider the first derivative, $j_I = \frac{\partial E}{\partial \Delta \theta_I}$, which is the current generated when applying a phase difference along direction $I$. We can see that, not far away from the origin, $j_1$ is always larger than $j_3$. From Appendix F, we know that the effective nearest-neighbor hopping along the major axis ($e_3$ direction) is zero in the nematic superfluid phase (within mean-field approximation). Only successive hopping along other directions will contribute to superflow in the $e_3$ direction. On the other hand, the large effective
nearest-neighbor hopping in the other two directions ($e_1$ and $e_2$) leads to larger superflow in those directions.

In sum, the anisotropy of the two macroscopic quantities, the superfluid stiffness and superflow, reveals breaking of discrete rotational symmetry and hence microscopic nematicity of the superfluid phase.

5.9. Summary

We have studied the emergence of nematic phases of interacting bosons in a Kagome lattice with a gapped flat band, obtained when a flux $\pi$ is threaded through each hexagon of the lattice. In the presence of onsite Hubbard interaction, we identified that, for close-packing filling, the ground state is an incompressible nematic loop crystal, in which particles occupy non-overlapping dimer-shape loops and completely avoid onsite interaction. This state does not only break the lattice translational symmetry but also the $C_6$ rotational symmetry down to $C_2$ symmetry, and hence is termed nematic. To study physics above close-packing, we projected the Hamiltonian into the gapped flat band and derived an effective Hamiltonian describing the interacting loops, in the manner similar to the lowest-Landau-level projection used in the context of fractional quantum Hall physics. We identified possible existence of a nematic superfluid and a nematic supersolid phase, which arise from the condensation of anisotropic loops. The nematicity originates from the consideration of energetics: particles tend to occupy the most compact and anisotropic loop orbitals to reduce the overlap of orbitals and hence the cost of interaction energy. In principle, such nematic states with nontrivial quantum entanglement due to the loop correlation can be captured by a tensor-network ansatz \cite{14, 85} in a generic way, which warrants further numerical study in future.
Generally speaking, the type of nematic ground states discovered by us is another example of self-organized liquid-crystal-like phases originating from a microscopic model, such as the electronic nematicity occurring in cuprates and iron pnictides [23, 50]. This research can be thought of as bridging the fields of hard condensed matter and soft matter. We have also shown that the nematic superfluidity can be revealed by the anisotropy of the superfluid stiffness, which can possibly be related to experimental observation in future.

Interesting future directions include the study of phases at higher density, especially the possibility of a featureless Mott insulator [76] at 1/3 filling, resonating valence bond states and fermionized ground states in the strong-interaction regime. Last but not least, more work needs to be done in the context of realization and detection of such physics in experiments. In the context of interacting photons in circuit-QED lattices, realistic consideration of drive and dissipation in the experiment is an important direction to pursue, in order to experimentally observe the non-equilibrium analog of the corresponding physics discussed in this chapter.
CHAPTER 6

Conclusion and Outlook

In the course of this thesis, we have explored the use of the circuit-QED architecture, coupled systems of superconducting qubits and resonators, as an analog quantum simulator. We have focused our study on both the elementary building blocks of such a simulator, as well as on the interesting many-body physics which may be simulated in a circuit-QED lattice.

First, we have studied in detail the properties of the fluxonium circuit when coupled to microwave photons. This coupling is governed by the fluxonium charge matrix elements. The absence of nearest-neighbor selection rules for these matrix elements makes it crucial to go beyond the description in terms of a two-level system when calculating dispersive shifts. Therefore, we developed a generalized Jaynes-Cummings model (Chapter 2) to describe the coupling between the fluxonium circuit (as a multi-level qudit) between the resonator. We then used the Schrieffer-Wolff transformation to formulate a perturbation theory of the coupled system in the dispersive regime, where “atomic” frequency and photon frequency are strongly detuned. This way, we have derived expressions for the dispersive shifts and Kerr nonlinearity, which contain contributions from all low-lying levels of the qudit, and hence can be sizable even when the spacing of the lowest two levels is strongly detuned from the photon frequency.

In Chapter 3, we derived analytical expressions for the fluxonium charge matrix elements and quasi-selection rules in the large inductance limit. In the experimental parameter regime, the quasi-selection rules lead to an approximate Λ-structure of the low-lying eigenstates, which can be particularly useful for the purpose of both quantum computation and quantum simulation.
We then switched to the study of the full quantum simulator: a circuit-QED lattice in which photons can hop between resonators due to capacitive coupling and interact locally with qubits through light-matter interaction. We explored the physics of strongly-interacting photons in two different directions which complemented each other. The first direction, discussed in Chapter 4, focused on novel quantum phases arising from the unusual properties of the light-matter interaction. The second direction, presented in Chapter 5, focused on the interesting physics arising from geometric frustration due to a specific choice of lattice.

In Chapter 4, we again used the Schrieffer-Wolff transformation to derive the effective interactions in a circuit-QED lattice (in the dispersive regime), including effective spin-spin interactions mediated by virtual photons, and effective photon-photon interactions mediated by virtual qubit excitations. In particular, it was shown that nontrivial ground states appeared in the ultrastrong coupling regime due to lack of conserved excitation number, including the emergence of interesting photon pairing and ferromagnetic states of photon-dressed spins.

In Chapter 5, we focused our study on interacting photons in a frustrated Kagome lattice. The interaction was considered in the dispersive regime, where qubit degrees of freedoms could be integrated out, and what remained was a simple onsite Hubbard interaction between photons. Interesting many-body physics can then arise from the existence of a gapped flat band in the single-particle spectrum. In this context, the conventional wisdom that bosons condense into the lowest single-particle state breaks down due to the macroscopic degeneracies of the flat band. Instead, we identified novel liquid-crystal like phases, including a nematic Wigner crystal, a nematic superfluid and supersolid as the ground states for appropriate fillings. The nematicity arises from the fact that the most compact localized loop states composing the flat band typically break the lattice rotational symmetry.
Several future research directions naturally connect to the research presented in this thesis. In Chapters 4 and 5 we discussed the physics of circuit-QED lattices in the context of a closed system and assumed a chemical potential for photons in the framework of a grand canonical description. However, photon number is not conserved due to the interaction with the bath, and one should normally assign photons a zero chemical potential. Except in the ultra-strong coupling regime as discussed in Chapter 4, there will be no photons inside the lattice at zero temperature without the presence of an external microwave drive. In that case, the ground state is usually a trivial vacuum state. There are two possible routes to circumvent this problem and observe nontrivial physics which might relate to the predictions made in this thesis:

The first approach is to engineer an effective chemical potential of photons and produce a quasi-equilibrium state. This could be achieved with specific methods of dissipation engineering, such as mentioned in Refs. [30] and [47]. For example, with such an approach, the nematic Wigner crystal phase mentioned in Chapter 5 could possibly be stabilized as the quasi-equilibrium states with nearly fixed total photon numbers.

The other approach is to consider the non-equilibrium steady-states of photons under coherent external drive. This approach is less demanding experimentally and could, for example, be realized with the current experimental devices made in Andrew Houck’s lab at Princeton [40]. Possible interesting phenomena will be dissipative phase transitions between non-equilibrium steady-states [49] when tuning certain parameters in the Hamiltonian. Definite-number states like the nematic Wigner crystal are unlikely to form the steady state under coherent driving. Nevertheless, superpositions and statistical mixtures of the nematic Wigner crystal and hard-core loop gas may possibly form a non-equilibrium steady state (incompressible when
increasing the driving strength), which distinguishes itself from higher average density steady states where interaction cannot be avoided.

With further developments in both experimental and theoretical techniques, strongly interacting photons and qubits in circuit-QED lattices will open up a new domain where condensed matter physics can be studied in and out of equilibrium. This exciting new field will require developments of new techniques and expertise from different areas, including condensed matter physics, quantum optics, quantum computation and quantum information. These developments will not only advance the field of quantum simulation of many-body systems, but perhaps also shed light on the ultimate goal of large-scale fault-tolerant quantum computation.
References


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APPENDIX A

Numerical diagonalization of the fluxonium Hamiltonian

It is straightforward to perform the numerical diagonalization of the fluxonium Hamiltonian $H_f$, Eq. (2.1), using the harmonic oscillator basis $\{|m\rangle\}$ which diagonalizes $H_f|_{E_J=0}$. The oscillator states $|m\rangle$ are generally not good approximations to the fluxonium eigenstates, however. Proper care must be taken to check convergence of results with respect to the cutoff in $m$. In the $\varphi$ representation (consider $\varphi$ as the position coordinate), the quantity $\varphi_0 = (8E_C/E_L)^{1/4}$ plays the role of the oscillator length. The corresponding eigenenergies are given by $\epsilon_m = \hbar \omega_p (c^\dagger c + 1/2)$, where $c^\dagger$ and $c$ are the usual raising and lowering operators and $\omega_p = \sqrt{8E_L E_C}/\hbar$ denotes the oscillator frequency.

In this basis, the Hamiltonian matrix has the form

$$H_{mm'} = \delta_{mm'} \epsilon_m - E_J \cos(2\pi \Phi/\Phi_0) \langle m | \cos \varphi | m' \rangle - E_J \sin(2\pi \Phi/\Phi_0) \langle m | \sin \varphi | m' \rangle.$$  \hfill (A.1)

The sine and cosine matrix elements can be expressed in terms of generalized Laguerre polynomials as [29]

$$\langle m | \cos \varphi | m + 2p \rangle = (-2)^{-p} \sqrt{\frac{m!}{(m+2p)!}} \varphi_0^{2p} e^{-\varphi_0^2/4} L_m^{2p}(\varphi_0^2/2)$$  \hfill (A.2)

$$\langle m | \sin \varphi | m + 2p + 1 \rangle = (-2)^{-p} \sqrt{\frac{m!}{2(m+2p+1)!}} \varphi_0^{2p+1} e^{-\varphi_0^2/4} L_m^{2p+1}(\varphi_0^2/2),$$
where \( m, p \in \mathbb{N} \).

As an alternative to the explicit calculation of \( \cos \varphi \) and \( \sin \varphi \) matrix elements, one may instead employ the direct evaluation of matrix-valued exponentials. Specifically, the cosine term may be re-expressed via

\[
\cos(\varphi - \varphi_{\text{ext}}) = \frac{1}{2} e^{i\varphi} e^{-i\varphi_{\text{ext}}} + \text{H.c.} = \frac{1}{2} \exp\left[\frac{i\varphi_0}{\sqrt{2}}(c + c^\dagger)\right] e^{i\varphi_{\text{ext}}} + \text{H.c.},
\]

Algorithms for matrix exponentiation are standard in commercial (Mathematica: \texttt{MatrixExp[]}, Matlab: \texttt{expm()}) and non-commercial packages (e.g., SciPy: \texttt{expm()} and \texttt{expm2()}).

Once the Hamiltonian matrix is diagonalized, \( H_l = \sum_l \epsilon_l |l\rangle\langle l| \), one obtains the charge matrix elements in the diagonalized basis, \( \langle l | N | l' \rangle \), as follows. The charge operator is rewritten in the oscillator basis via \( N = -\frac{i}{\sqrt{2}\varphi_0}(c - c^\dagger) \) and thus one finds

\[
\langle m | N | m' \rangle = -\frac{i}{\sqrt{2}\varphi_0}(\sqrt{m'}\delta_{m,m' - 1} - \sqrt{m}\delta_{m,m' + 1}).
\]

Finally, one obtains

(A.3) \[
\langle l | N | l' \rangle = \sum_{mm'} \langle l | m \rangle \langle m | N | m' \rangle \langle m' | l' \rangle,
\]

where \( \langle l | m \rangle \) and \( \langle m' | l' \rangle \) are eigenvector amplitudes in the harmonic basis.
APPENDIX B

Schrieffer-Wolff transformation and its application to the generalized Jaynes-Cummings model

We consider a quantum mechanical system described by a Hilbert space $\mathcal{H}$, which is composed of several subspaces, $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 + \ldots$ For our following treatment, it is convenient to introduce the projectors

\begin{equation}
  P_\alpha = \sum_j |\alpha, j\rangle \langle \alpha, j|
\end{equation}

onto these subspaces. Here, the index $j$ enumerates the eigenstates within each subspace $\mathcal{H}_\alpha$. The projectors satisfy the completeness condition

\begin{equation}
  \sum_\alpha P_\alpha = 1.
\end{equation}

The goal of Schrieffer-Wolff transformation is to construct a Hamiltonian $H'$ with the same eigenenergies as the original Hamiltonian but without coupling between the specified subspaces. The elimination is facilitated by a unitary transformation,

\begin{equation}
  H' = e^{iS} H e^{-iS},
\end{equation}

where the generator $S$ is chosen such that

\begin{equation}
  P_\alpha H' P_\beta = P_\alpha e^{iS} H e^{-iS} P_\beta = 0 \quad (\alpha \neq \beta),
\end{equation}
which eliminates all coupling between subspaces. Condition (B.4) only determines the off-diagonal elements of $H'$. To remove the remaining ambiguity, one imposes the constraint that the diagonal elements of the generator $S$ be zero,

\[(B.5)\quad P_{\alpha}SP_{\alpha} = 0.\]

Conditions (B.4) and (B.5) then uniquely determine $S$ and $H'$.

To construct $S$ and $H'$ perturbatively and order by order, we decompose $S$ into a series,

\[(B.6)\quad S = \sum_{n=1}^{\infty} \lambda^n S_n,\]

where $\lambda$ is an auxiliary parameter for order counting. Using a variation of the Baker-Campbell-Hausdorff relations we rewrite

\[(B.7)\quad \begin{aligned} H' = & \, H + [iS, H] + \frac{1}{2!} [iS, [iS, H]] + \cdots = \sum_{n=0}^{\infty} \frac{1}{n!} [iS, H]_n. \end{aligned}\]

Decomposing $H'$ in a similar series

\[(B.8)\quad \begin{aligned} H' = & \, H_0 + \sum_{n=1}^{\infty} \lambda^n H'_n, \end{aligned}\]

substituting into Eq. (B.7) and consistently collecting terms up to $\lambda^2$, one obtains

\[(B.9)\quad \begin{aligned} H' = & \, H + [iS, H] + \frac{1}{2} [iS, [iS, H]] + O(\lambda^3) \\ = & \, H_0 + \{\lambda V + [i\lambda S_1, H_0]\} + \{[i\lambda^2 S_2, H_0] + [i\lambda S_1, \lambda V] \\ & \, + \frac{1}{2} [i\lambda S_1, [i\lambda S_1, H_0]]\} + O(\lambda^3). \end{aligned}\]
After imposing conditions (B.4) and (B.5), the resulting expression for $H'$ up to (and including) second order is given by [17]

\begin{equation}
H' = H_0 + V^{\text{diag}} + \frac{1}{2} \sum_\alpha P_\alpha [iS_1, V^{\text{nd}}] P_\alpha + \mathcal{O}(\lambda^3).
\end{equation}

Here, the diagonal components of $V$ are $V^{\text{diag}} = \sum_\alpha P_\alpha V P_\alpha$, and the off-diagonal elements $V^{\text{nd}} = V - V^{\text{diag}}$. To first order, the generator is obtained as

\begin{equation}
P_\alpha i S_1 P_\beta = \frac{P_\alpha V P_\beta}{E_\alpha - E_\beta}.
\end{equation}

We then apply Eq. (B.10) to a system composed of a multi-level qudit coupled to harmonic modes (such as the ones realized by a resonator). The non-interacting and interaction contributions to the Hamiltonian, $H_0$ and $V$, are given by Eqs. (2.4) and (2.5). By our choice, the individual subspaces are one-dimensional each and spanned by one of the eigenstates of $H_0$, i.e., $|nl\rangle_0$. The integer components of $n = (n_j)$ denote the photon numbers of the harmonic modes (indexed by $j$), and $l = 0, 1, \ldots$ enumerates the qudit levels.

Since $V$ involves an increase or decrease in photon number, its diagonal part vanishes, $V^{\text{diag}} = 0$, and thus one finds $V = V^{\text{nd}}$. From Eq. (B.11), we obtain the explicit form of the first-order generator

\begin{equation}
S_1 = -i \sum_j \sum_{ll'} \left[ \frac{g_{j,l'l}a_j}{\epsilon_{l'l} - \omega_j} - \frac{g_{j,l'l}^\dagger a_j^\dagger}{\epsilon_{l'l} - \omega_j} \right] |l\rangle_0 \langle l'|_0,
\end{equation}
where $\epsilon_{t,l} \equiv \epsilon_{t} - \epsilon_{l}$ is a transition energy. (Note that $S_{1}^{\dagger} = S_{1}$.) Finally, Eq. (B.10) yields the following second-order expression for $H'$:

\begin{equation}
H' = H_0 + \sum_{uu'} \sum_{j} [(\chi_{j;tt'} - \chi_{j;tt'})a_{j}^{\dagger}a_{j} + \chi_{j;tt'}] |l\rangle_{00} \langle l|.
\end{equation}

(B.13)

Here, we have abbreviated the partial dispersive shifts by

\begin{equation}
\chi_{j;tt'} = \frac{|g_{j;tt'}|^2}{\epsilon_{tt'} - \omega_{j} - i\gamma_{j;tt'}}
\end{equation}

(B.14)

By construction, $H'$ [Eq. (B.13)] is turned into the effective Hamiltonian $H_{\text{eff}}$ in Eq. (2.14) by replacing bare operators by dressed ones, $a_{j} \rightarrow a_{j}$ etc. The expression for the second-order shifts in Eq. (B.14) agrees with the one derived in the main text [Eq. (2.18)].
APPENDIX C

Two-photon vacuum Rabi splitting

In this appendix, we consider a multi-level qudit coupled to a single resonator mode $a$ in a configuration where the bare states $|l_1, n_a \rangle_0$ and $|l_2, n_a + 2 \rangle_0$ are degenerate. The leading order coupling between them is through a two-photon process involving the intermediate states $|l', n_a + 1 \rangle_0$. We derive the effective two-photon coupling by adiabatic elimination of the intermediate states $|l', n_a + 1 \rangle_0$ and obtain an effective Hamiltonian $H'_\alpha$ for the subspace spanned by the two states $\alpha = \{|l_1, n_a \rangle$ and $|l_2, n_a + 2 \rangle\}$. By applying Eqs. (B.10) and (B.12) and using the projector $P_\alpha$ for the relevant subspace, we find

$$H'_\alpha = \sum_{l' \prime} \frac{g_{a;l_2;l'} g_{a;l'_1} a^\dagger a^\dagger}{\Delta_{a;l_2;l'}} |l_2 \rangle \langle l_1 | + \text{H.c.} \quad \text{(C.1)}$$

Here, the detuning is $\Delta_{a;l_2;l'} = \epsilon_{l_2;l'} - \omega_a$ as defined previously. Note that the effective coupling indeed involves the emission or absorption of two photons. Diagonalization of $H'_\alpha$ yields the splitting

$$\sum_{l'} \frac{2\sqrt{(n_a + 1)(n_a + 2)} g_{a;l_2;l'} g_{a;l'_1} a^\dagger a^\dagger}{\Delta_{a;l_2;l'}}$$

for initial photon number $n_a$. With $n_a = 0$, $l_1 = 4$ and $l_2 = 0$, we recover the expression for the two-photon vacuum Rabi splitting presented in the main text.
APPENDIX D

Construction of orthogonal Wannier Orbitals

For the \( \pi \)-flux case, the unit cell is doubled with respect to the 0-flux case and hence includes 6 sites (labeled as A, B, C, D, E, and F), as shown in Fig. D.1(a). Hence, the lowest flat bands are doubly degenerate, which means that there is an arbitrary choice to decompose the two flat bands, since for each \( k \) one can arbitrarily choose two orthogonal Bloch vectors in the 2-dimensional degenerate subspace. Sensible choice of basis has to be physically motivated and has to respect certain symmetries.

For the sake of convenience, we choose loops along the \( e_3 \)-direction as our preferred flat band basis (total number \( N_{\text{site}}/3 \) equals the number of flat-band degeneracy). The operators \( L^\dagger_{s,R} \) which create the two types of loops within each unit cell can be represented by the original lattice boson operators as:

\[
L^\dagger_{1,R} = b^A_R - b^B_R + b^C_R - b^E_R - b^E_{R-a_2} + b^E_{R-a_1} - b^F_{R-a_1+a_2} + b^B_{R+a_2} - b^A_{R+2a_2} + b^C_{R+a_2},
\]
\[
L^\dagger_{2,R} = b^B_{R+a_1} - b^B_{R+a_1-a_2} - b^C_R - b^C_{R+a_2} + b^D_R - b^D_{R+2a_2} + b^E_{R+a_2} - b^E_{R} + b^E_{R+2a_2} - b^F_{R} + b^F_{R+a_2}.
\]

Here, the index \( s = 1, 2 \) labels the loops encircling left/right hexagons. The wavefunctions of the two types of loops are already shown in Fig. 5.8(a). Here, the lattice vectors \( R \equiv (m, n) \) labels the enlarged 6-site unit cell and the lattice vectors \( a_1 \equiv (1, 0) \) and \( a_2 \equiv (0, 1) \) translate the cells in the two oblique directions [shown in Fig. D.1(a)].
One can construct two classes of Bloch states by translationally-invariant superposition (with a particular wavevector $\mathbf{k}$) of the two types of loop states respectively, i.e.

\begin{equation}
L_{s,k}^\dagger = \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{R}} L_{s,\mathbf{R}}^\dagger.
\end{equation}

Here, left/right label $s=1,2$ can also be thought as the band index and in this particular case labels the two degenerate flat bands. The generated state $L_{s,k}^\dagger |0\rangle = \sum_l u_{s,k}^l b_{l}^{\dagger} |0\rangle$ can be represented by a 6-component Bloch vector $\vec{u}_{s,k}$, where we have $l = A, B, ..., F$ and $b_{l}^{\dagger} = \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{R}} b_{l}^{\dagger}$. The two Bloch vectors got from the two chosen loop states are represented as

\begin{equation}
\vec{u}_{1,k} = (1 - e^{-i2\mathbf{k} \cdot \mathbf{R}_2}, -1 + e^{-i\mathbf{k} \cdot \mathbf{R}_2}, 1 + e^{-i\mathbf{k} \cdot \mathbf{R}_2}, 0, -1 - e^{-i\mathbf{k} \cdot \mathbf{R}_2}, e^{i\mathbf{k} \cdot \mathbf{R}_1} - e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)})^T,
\end{equation}

\begin{equation}
\vec{u}_{2,k} = (0, e^{-i\mathbf{k} \cdot \mathbf{R}_1} - e^{-i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)}, -1 - e^{-i\mathbf{k} \cdot \mathbf{R}_2}, 1 - e^{-i2\mathbf{k} \cdot \mathbf{R}_2}, 1 + e^{-i\mathbf{k} \cdot \mathbf{R}_2}, -1 - e^{-i\mathbf{k} \cdot \mathbf{R}_2})^T.
\end{equation}
However, the Bloch vector $\vec{u}_{s,k}$ is not yet normalized. We call the normalized Bloch vectors $\vec{\beta}_{s,k}$, and define the normalized Bloch state as $|\beta_{s,k}\rangle = \tilde{L}_{s,k}^\dagger |0\rangle = \sum_l \beta_{s,k}^l b_l^\dagger |0\rangle$, where the redefined operator $\tilde{L}_{s,k}^\dagger$ now becomes canonical Bosonic operators satisfying the commutation relation $[\tilde{L}_{s,k}^\dagger, \tilde{L}_{s,k'}^\dagger] = \delta_{k,k'}$. Thus, we get a set of orthonormal Bloch states for each of the two flat bands, and can be transformed into two sets of Wannier states as:

$$w_{s,R}^\dagger = \frac{1}{\sqrt{N_{\text{site}}}} \sum_k e^{ik \cdot R} \tilde{L}_{s,k}^\dagger = \sum_{R',l} w_{s,R}^l (R') b_{R'}^l,$$

where the Wannier wavefunction is given by

$$w_{s,R}^l (R') = \frac{1}{\sqrt{N_{\text{site}}}} \sum_k e^{ik \cdot R} \beta_{s,k}^l e^{-ik \cdot R'}.$$

Here, the Wannier wavefunction sits on the coordinate $(R', l)$. The coordinate $(R, s)$ labels where the center of the wavefunction locates. We note that the more detailed notations, $w_{s,R}^\dagger$ and $w_{s,R}^l (R')$, which we use here, are equivalent to the more compact notations we have used in the main text, namely $w_j^\dagger$ and $w_j(r)$. The direct correspondence is $r \equiv (R', l)$ and $j \equiv (R, s)$. The two sets of wavefunctions are illustrated in Fig. D.1(b), where the $s=1$ one encircles only the left hexagons in every unit cell and the $s=2$ one encircles only the right hexagons. The major part of the real-valued Wannier functions are essentially the two dimer loop states which we start with. The amplitude tail spreads out and decays exponentially along the major axis of the loop which ensures orthogonalization. However, the two sets of Wannier functions are not mutually orthogonal to each other (for example, those neighboring ones will still have finite overlap) since the two sets of Bloch vectors are not mutually orthogonalized yet.
For each $k$, one can orthogonalize the two Bloch vectors through the Gram-Schmidt process, i.e.

\begin{equation}
|\gamma_{1,k}\rangle = \frac{|\beta_{2,k}\rangle - |\beta_{1,k}\rangle \langle \beta_{1,k}| \beta_{2,k}\rangle}{\sqrt{\langle |\beta_{2,k}\rangle - |\beta_{1,k}\rangle \langle \beta_{1,k}| \beta_{2,k}\rangle}},
\end{equation}

which generates a normalized $|\gamma_{1,k}\rangle$ orthogonal to $|\beta_{1,k}\rangle$. Similarly, one can get a normalized $|\gamma_{2,k}\rangle$ which is orthogonal to $|\beta_{2,k}\rangle$. Therefore, one can choose either orthogonal pair as the flat-band basis. However, from either choice, the acquired Wannier wavefunctions belonging to the two bands have completely different shapes and hence lose translational symmetry. To preserve translational symmetry and being closer to a dimer shape, we can make a symmetric superposition as:

\begin{equation}
|\alpha_{1,k}\rangle = \frac{1}{\sqrt{2}} \left[ |\beta_{1,k}\rangle + e^{i\theta_k}|\gamma_{2,k}\rangle \right],
|\alpha_{2,k}\rangle = \frac{1}{\sqrt{2}} \left[ |\beta_{2,k}\rangle + e^{i\theta_k}|\gamma_{1,k}\rangle \right],
\end{equation}

where $|\alpha_{1,k}\rangle$ and $|\alpha_{2,k}\rangle$ are the mutually-orthogonal sets of Bloch states we choose. The additional free choice of phase factor $e^{i\theta_k}$ will give rise to different Wannier states. The sensible choice of the phase factor makes sure that the Bloch vectors are analytically continuous in $k$-space, which ensures that the generated Wannier function is exponentially localized \cite{55} and hence is more compact.

The Bloch states generated from the Gram-Schmidt process, $|\gamma_{s,k}\rangle$, are unfortunately not analytically continuous. For example, as shown in Fig. \ref{fig:D.1}(c), the $A$-component of one of the Bloch vectors, $|\gamma_{1,k}\rangle_{A}$, has a diagonal discontinuity cut in its real part. Same cut happens for its imaginary part and most of the other components of $|\gamma_{1,k}\rangle$, and $|\gamma_{2,k}\rangle$.

Thus, one has to take advantage of the additional phase factor $e^{i\theta_k}$ to remove the discontinuity. In this particular case, a simple sign flip of every other strip in the $k$-space, which
can be expressed as a square-wave function: \( \text{sgn}[\sin((k_x, k_y) \cdot (1, \sqrt{3}))] \), is able to remove the discontinuity [see Fig. D.1(d)]. In addition, we employ an extra phase factor \( e^{ik \cdot a_2} \) to ensure no breaking of TR symmetry and closeness in shape to the dimer loop state. Thus, our choice of phase factor \( e^{i\theta k} \) for Eq. (D.7) is \( e^{ik \cdot a_2} \text{sgn}[\sin((k_x, k_y) \cdot (1, \sqrt{3}))] \) (a \( k \)-independent relative sign or phase factor does not affect the probability distribution of the Wannier functions). This particular choice yields the complete Wannier basis illustrated in Fig. 5.8(b).

Our Wannier Orbitals (WOs) preserve the mirror symmetry (in terms of probability) with respect to its major axis, similar to the original Loop Orbitals (LOs) which they are based on. However, due to the additional phase factor we choose to keep the analytical continuity, the mirror symmetry along the minor axis is slightly broken. We can see that the lower part of the WO has slightly larger probability than the upper part. If we replace part of the phase factor \( e^{ik \cdot a_2} \) with \( e^{-ik \cdot a_2} \), the shape of the WO will be flipped with respect to the minor axis, namely the higher part will have larger probability. We also note that we do not claim that we have found the maximally compact WOs, even though the construction is based on the maximally compact LOs. In general, it should be possible to numerically/analytically determine such maximally compact WO which also preserve both types of mirror symmetries. Thus, our current approach is just a simple mathematical construction which aims to approximate the maximally compact WOs, since the shape we have acquired is not too far from the original LOs which they are based on.

Finally we note that, since we have successfully found a complete orthogonal Bloch or Wannier basis from superposition of the dimer loop states, we have proved the completeness of the loop states which is mentioned in property 2 of Sec. 5.4.
APPENDIX E

Localized orbitals preserving $C_6$ symmetry

We show that it is possible to construct a localized orbital which preserve the $C_6$ rotational symmetry of probability. The most compact $C_6$-symmetric orbital can be constructed by the superposition of six dimer loop orbitals as shown in Fig. E.1. In panel (a), we have six dimer loop orbitals (with the amplitude labeled for each site) sharing the same left hexagon. The superposition of the six orbitals generate a $C_6$-symmetric orbital in panel (b), centered on the left hexagon. We note that in order to preserve the $C_6$-symmetry of probability, one has to introduce relative phase between the orbitals, and in this example a $\pi/2$ phase. This leads to the imaginary number $i$ in certain amplitudes and breaking of TR symmetry. In this case, another

![Diagram](image)

Figure E.1. (a) Six dimer loop orbitals (with amplitudes labeled for each site) sharing the same left hexagon. (b) A $C_6$-symmetric localized orbital centered on the left hexagon. The orbital is superimposed by the six dimer loop orbitals in panel (a). (c) A $C_6$ symmetric localized orbital centered on the right hexagon. The orbital has the same probability distribution as the one in panel (b).
possible choice is obtained by turning $i$ into $-i$. This orbital also preserves the $C_6$-symmetry and has the opposite current. The reason of this is that the $C_6$-symmetric orbital includes seven (odd number) $\pi$-fluxes, which gives rise to the doubly degenerate eigenstates with opposite chirality. A similar construction can generate a $C_6$-symmetric orbital centered on the right hexagon, by the superposition of the six surrounding dimer loops. Thus, for each hexagon, one can generate a $C_6$-symmetric orbital centered on right hexagons with the same probability distribution. These orbitals form a complete and spatially uniform basis of the gapped flat band and can also be orthogonalized to form Wannier orbitals.

The reason that we do not choose these $C_6$-symmetric orbitals as our basis for flat-band projection and mean-field theory is that they have much larger overlaps compared to the dimer loop orbitals. Therefore, at low density ($\nu < 1/3, \nu_{\text{eff}} < 1$) when the hard-core approximation holds, a mean-field product state of particles occupying such orbitals, in the form of $|\psi_{\text{MF}}\rangle=\prod_j (f_{j,0}+f_{j,1}w_j) |0\rangle$, will cause much more interaction energy than using more compact and anisotropic orbitals, and hence is not energetically favorable. However, when going up to high density ($\nu \gg 1/3, \nu_{\text{eff}} \gg 1$), namely on average more than 1 particle per orbital, the hard-core approximation breaks down and there will be large interaction energy cost for particles in the same orbital. Hence there is no obvious advantage for particles to occupy more compact orbitals. Thus, one may expect a phase transition from nematic phase to isotropic (also chiral) phase at high filling, which will be studied more systematically in future works.
APPENDIX F

Summary of terms in the flat-band effective Hamiltonian

Here we classify all types of effective interaction $\sum_{ijkl} I_{ijkl} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{k} \hat{w}_{l}$, not limited by the hard-core constraint. The types of terms are listed below:

(1) On-site repulsion:

(F.1) \[ V_{\text{onsite}} = \sum_{j} U' \hat{w}_{j}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{j} \hat{w}_{j}, \]

where $U' = I_{jjjj} \approx 0.11U$ is the largest energy scale in the effective Hamiltonian.

(2) Density-density repulsion:

(F.2) \[ V_{\text{DD}} = \sum_{(i,j)} 2I_{ij}^{d} \hat{w}_{i}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{j} = \sum_{i,j} I_{ij}^{d} \hat{w}_{i}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{j} , \]

where $(i,j)$ means sum over pairs of sites $(i \neq j)$. Thus, $(i,j)$ and $(j,i)$ correspond to the same term and should not be double counted. Now we determine the coefficients $I_{ij}^{d}$ of the effective interaction. Four terms in the effective interaction correspond to the pair $(i,j)$, namely $I_{ij}^{d} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{i} \hat{w}_{j} + I_{jj}^{d} \hat{w}_{i}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{j} + I_{ij}^{d} \hat{w}_{j}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j} \hat{w}_{i} + I_{ji}^{d} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{j} \hat{w}_{i} = 4I_{ij}^{d} \hat{w}_{i}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j}^{\dagger} \hat{w}_{j}$. Thus, we get $I_{ij}^{d} = 2I_{jj}^{d}$.

(3a) Onsite pair-hopping (involving two different sites):

(F.3) \[ V_{\text{PHA}} = \sum_{(i,j)} I_{ij}^{p}(\hat{w}_{i}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j} \hat{w}_{j} + \text{H.c.}) = \sum_{i,j} I_{ij}^{p} \hat{w}_{i}^{\dagger} \hat{w}_{i}^{\dagger} \hat{w}_{j} \hat{w}_{j}, \]
Figure F.1. Table summarizing the leading terms and their coefficients (in units of Hubbard interaction strength $U$) of the effective onsite repulsion and the other three types of effective interactions which survive under the hard-core constraint.
where \( I^p_{ij} = I^p_{ijj} \)

(3b) Off-site pair-hopping (involving three different sites):

\[
V_{PHb} = \sum_{\substack{(i,j) \ k \neq i,j}} \sum_{k} [P^p_{ijk}(w_i^\dagger w_j^\dagger w_k + w_j^\dagger w_i^\dagger w_k + H.c.)] = \sum_{i,j,k} P^p_{ijk}[w_i^\dagger w_j^\dagger w_k w_k + H.c.],
\]

where \( P^p_{ijk} = I^p_{ijj} \).

(4a) Assisted-hopping (involving three different sites):

\[
V_{AHa} = \sum_{\substack{(i,j) \ k \neq i,j}} \sum_{k} I_{ijj}^{ah}(w_i^\dagger w_j^\dagger w_k + H.c.) = \sum_{i,j,k} I_{ijj}^{ah}w_i^\dagger w_j^\dagger w_k w_k.
\]

Four terms (and their H.c.) in the effective interaction correspond to the pair \((i,j)\), namely

\[
I_{ikjk}w_i^\dagger w_j^\dagger w_k + I_{ikjk}w_i^\dagger w_j^\dagger w_k + I_{ikjk}w_i^\dagger w_j^\dagger w_k + I_{ikjk}w_i^\dagger w_j^\dagger w_k = 4I_{ikjk}w_i^\dagger w_j^\dagger w_k.
\]

Thus, we get \(I_{ijj}^{ah} = 4I_{ikjk} (i \neq j \neq k)\).

(4b) Assisted-hopping (involving only two different sites):

\[
V_{AHb} = \sum_{\substack{(i,j) \ k \neq i,j}} \sum_{k} I_{ijj}^{ah} w_i^\dagger w_j^\dagger w_j + H.c.)w_j^\dagger w_j = \sum_{i,j} I_{ijj}^{ah} w_i^\dagger w_j^\dagger w_j w_j.
\]

Here, we have \(I_{ijj}^{ah} = 2I_{ijjj}\), due to the presence of two terms of each type, e.g. 

\[
I_{ijjj}w_i^\dagger w_j^\dagger w_j + I_{ijjj}w_i^\dagger w_j^\dagger w_j = 2I_{ijjj}w_i^\dagger w_j^\dagger w_j.
\]

(5) Ring-exchange interaction:

\[
V_{Ring} = \sum_{\substack{(i,j) \ k,l}} I_{ijj}^{Ring}(w_i^\dagger w_j^\dagger w_k w_l + H.c.).
\]

Here, \(\sum_{\substack{(i,j) \ k,l}}\) means each term in the sum selects two pair of sites (none of the four sites coincide), one pair with creation operators and the other pair with annihilation operators. Due
to the fact that \((i, j)\) and \((j, i)\) correspond to the same thing, there are \(2 \times 2 = 4\) terms from effective interaction correspond to the same type. Thus, we get \(I_{ij,kl}^{\text{Ring}} = 4I_{ijkl}\). Note that, for each plaquette \((i, j, k, l)\), there are \(\binom{4}{2} = 4\) different types of terms, due to the different choices of creation and annihilation operators.

After imposing the hard-core approximation, namely replacing the Wannier operators \(w_j^\dagger\) by the Pauli operator \(\sigma_j^+\), only the density-density repulsion (2), assisted hopping involving three different sites (4a) and the ring-exchange interaction (5) survive. Other types of term vanish due to the doubling of Pauli operators on the same site, namely \((\sigma_j^+)^2 = 0\). We list the leading terms of these types in Fig. F.1.

There are certain pairs of effective terms illustrated in Fig. F.1 which are associated with a mirror reflection along the major axis \((e_3)\). For the density-density repulsion, terms in such pair have exactly the same coefficients. For the assisted hopping, terms in the mirror pair have the same magnitude for coefficients, but may have opposite signs. In particular, for the assisted hopping in row (b) (hopping along the major axis \(e_3\)), terms in all the mirror pairs have opposite signs. One can see that for uniform density case (e.g. nematic superfluid) and within the mean-field approximation, the assistive number operator of the dimer (green) can be replaced by a constant number. Thus, the mirror terms will cancel out exactly and there will be no effective hopping along the major axis \((e_3)\) of the dimer. The finite effective hopping of the dimers only occur in the other two directions \((e_1\) and \(e_2)\). Therefore, in a nematic superfluid, the hopping of the bosons is anisotropic.
APPENDIX G

Details of the self-consistency mean-field theory on a large lattice

With the decoupling of effective interaction mentioned in the main text, we search for the self-consistent solution on a large periodic lattice (torus) with randomized initial distribution of the mean-field order parameters. We use a local update algorithm: (1) randomly pick up a site $i$ in each step and find the local ground state $|g\rangle_i$ of the decoupled Hamiltonian $h_i(\{\psi_j\}, \{n_j\})$;

Figure G.1. (a,b,c) The nematic Wigner crystal ground states from self-consistent mean-field calculations on three different lattices. The periodic boundary condition is illustrated by the wires. The lattices contain 200, 225 and 225 sites respectively. (d,e) The nematic supersolid and nematic superfluid states calculated form the self-consistent mean-field theory on the periodic lattice shown in panel (a).
(2) Calculate the expectation values of the corresponding Wannier operator and Wannier number operator and use them as updated order parameters for site \( i \), i.e. \( \psi_i = \langle g | w_i | g \rangle_i \) and \( n_i = \langle g | n_i | g \rangle_i \); (3) Repeat the previous two steps until the order parameters on each site have converged and hence reach the self-consistent mean-field solution.

We have done calculations on lattice with different types of geometry, as shown in Fig. G.1(a-c) (with the periodic boundary conditions illustrated by the wires). For all the cases, the nematic Wigner crystal states are produced (as shown in the figure), as well as the other two phases. However, the convergence time of the simulation differs from the lattice geometry. We find lattice (a) has the fastest convergence, possibly due to the fact that it respects the mirror symmetry of the dimers along their major axis. Therefore, we use lattice (a) to calculate all the curves shown in Fig. 5.9(a). For each chemical potential, we do several independent simulations with different randomized initial conditions and pick the one with the lowest energy as our solution. This is due to the fact that sometimes the configuration may be trapped in certain local energy minimum and stop evolving into the true mean-field solution. The complete image of the simulation results (a nematic supersolid state and a nematic superfluid state) from Fig. 5.9(c,d) is shown in Fig. G.1(d,e).