Abstract

This thesis comprises an intensive investigation of the Jaynes-Cummings-Hubbard (JCH) system. This Hamiltonian describes a system of coupled photonic cavities, each cavity contains a single two-level system. This system is rich in the physics it contains. The presence of the two-level system provides a mechanism by which the photons may interact with each other, providing an interesting array of non-linear phenomena. Using the mean-field approximation, the phase diagram of this system has been shown to display what are effectively two different phases - a superfluid phase, and a Mott-insulator phase. In this thesis we show that by using exact diagonalisation for a finite number of cavities, there is a rich structure to the phases that goes beyond this dual division of phases. We also generate phase diagrams that could be experimentally realised using an ion trap system.

Investigating the time dependent properties of the one-dimensional JCH system, we obtain both localised and delocalised behaviour, despite having only one excitation in the system. In certain limits the 1D JCH system approximates two Heisenberg spin chains. We find it is also possible in the one excitation, one-dimension time dependent case to actively control the location of the excitation, by means of a potential, thus creating all standard components of linear optics: we specifically investigate waveguides and beamsplitters. Finally, we investigate the use of matrix product states (MPS) to study the one-dimensional JCH system in the time domain. MPS is used to show how two colliding excitations can show the signature of photon blockade.
DECLARATION

This is to certify that:

(i) the thesis comprises only my original work towards the PhD except where indicated,

(ii) due acknowledgement has been made in the text to all other material used,

(iii) the thesis is less than 100,000 words in length, exclusive of tables, maps, bibliographies, and appendices.

Melissa Irene Makin
During the course of this project, the following articles have been published, which are based on the work presented in this thesis. They are listed here for reference.


**James Quach, Melissa I. Makin, Chun-Hsu Su, Andrew D. Greentree, Lloyd C. L. Hollenberg** *Band structure, phase transitions, and semiconductor analogs in one-dimensional solid light systems*, Physical Review A, **80** (2009) 063838
Andy Greentree was my primary supervisor for this thesis, and deserves an enormous thankyou. Not only has he had a wealth of enthusiastic support for the science I’ve produced during this thesis, he also supported my decision to move from being an ideal-student-who-works-a-lot to a more-well-rounded-human-being-who-has-a-baby-while-she-is-young-and-healthy. My second and third supervisors, Lloyd Hollenberg and Andy Martin have also been fantastic help, with both reading and making comments on various papers as well as chapters of this thesis.

Thanks also needs to go to the postdocs who helped me over the course of this thesis: Jared Cole and Charles Hill. They have both had lots of time for me over the years, and have been especially helpful with questions I’m sure are too simple for supervisors, but too complicated to work out on my own. Thanks also to my “thesis Friday” partner Lila Warszawski, it is lovely to have someone who is going through the same stresses at the same time.

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I recognise that many people who see a copy of this thesis will read only these acknowledgements, and only flick through the rest, so, thanks for reading these acknowledgements. If your name isn’t mentioned above, but you think it should be, sorry. I probably think you are truly awesome, just you probably didn’t help with my thesis that much.
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Normally, photons do not interact with each other. This can make them difficult to control. For a photon to interact with another photon, the first photon would have to change either the momentum or the phase of the second photon. However, even when shining two very powerful lasers through each other, nothing happens at the intersection point - no sparks fly, the beams do not bend or buckle - the photons merely ignore each other. In the system studied in this thesis however, photons can interact (this is not the only way of getting photons to interact with each other: the optical Kerr effect is one example of a means by which photons may interact with each other, however in practice this is a very lossy process). These interactions lead to behaviour reminiscent of condensed matter systems. As such, many interesting effects may occur: for example, a phase transition from the superfluid (gaseous, “normal”) phase of light to a Mott-insulator (solid) phase of light; transport of a single photon through a medium may be slowed or stopped; and single photons may be guided through such a medium in a controlled fashion via dynamic control. This system is described by the Jaynes-Cummings-Hubbard (JCH) model, which is the primary theme of this thesis.

The JCH model describes a number of coupled photonic cavities, each containing a single two-level system. This system, at least in restricted implementations, is on the cusp of realisation experimentally. As such, the theoretical investigations performed in this thesis will be important for guiding the first experiments performed for this system. The JCH system is important because it can contain and manipulate small numbers of photons - this will be invaluable in the development of various quantum devices, including quantum
emulators.

This thesis has two main parts: investigation of phase diagrams of the system occur in chapters 3 and 4, and investigation of time evolution occurs in chapters 5, 6 and 7.

1.1 Layout and publication of material in this thesis

Chapter 2 gives a brief introduction to the Jaynes-Cummings-Hubbard Hamiltonian: exploring the origins of this model, its construction as a composite of many Jaynes-Cummings Hamiltonians, and its relationship to the more traditional Bose-Hubbard Hamiltonian. We outline the importance and relevance of the chemical potential term, and also explore how this Hamiltonian changes in the limit of one excitation. Finally, we discuss the possibilities for experimental realisation of this model.

The work in chapter 3, excluding the work on the mean-field approximation (which is review) and perturbation theory (which is largely review), has been published in references [66, 64]. This chapter focuses on phase diagrams of the JCH system, using the exact diagonalisation method, for small numbers of cavities. These phase diagrams are compared to phase diagrams generated using the mean-field technique. This chapter leads directly to the next, chapter 4, which investigates a system of ions individually trapped in a one-dimensional array, which with minor modifications can also be described by the JCH Hamiltonian. Thus, phase diagrams specific to the ion trap system can be generated, which may be amenable to experimental verification in coming experiments.

Time evolution of the JCH Hamiltonian in one dimension is investigated in chapter 5, which was published in [65]. Here, we initiate the system in one of two initial states, and investigate the time evolution of the system in various limits of the system. We consider both uniform coupling between cavities, as well as a parabolic coupling profile, with coupling between the middle cavities stronger than the coupling between cavities at the end of the chain. We find that in certain limits of the system, the Hamiltonian behaves like two separate Heisenberg spin chains - one chain being the atomic evolution, the other the photonic evolution. This work inspired the next chapter, on time evolution via the utilisation of a time dependent Hamiltonian.
Chapter 6 investigates the virtual waveguides and beamsplitters in the one-dimensional JCH system. These are generated by forming an effective potential of the detuning along the chain. These Gaussian potentials can trap, and move excitations along the chain - thus forming a \textit{virtual} waveguide. By placing two such virtual waveguides in close vicinity, a beamsplitter may be constructed. These virtual waveguides and beamsplitters supersede normal waveguides and beamsplitters because rather than existing in two spatial dimensions, they exist in one spatial and one time dimension, and as such can be modified easily on an experiment-by-experiment basis.

While chapters 5 and 6 focus on the time evolution of \textit{one} excitation in the one dimensional system, chapter 7 introduces and investigates the use of matrix product states, which is an excellent method for exploring the time evolution of \textit{multiple} excitations in the one dimensional JCH system. Matrix product states are an excellent method for manipulating quantum states: the representation, the generation of single site expectation values, time evolution and the generation of ground states can all be found efficiently. Finally the thesis is concluded in chapter 8.
1. Introduction
A photonic cavity is a volume in space which can contain, for some amount of time and for various frequencies, one or more photons. We assume throughout this thesis that the photonic cavity is only capable of supporting a single photonic mode, that is, that it can only trap photons of a single specific frequency. In isolation from its neighbours, each cavity is described by the Jaynes-Cummings (JC) Hamiltonian, which was first described in 1963 [50]. The JCH Hamiltonian describes a system of \( N \) coupled photonic cavities, each of which contains a single two-level system. Without loss of generality, we refer to the two-level system as a two-level atom. The JC Hamiltonian is introduced in section 2.1, and the JCH Hamiltonian in section 2.3. The general theoretical description can apply to any of a number of possible experimental configurations, we review some of these in section 2.4.

### 2.1 Jaynes-Cummings model

The Jaynes-Cummings (JC) Hamiltonian describes a single photonic cavity containing a single two-level system, first introduced in [50]. A possible representation of a photonic cavity shown in figure 2.1: the outer curved lines represent two concave mirrors facing each other, which trap a photon of energy \( \omega \) (a single mode cavity is assumed). The atom has energy gap \( \epsilon \), and (not shown in the diagram) the photon may convert to an excited atom, and vice versa, with strength \( \beta \). The JC Hamiltonian [50] is given by
2. The Jaynes-Cummings-Hubbard model

\[ \mathcal{H}_{JC} = \epsilon \sigma^+ \sigma^- + \omega a^\dagger a + \beta (\sigma^+a + \sigma^- a^\dagger), \]  
\tag{2.1} \]

where \( \sigma^+ \) and \( \sigma^- \) are the atomic raising and lowering operators (which may also be written \( |e\rangle \langle g| \) and \( |g\rangle \langle e| \)), and \( a^\dagger \) and \( a \) are the photonic raising and lowering operators. The operator \( \sigma^+ \sigma^- \) is the number operator for the number of atomic excitations (eigenvalues are zero or one only). The operator \( a^\dagger a \) is the number operator for the number of photonic excitations (eigenvalues are any positive integer, including zero). The coefficient \( \epsilon \) is the atomic energy difference, \( \omega \) is the energy of the trapped photon (equivalent to the cavity frequency), and \( \beta \) is the coupling between the cavity and its resident atom. The difference \( \Delta = \omega - \epsilon \) is the atom-cavity detuning, which is important for setting the characteristic energy scales for the system.

Equation (2.1) utilises both the dipole approximation and the rotating wave approximation (RWA), see for example chapter 5 of [53]. The dipole approximation assumes that the dimensions of the atomic system are small when compared to the wavelength of the photons. The RWA ignores counter-rotating terms: it assumes that the terms which oscillate with frequency \( \omega + \epsilon \) (specifically the terms \( \beta (\sigma^+a^\dagger + \sigma^- a) \), which disobey particle number conservation) are discarded, and the terms which oscillate with frequency \( \omega - \epsilon \), namely \( \beta (\sigma^+a + \sigma^- a^\dagger) \), are kept. The RWA is valid when the Rabi frequency is much less than the photonic frequency, that is, \( \beta \sqrt{n} \ll \omega \).

![Figure 2.1: Representation of a photonic cavity described by the JC model. The two outer curved lines represent two concave mirrors, which form the photonic cavity. The oval represents a photon with frequency \( \omega \). The two horizontal lines represent the energy levels of a two-level atom with energy gap \( \epsilon \). Not shown is the coupling between the cavity and the atom, which has strength \( \beta \).](image-url)
Table 2.1: Some examples of elements of the bare and dressed bases, in order of increasing total number of excitations.

\[
\begin{array}{|c|c|}
\hline
\text{Bare basis} & \text{Dressed basis} \\
\hline
|g, 0\rangle & |g, 0\rangle \\
|e, 0\rangle & |-, 1\rangle \\
|g, 1\rangle & |+, 1\rangle \\
|e, 1\rangle & |-, 2\rangle \\
|g, 2\rangle & |+, 2\rangle \\
\vdots & \vdots \\
\hline
\end{array}
\]

The bare basis for the JC Hamiltonian is given by states \(|s, n\rangle\), where \(s = g\) (e) represents the atom in the ground (excited) state, and the Fock states \(n = 0, 1, \ldots\) represent the number of photons in the cavity. The matrix form of the Hamiltonian written in the bare basis, in the order shown in table 2.1, is

\[
\mathcal{H}^{JC} = \begin{pmatrix}
0 \\
\epsilon & \beta & \omega \\
\beta & \omega & \sqrt{2}\beta \\
\epsilon + \omega & \sqrt{2}\beta & 2\omega \\
\end{pmatrix},
\]

which is block diagonal, where the horizontal and vertical lines indicate the blocks. All matrix elements outside of these lines are zero. The column vector on the right shows the basis used. The blocks (apart from the first, which is a 1×1 matrix consisting of a single zero) can be written

\[
\mathcal{H}^{JC}_{(n)} = \begin{pmatrix}
\epsilon + (n - 1)\omega & \sqrt{n}\beta \\
\sqrt{n}\beta & n\omega \\
\end{pmatrix},
\]

in the basis \(|e, n - 1\rangle, |g, n\rangle\), hence

\[
\mathcal{H}^{JC} = \text{diag}[0, \mathcal{H}^{JC}_{(1)}, \mathcal{H}^{JC}_{(2)}, \ldots],
\]

(2.4)
The Jaynes-Cummings-Hubbard model

As such diagonalisation of the JC Hamiltonian is straightforward, as it is just a case of diagonalising each $2 \times 2$ submatrix independently.

The energy eigenbasis is commonly referred to as the dressed basis, with states given by $|\pm, n\rangle$, where $n$ now refers to the total number of excitations in the cavity (photonic plus atomic). The state $|g, 0\rangle$ belongs to both the bare basis and the dressed basis, examples of some states for both the bare and dressed basis are shown in table 2.1. Other dressed basis states are related to the bare basis by

$$|\pm, n\rangle = \frac{\beta \sqrt{n}|g, n\rangle + \left[\left(-\Delta/2\right) \pm \chi(n)\right]|e, n-1\rangle}{\sqrt{2\chi^2(n) + \chi(n)\Delta}} \quad \forall n \geq 1,$$

with eigenvalues, (as plotted in figure 2.2)

$$E_{|g, 0\rangle} = 0, \quad E_{|\pm, n\rangle} = n\omega \pm \chi(n) - \Delta/2,$$

where we have used the generalised Rabi frequency

$$\chi(n) = \sqrt{n \beta^2 + \Delta^2/4} \quad \forall n \geq 1.$$

The Rabi frequency is the frequency with which any two-level system oscillates between its ground and excited state, when in the presence of a photon field. It is different from the quantity $\epsilon$, which is the energy difference between the ground and excited states.

Photon blockade is a dramatic effect in the Jaynes-Cummings model [46]. Photonic blockade (analogous to Coulomb blockade of electron transport [77, 11]) is the phenomenon whereby the presence of a single photon inside a JC cavity prevents the intrusion of subsequent photons of the same energy. This occurs because of the shifted energy levels due to the presence of the atom inside the cavity. The first photon enters the cavity by exciting the $|g, 0\rangle - | - 1\rangle$ transition. The next available state is $| -, 2\rangle$, which requires a transition energy of $\omega - \sqrt{2\beta^2 + \Delta^2/4} + \sqrt{\beta^2 + \Delta^2/4}$. Because this is different from the first transition energy, the presence of a second photon in the cavity is suppressed (provided that $\beta$ is sufficiently large). This effect has been analyzed for four-state systems [46, 28, 34] and two-state systems [82, 99]. More recently photon blockade has been observed [13, 21],
2. The Jaynes-Cummings-Hubbard model

Figure 2.2: Eigenenergies as a function of the detuning $\Delta$ of the JC Hamiltonian, the vertical axis of (a) is different to that of (b). (a) (with an arbitrary choice of $\omega = 12\beta$) shows the energies in full, while (b) shows the energies with the photon energy, $n\omega$ subtracted, creating a much more concise yet sometimes misleading plot. The left plot clearly shows the relative arrangement of energy levels, while the right clearly shows how the anti-crossings increase in size with increasing $n$, which is the signature of the nonlinear interaction.

adding substantial impetus to apply this effect to a range of applications. Arguably the most important case is that described here, namely one atom per cavity with few excitations. This is because this regime maximises the non-linear (photon-photon) interactions, and is therefore the most experimentally accessible regime.

2.2 Bose-Hubbard model

It is pertinent, before introducing the Jaynes-Cummings-Hubbard Hamiltonian, to introduce the Bose-Hubbard Hamiltonian [44, 84]. This model pre-dates the JCH model, and while the JCH model has both photons and atoms, and the Bose-Hubbard has only bosons, some aspects of the analysis are similar. The Bose-Hubbard model describes bosons hopping around a lattice of fixed positional states. The Hamiltonian is given by

$$H^{BH} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$ (2.8)

where $t$ represents the coupling between cavities (which can determined by the overlap
2. The Jaynes-Cummings-Hubbard model

Figure 2.3: Diagram representing the JCH model in one spatial dimension. The bottom row of circles represents the photonic cavities, and the top row of circles represents each cavity’s resident atom. The coupling between each cavity and its resident atom has strength $\beta$, while the inter-cavity coupling rate is given by $\kappa$.

integral between sites), $(i, j)$ sums over nearest neighbour pairs, $U$ is the on-site repulsion energy, $\hat{n}_i = a_i^\dagger a_i$ is the number operator for the bosons, and $\mu$ is the chemical potential. This Hamiltonian assumes the tight binding approximation (each site can be (apart from bosonic hopping) isolated).

The tight binding approximation is utilised in equation (2.8) - this assumes that the eigenstates of the system are superpositions of eigenstates of the individual sites (i.e. sites are sufficiently isolated from each other). As such, the coupling between cavities $t$ can be determined by the overlap integral between sites. An example of a system which is described by the Bose-Hubbard model is an ultracold atom system, see for example [61] and references therein.

Numerous facets of the Bose-Hubbard model have been considered including the prediction of glassy phases [25], Hilbert-space optimisation [32], and implementations of topological quantum computing [26]. One of the most dramatic and beautiful examples of the Bose-Hubbard model is the prediction [25] and demonstration [35] of the quantum phase transition in an ultra-cold atomic gas. Such demonstrations are significant for applying canonical solid-state treatments to the more controllable regime of atom optics, allowing new predictions to be tested (e.g. the supersolid phase [86]). Recent work on quantum phase transitions in photonic band-gap lattices does the same for the photonics–solid-state crossover [37, 49, 33, 7, 83, 39, 69, 17, 55, 40].
2.3 Jaynes-Cummings-Hubbard model

The Jaynes-Cummings-Hubbard (JCH) model describes a system of $N$ JC cavities, each of which is connected to its nearest neighbours via photonic coupling; it is diagrammatically represented in figure 2.3. The basis states for the JCH Hamiltonian are given by tensor products of the JC basis states. That is, $\{ |g, 0\rangle, |e, 0\rangle, |g, 1\rangle, \ldots \} \otimes N$ for the bare basis and $\{ |g, 0\rangle, |-, 1\rangle, |+, 1\rangle, \ldots \} \otimes N$ for the dressed basis. For example when $N = 2$, some example basis states are $|g, 0\rangle \otimes |g, 0\rangle$, $|g, 0\rangle \otimes |e, 0\rangle$, $|e, 0\rangle \otimes |g, 0\rangle$ and so forth. The JCH Hamiltonian is given by

$$H^{\text{JCH}} = \sum_{i=1}^{N} H^{\text{JC}}_i - \kappa \sum_{i,j=1}^{N} A_{i,j} a_i^\dagger a_j - \sum_{i=1}^{N} \mu_i (\sigma_i^+ \sigma_i^- + a_i^\dagger a_i).$$ (2.9)

The above equation contains three terms. The first term describes the JC nature of each cavity individually (as discussed above in section 2.1). The second term describes the coupling of the photons between cavities, in practice these can be effected by either evanescent fields between cavities, or optical fibres. Evanescent fields decay exponentially with distance between cavities, as such we assume only nearest neighbour coupling between cavities. The tight binding approximation (which is also utilised in the Bose-Hubbard model, section 2.2) assumes that the eigenstates of the system are superpositions of eigenstates of the individual cavities - each cavity-atom system can be considered isolated (apart from photonic hopping). The sign of $\kappa$ is chosen to be negative (chosen to be connected to the Bose-Hubbard model, equation (2.8)), however if it were instead positive (or any other phase factor), the underlying physics remains the same (the two are related by a time independent unitary transformation). $A$ is an adjacency matrix, which encodes the geometry of the system, it is given in general by

$$A_{i,j} = \begin{cases} 1 & \text{if cavity } i \text{ is connected to cavity } j \\ 0 & \text{otherwise.} \end{cases}$$ (2.10)

For example, if we consider a one-dimensional system of cavities with hard wall boundary conditions, where the cavities are labelled $1, 2, 3, \ldots, N$, the adjacency matrix is
2. The Jaynes-Cummings-Hubbard model

\[ A_{ij} = \begin{cases} 
1, & \text{if } |i - j| = 1 \\
0, & \text{otherwise.}
\end{cases} \tag{2.11} \]

The third term in equation (2.9) is the chemical potential \( \mu_i \) for each cavity, throughout this thesis it is set such that it is equal for all cavities, \( \mu_i = \mu, \forall i \). Chemical potential for a system of photons is zero, however as the particles we are dealing with here are composite particles\(^\ast\), particles which are neither bosons nor fermions, these may have a non-zero chemical potential defined. This is a subtle point, and is further discussed in section 2.3.1. The sign of \( \mu \) is negative, this corresponds with the negative sign introduced for the chemical potential in the Bose-Hubbard model [equation (2.8)], and is also discussed in section 2.3.1. Physically, when another excitation is added to the system, according to the chemical potential term, the total energy of the system is lowered.

The non-bosonic nature of the particles in the Hamiltonian of equation (2.1) requires further discussion. Normally one can divide all particles in the universe into two categories: either bosonic or fermionic. However, neither the composite particles of the JCH system nor the four state system with few atoms per cavity [37, 38] obey bosonic (or fermionic) commutation relations. The limits where we can view the system as being comprised of interacting bosons are many atoms per cavity (holds for both the Jaynes-Cummings and four state systems [69, 47, 37]), large detuning [33], and large excitation number.

The field of the JCH Hamiltonian was initiated in 2006 [37, 33, 7]. These three works, published within a short time frame, started this field, by showing that quantum phase transitions are possible in this system. There are of course variations between these three papers, specifically [37] uses four level rather than two-level atoms. Another common extension to the standard JCH model is to use multiple atoms inside each cavity, called the Dicke model [69], however this reduces the Mott-insulator phases of the phase diagram [29, 28, 34].

\(^\ast\)These particles are also called polaritons. This is the only time we refer to polaritons in this thesis. While the concept of a polariton has taken hold in the literature, in this thesis we are largely restricted to one excitation, and as such do not need to invoke polaritons.
2.3.1 Chemical potential in the JCH model

In this section we show, through arguments of statistical mechanics, that the parameter $\mu$ from equation (2.9) indeed represents the chemical potential. Let us decompose the full JCH Hamiltonian into two parts:

$$\mathcal{H}^{JCH} = \mathcal{H} - \mu \hat{L},$$

(2.12)

that is, $\mathcal{H}$ is the JCH Hamiltonian without the chemical potential term, and $\hat{L}$ is the operator representing the total number of excitations, $\hat{L} = \sum_{i=1}^{N} \sigma_i^+ \sigma_i^- + a_i^+ a_i$. We assume that the entire $N$ cavity system with $l$ total excitations exists in the ground energy eigenstate $|\psi_g\rangle$, so that $\mathcal{H}^{JCH}|\psi_g\rangle = E_g|\psi_g\rangle$ and $\hat{L}|\psi_g\rangle = l|\psi_g\rangle$ (i.e. $[\mathcal{H}^{JCH}, \hat{L}] = 0$, these two operators commute).

To show that $\mu$ has the general form of a chemical potential, we begin with the usual definition of free energy $F = E - TS$, where $E$ is the energy of the system $\mathcal{H}$ (before chemical potential has been included), $T$ is temperature and $S$ is entropy. Assuming that $T = 0$ (which is always the case for the JCH system in this thesis), we use the definition of chemical potential as the derivative of the free energy with respect to number of excitations, hence

$$\mu \equiv \left( \frac{\partial F}{\partial l} \right)_{T,V} = \left( \frac{\partial E}{\partial l} \right)_{T,V}. \quad (2.13)$$

The Hellmann-Feynman theorem \cite{42, 24} describes how the derivative of the energy eigenvalue with respect to an arbitrary parameter $\lambda$ relates to the expectation value of the Hamiltonian:

$$\frac{\partial E_\lambda}{\partial \lambda} = \langle \psi(\lambda) | \frac{\partial H_\lambda}{\partial \lambda} | \psi(\lambda) \rangle. \quad (2.14)$$

Hence to calculate the derivative of the energy with respect to number of excitations

$$\frac{\partial E}{\partial l} = \langle \psi_g | \frac{\partial \mathcal{H}}{\partial l} | \psi_g \rangle = \langle \psi_g | \frac{\partial}{\partial l} (\mathcal{H}^{JCH} + \mu l) | \psi_g \rangle = \mu. \quad (2.15)$$
2. The Jaynes-Cummings-Hubbard model

Hence provided that $T = 0$, the $\mu$ of equation (2.12) represents chemical potential as defined by the free energy equation.

2.3.2 One excitation JCH Hamiltonian

We construct a restricted basis of the full $N$ cavity bare basis, by limiting the system to one excitation (atomic or photonic, or some superposition of the two). The total number of excitations in the JCH system is conserved, hence this is a restriction, not an approximation. We write the restricted one excitation basis as $|Q\rangle \otimes |g,1\rangle (|Q\rangle \otimes |e,0\rangle)$, where $Q \in \{1, \ldots, N\}$, represents a photonic (atomic) excitation at cavity number, $Q$, and $|g,0\rangle$ at every other cavity position. That is,

\begin{align*}
|Q\rangle \otimes |g,1\rangle &= |g,0\rangle^{\otimes (Q-1)} \otimes |g,1\rangle \otimes |g,0\rangle^{\otimes (N-Q)} \quad (2.16) \\
|Q\rangle \otimes |e,0\rangle &= |g,0\rangle^{\otimes (Q-1)} \otimes |e,0\rangle \otimes |g,0\rangle^{\otimes (N-Q)} \quad (2.17)
\end{align*}

The states $\{|Q\rangle \otimes |g,1\rangle, |Q\rangle \otimes |e,0\rangle\}$, for $Q = 1, \ldots, N$ form a valid Hilbert space. In this restricted basis and under these conditions, the Hamiltonian (2.9) is greatly simplified, and can be represented

$$
\mathcal{H}_{\text{JCH}}^{\text{1exc}} = \frac{\Delta}{2} I_N \otimes Z + \beta I_N \otimes X - \kappa A \otimes \frac{I_2 + Z}{2}, \quad (2.18)
$$

where $I_m$ is the $m \times m$ identity matrix, and $X$ and $Z$ are the usual Pauli matrices acting on the atom-photon cavity subspace. The operator $A$ in matrix form is given by the adjacency matrix of the connectivity graph, in general given by equation (2.10). In this form, the first and second terms affect only the atomic/photonic modes locally, but do not move the excitation to any other cavity. The first term describes the detuning and the second term the coupling between photonic and atomic excitation modes. The third term describes photonic coupling between cavities, remembering that only photonic excitations may move between cavities, and that atomic excitations are fixed. This Hamiltonian, equation (2.18), is now in the form of tensor products of $2 \times 2$ matrices by $N \times N$ matrices. Two of the
$N \times N$ matrices are identity matrices, and the third is the adjacency matrix $A$. As such, if $A$ is diagonalisable then the entire Hamiltonian is diagonalisable.

The chemical potential is only important when the number of excitations is allowed to vary. This can be understood mathematically in the one excitation Hamiltonian because, in this restricted basis, the term $\sum_{i=1}^{N} (\sigma_{i}^{+} \sigma_{i}^{-} + a_{i}^{\dagger} a_{i})$ [from equation (2.9)] is equivalent to the identity operator (which of course is relevant only under the assumption that $\mu_{i} = \mu \ \forall i$). Since any identity operator added to any Hamiltonian makes no physical difference to that Hamiltonian, the chemical potential under the restriction of one excitation is not mathematically or physically meaningful, and as such will be excluded. Further to this, when the JCH Hamiltonian is restricted to $l$ excitations, the term $\sum_{i=1}^{N} (\sigma_{i}^{+} \sigma_{i}^{-} + a_{i}^{\dagger} a_{i})$ is equivalent to the identity operator multiplied by $l$. As such, for any number-restricted form of the JCH Hamiltonian, the chemical potential may be excluded.

The one excitation JCH Hamiltonian is utilised in two chapters of this thesis. In chapter 5, time evolution of the one excitation JCH model in one spatial dimension is investigated. In chapter 6, it is used to investigate the ability of the 1D JCH model to actively move a single excitation, in the form of virtual waveguides.

### 2.4 Experimental realisation

Here we discuss potential experimental platforms for the JC and JCH models, to highlight how this work relates to current experimental technologies. For many of the phenomenon discussed in this thesis to be realised experimentally, there are a few requirements of whichever setup is chosen. Specifically, the quality-factor $Q$ of the cavities must be high, and the main photon leakage channel must be into neighbouring cavities, rather than absorption or loss out of the system. The coupling between each cavity and its resident atom, $\beta$, must be much stronger than the hopping rate between cavities, $\kappa$ for the photon blockade regime to be realised. There are numerous ways in which to realise such a system depending on the available experimental configurations and desired topologies. Possible two-state systems include colour centres in diamond [30], quantum dots [69, 36],

*assuming $\lambda = 420$ nm from [71].
Table 2.2: Photonic cavities: some typical values of the parameters $Q$, $\omega$, and $\beta$ used in various experiments. Values given in brackets are measured, all other values in this table are theoretical predictions.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Reference</th>
<th>$Q$</th>
<th>$\omega/2\pi$</th>
<th>$\beta/\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transmission line resonators (3D optical)</td>
<td>[15]</td>
<td>$3 \times 10^7$</td>
<td>350 THz</td>
<td>220 MHz</td>
</tr>
<tr>
<td>Transmission line resonators (3D microwave)</td>
<td>[15]</td>
<td>$3 \times 10^8$</td>
<td>51 GHz</td>
<td>47 kHz</td>
</tr>
<tr>
<td>Transmission line resonators (1D circuit)</td>
<td>[15]</td>
<td>$10^4$</td>
<td>10 GHz</td>
<td>100 MHz</td>
</tr>
<tr>
<td>Silicon photonic crystal cavities</td>
<td>[72][71]</td>
<td>$10^9(2 \times 10^6)$</td>
<td>(29.8 THz)</td>
<td>-</td>
</tr>
<tr>
<td>Diamond photonic crystal cavities</td>
<td>[100][111]</td>
<td>$10^7(10^2)$</td>
<td>2.4 PHz$^*$</td>
<td>-</td>
</tr>
</tbody>
</table>

Spontaneous emission in a JCH system can occur either from the atom (either into the cavity, or into space), and/or from the photonic cavity (this effect will increase for more photons in the cavity, and is taken into account by the quality factor $Q$). This issue is explored in, for example, [54]. The effects of spontaneous emission from a cavity will be minimised for high $Q$ and low mode volume due to the Purcell effect [80]. In this regime, spontaneous emission to the vacuum (i.e. modes not supported by the cavity) will be suppressed in favour of the cavity modes. In this way the effective spontaneous emission rate is reduced relative to free space. Ultimately, if the spontaneous emission can be reduced to be less than the cavity loss rate, then it is no longer a significant problem (providing repopulation can be achieved). In this thesis, the calculations largely ignore the effects of both forms of spontaneous emission. Certainly, there are parameter regimes where spontaneous emission can be ignored - this has been shown experimentally...
Table 2.3: Two-level systems: some typical values of the parameters $\epsilon$ and $\beta$ used in various experiments. The numbers for the NV and NE8 centres, and the values of $\epsilon/2\pi$ for the SiV and Cr-1 and Cr-2 centres are theoretical predictions, all other values in this table are measured.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Reference</th>
<th>$\epsilon/2\pi$</th>
<th>$\beta/\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Superconducting transmon qubits</td>
<td>[14]</td>
<td>340-400 MHz</td>
<td>347 MHz</td>
</tr>
<tr>
<td>NV centre</td>
<td>[95]</td>
<td>74.9 THz</td>
<td>28 GHz</td>
</tr>
<tr>
<td>NE8 centre</td>
<td>[95]</td>
<td>59.6 THz</td>
<td>127 GHz</td>
</tr>
<tr>
<td>SiV centre</td>
<td>[95, 110]</td>
<td>64.6 THz</td>
<td>108 GHz</td>
</tr>
<tr>
<td>Cr-1 centre</td>
<td>[95, 1]</td>
<td>63.1 THz</td>
<td>270 GHz</td>
</tr>
<tr>
<td>Cr-2 centre</td>
<td>[95, 1]</td>
<td>63.7 THz</td>
<td>250 GHz</td>
</tr>
</tbody>
</table>

In table 2.2 we show some typical values of quality $Q$, cavity frequency $\omega$ and coupling to a resident two-level system $\beta$ for a number of different photonic cavities. The coupling between cavities, $\kappa$ is not shown either because multiple cavity systems are yet to be built or because this parameter can be varied over such a wide range as that displaying one value in this case would be meaningless. There is no parameter $\beta$ displayed for silicon because the quantum dots which could be placed on the silicon surface show significant variability. There is no parameter $\beta$ displayed for diamond because these are shown in table 2.3 as NV and NE8 centres.

In table 2.3 we show some typical values of transition frequency $\epsilon$ and coupling to its photonic cavity $\beta$ for a number of different two-level systems which are suitable for placement inside photonic cavities.

The final two entries of table 2.2 describe photonic cavities, in figure 2.4 we show a schematic diagram of such a photonic crystal. A photonic crystal is a thin sliver of dielectric medium punctured by a regular array of holes. The distance between holes is of order the wavelength of the light that is to be trapped. Transport of the light between the holes is thus repressed due to the Bragg condition. Every time a hole is not drilled (a defect in the imposed photonic crystal), a cavity is formed. In each hole, a single two-level atom is placed (for example a nitrogen-vacancy centre if the dielectric medium was diamond).

The systems shown in tables 2.2 and 2.3 are just a few of the possible experimental
2. The Jaynes-Cummings-Hubbard model

Figure 2.4: A JCH system represented as a photonic crystal. The yellow represents some dielectric medium: the periodic array of holes drilled forms a photonic crystal. Lattice locations where holes are not drilled form photonic cavities, into each cavity is placed a single two-level atom (represented by a red sphere).

platforms for demonstrating the JCH phenomena described in the subsequent chapters of this thesis.

2.5 Summary

The JC model describes a photonic cavity containing a single two-level system, and the JCH model describes a set of such cavities, connected by photon hopping. This is based on and extends the Bose-Hubbard model, which consists of a number of sites each able to contain one or more bosons. The JCH Hamiltonian contains a chemical potential term, which disappears under the restriction of one excitation: the one excitation Hamiltonian simplifies the mathematics considerably. The theoretical study of the JCH model is important both because it is an excellent system for slowing and stopping photons, which will be incredibly useful in the near future of a multitude of quantum devices, but also because these devices are so very near to being experimentally realised.
In this chapter, we use the word *phase* to mean some region of a material with uniform properties. One does not usually consider light to be able to change phase. For example water has three phases: liquid, solid and gas. The normal phase of light best resembles a gas, technically it is called a superfluid. It is theoretically possible in our Jaynes-Cummings-Hubbard system to access another phase of light: that resembling a solid (technically a Mott-insulator state). This work is different from the phase transitions of an optical field in a cavity, e.g. Refs. [88, 96], which are for a driven, damped, far from equilibrium system.

We can draw comparisons to calculations done previously with the Bose-Hubbard model, which describes bosons hopping around a lattice of allowed positional states, and was described in section 2.2. A quantum phase transition is observed between delocalised particles (superfluid phase) and localised particles (Mott-insulator phase) depending on the strength of the hopping term relative to the onsite interaction [84]. Differences between the JCH and Bose-Hubbard systems are interesting topics for investigation, and a study of the particle nature (whether the particles are bosons, as in the Bose-Hubbard model, or fermions, or something else) should prove fruitful, but goes beyond our present work. We may understand some of the differences by comparing the onsite repulsion in the Bose-Hubbard and JCH cases. The Bose-Hubbard Hamiltonian is given by
3. Phase diagram of the JCH in the ground state

$$\mathcal{H}^{\text{BH}} = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j^\dagger + a_j a_i^\dagger) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$  \hspace{1cm} (3.1)

where $\hat{n}_i = a_i^\dagger a_i$ is the number operator for the number of bosons at lattice site number $i$. For comparison, we repeat the JCH Hamiltonian, equation (2.9), here also:

$$\mathcal{H}^{\text{JCH}} = \sum_{i=1}^{N} \mathcal{H}^{\text{JC}}_i - \kappa \sum_{i,j=1}^{N} A_{i,j} a_i^\dagger a_j - \sum_{i=1}^{N} \mu_i (\sigma_i^+ \sigma_i^- + a_i^\dagger a_i).$$  \hspace{1cm} (3.2)

In the Bose-Hubbard system, the interaction $U$ is a constant, however in the JCH model this can be seen as having a particle number dependence, i.e. $U_\pm(n) = \chi(n+1) - \chi(n)$ [where $\chi(n) = \sqrt{n^2 + \Delta^2} / 4 \forall n \geq 1$], as in equation (2.7)]. In the large photon limit, we obtain a non-interacting Bose gas, as $U_\pm(n) \to 0$, (because $\sqrt{n+1} \approx \sqrt{n}$ as $n \to \infty$), and in the large detuning limit, $U_\pm(n) \to \pm \beta^2 / \Delta$, which is a constant bosonic Hubbard type repulsion [47, 69]. There is also no ideal Kerr-type $[n(n-1)]$ term to generate an exact quartic interaction in the large $\Delta$ limit. Nonetheless, as has been shown, qualitative similarity between the phase diagrams of JCH and Bose-Hubbard systems is found, and the analysis of these phase diagrams is a major topic of this chapter.

In chapter 2 we introduced the system of coupled JC cavities (the JCH model) that will be investigated in the present chapter for quantum phase transitions. The Mott-insulator phase has previously been studied in the JCH system with the mean-field approximation [33], which we shall review in section 3.1. We review how perturbation theory can be applied to the mean-field Hamiltonian in subsection 3.1.1, [55]. The remainder of the chapter is entirely original work, published as [66, 64]. In section 3.2 we present the exact diagonalisation techniques for up to six cavities, and results, for quantum phase diagrams. In the Bose-Hubbard model, the extent of the lobe is constant with respect to the chemical potential, and decreases with inter-site coupling. We find an analogous phase diagram for the JCH: the extent of the lobes decreases with both chemical potential and inter-cavity coupling. In section 3.3 comparisons are made between the two methods (exact diagonalisation and mean-field) for generating the phase diagrams. Disorder and the implications for effective model temperature are considered in section 3.4. By directly
connecting these small scale cases (solved by exact diagonalisation) with the thermodynamic limit (solved by mean-field), our results serve as a guide to coming proof-of-concept experiments. We are also able to compare our finite cases with the thermodynamic limit [33, 69, 92, 104, 41, 59, 89, 60, 18]. In chapter 4 we shall discuss a possible experimental protocol for observing the two phases.

3.1 Mean-field approximation

We now introduce the mean-field Hamiltonian for the JCH model. The mean-field approximation focuses attention on one particular JC cavity, from an infinite field of such cavities, and assumes that its $z$ nearest neighbors all behave like it. To invoke the mean-field, we use the decoupling approximation to decouple the photons:

$$a_i^\dagger a_j \approx \langle a_i^\dagger \rangle a_j + \langle a_j \rangle a_i^\dagger - \langle a_i^\dagger \rangle \langle a_j \rangle,$$  (3.3)

and introduce the superfluid order parameter $\psi = \langle a_i \rangle = \langle a_i^\dagger \rangle$ (which we assume is real). This decoupling approximation breaks the double sum term in the JCH Hamiltonian, equation (3.2), to be a single sum term. Under this approximation, the Hamiltonian is now a sum over an infinite number of identical JC cavities, the Hamiltonian on one such cavity is the mean-field Hamiltonian. In this way, only the coupling which occurs between JC cavities is approximated, and the full JC Hamiltonian is still included. The mean-field Hamiltonian is hence given by

$$\mathcal{H}^{MF} = \mathcal{H}^{JC} - z\kappa \psi (a^\dagger + a) + z\kappa \psi^2 - \mu \hat{L},$$  (3.4)

where $\hat{L} = a^\dagger a + \sigma^+ \sigma^-$. The basis for this Hamiltonian is the single cavity bare basis \{|g,0\}, |e,0\}, |g,1\}, \ldots \}$ (table 2.1), but the system (approximately) describes an infinite number of cavities. Note that the number of nearest neighbors $z$ effectively “rescales” the mean-field coupling, i.e., $\kappa \rightarrow z\kappa$ (as $z$ and $\kappa$ always appear together). We can write this Hamiltonian as a matrix as
where $I$ is the identity matrix. When $\kappa = 0$, the coupling between cavities switches off, and we recover a block diagonal matrix, with $\mu = 0$ this is identical to that of the single cavity JC Hamiltonian $H^{JC}$, equation (2.2).

The phase diagram using the mean-field approach is determined via the following method [33]. Firstly, choose values of $\Delta$, $\kappa$, $\mu - \omega$, and $\beta$. Then, minimise the smallest eigenvalue of the mean-field matrix truncated at a sufficiently large $n_{\text{max}}$ with respect to the superfluid order parameter $\psi$ (one should check that the value of $\psi$ has converged by increasing $n_{\text{max}}$ until $\psi$ no longer changes). We plot $\psi$ as a function of the energy scales of the system. This makes physical sense, as we are searching for some parameter which finds the system ground state (minimising the smallest eigenvalue) at each point in phase space.

We have also considered using a larger unit cell - for example, using two cavities, each with $z$ nearest neighbors. We found that while this is more difficult to calculate (finding eigenvalues of larger matrices) this exactly replicates the results of the original mean-field - which is not surprising. However, this technique could be used to include some form of disorder, or more complicated topologies, in the infinite cavity limit.

Figure 3.1 shows the mean-field phase diagram for $\Delta = 0$. In this phase diagram, two distinct phases are shown: Mott-insulator phases are shown by the black lobes corresponding
to $\psi = 0$. The quantum phase transition occurs when $\psi$ becomes positive. The superfluid phase exists in the region $\psi > 0$. The lowest Mott-insulator lobe corresponds to the state $|g,0\rangle$ on every cavity, the next lobe up corresponds to the state $|-,1\rangle$, the next lobe to $|-,2\rangle$, and so on (if spontaneous emission were included, the top lobes could not be seen due to the blurring of the spectral resolution). This makes good physical sense in the horizontal (inter-cavity coupling) and vertical (chemical potential) direction. In the horizontal direction, increasing the coupling between cavities increases the tendency for excitations to hop between cavities: at some point, a transition is seen from the Mott-insulator (solid) to the superfluid phase. In the vertical direction, by increasing the chemical potential, one effectively adds particles to the system: the Mott-insulator lobes also increase in number of particles per cavity, by one excitation each lobe. The small inverted lobe at the top left of the diagram is not physical: it results from an insufficiently large $n_{\text{max}}$.

### 3.1.1 Perturbation theory to explore phase boundaries

We have shown above how to use the mean-field approximation to find, numerically, the phase diagram for the JCH system. This section aims to utilise time independent perturbation theory, applied to the mean-field Hamiltonian, to find the boundaries of the Mott-insulator phase analytically. This subsection follows closely the work in references...
3. Phase diagram of the JCH in the ground state

[55, 103], except where stated.

In general, perturbation theory splits the Hamiltonian $H$ into two parts: $H_0$ has known eigenvalues and eigenvectors, and the perturbation $V$ does not:

$$H = H_0 + \lambda V,$$

where $\lambda$ is a small dimensionless parameter. In this calculation, the mean-field JCH Hamiltonian, equation (3.4), is split into two and made dimensionless by dividing through by $\kappa$ as

$$H_{0}^{\text{MF}} = -\bar{\mu}a^\dagger a - (\bar{\Delta} + \bar{\mu})\sigma^+\sigma^- + \bar{\beta}(a^\dagger\sigma^- + a\sigma^+) + \psi^2$$

$$V_{\text{MF}} = -(a^\dagger + a),$$

where the unitless parameters $\bar{\mu}$, $\bar{\Delta}$, and $\bar{\beta}$ are given by

$$\bar{\mu} = (\mu - \omega)/\kappa$$

$$\bar{\Delta} = (\omega - \epsilon)/\kappa$$

$$\bar{\beta} = \beta/\kappa$$

and $\psi$ acts as the perturbation parameter $\lambda$. The eigenstates of $H_{0}^{\text{MF}}$ are given by the dressed states, as discussed in section 2.1, of a single JC cavity, $\{|g,0\rangle, |\pm,1\rangle, |\pm,2\rangle, \ldots \}$. The (unitless) eigenvalues of $H_{0}^{\text{MF}}$ are given by

$$E_{|\pm,n\rangle}^{\text{MF}} = -n\bar{\mu} \pm \bar{\chi}(n) - \bar{\Delta}/2 + \psi^2$$

$$E_{|g,0\rangle}^{\text{MF}} = \psi^2$$

where $\chi(n)$ was first introduced as equation (2.7) and its dimensionless counterpart $\bar{\chi}(n)$ is
The general eigenvalues and eigenvectors of an arbitrary Hamiltonian $H = H_0 + \lambda V$ in a perturbative expansion are given by [85]

$$E_n = E^{(0)}_n + \lambda E^{(1)}_n + \lambda^2 E^{(2)}_n + \ldots$$

$$|\psi_n\rangle = |\phi^{(0)}_n\rangle + \lambda |\phi^{(1)}_n\rangle + \lambda^2 |\phi^{(2)}_n\rangle + \ldots$$

where the eigenvalues are given by

$$E^{(0)}_n = \langle \phi^{(0)}_n | H_0 | \phi^{(0)}_n \rangle$$

$$E^{(1)}_n = \langle \phi^{(0)}_n | V | \phi^{(0)}_n \rangle$$

$$E^{(2)}_n = \sum_{k=1}^{N} \frac{|\langle \phi^{(0)}_k | V | \phi^{(0)}_n \rangle|^2}{E^{(0)}_n - E^{(0)}_k}.$$  

(3.11)

(3.12a)

(3.12b)

(3.12c)

To find the phase boundaries, we need to find an expression for the energy of the negative branch eigenstates \{ |g, 0\rangle, |-, 1\rangle, |-, 2\rangle, \ldots \}, as informed by the mean-field phase diagrams, e.g. that shown in figure (3.1), and then minimise that expression as a function of $\psi$. As such, we write the system ground state energy as an expansion in $\psi$:

$$\tilde{E}_{[-, n]}(\psi) = a_0(\bar{\mu}, \bar{\Delta}, \bar{\beta}) + a_1(\bar{\mu}, \bar{\Delta}, \bar{\beta})\psi + a_2(\bar{\mu}, \bar{\Delta}, \bar{\beta})\psi^2 + O(\psi^3),$$

(3.13)

where $a_1 = 0$. This is because $\tilde{E}_{[-, n]}^{(1)}$ is zero by inspection, as the perturbation $\tilde{V}_{\text{MF}}$ adds or removes a particle. Let us focus on the sign of $a_2$. If $a_2 > 0$, $\tilde{E}_{[-, n]}(\psi)$ is an upright parabola, with a minimum which occurs at $\psi = 0$. If $a_2 < 0$, $\tilde{E}_{[-, n]}(\psi)$ is an inverted parabola, which has no minimum — the term of order $\psi^3$ or higher must act to generate some minimum, which may or may not occur at $\psi = 0$. As such, $a_2 = 0$ indicates the boundary between the insulator $\psi = 0$ and superfluid $\psi > 0$ phases. In our case,
3. Phase diagram of the JCH in the ground state

\[ a_2(\mu, \Delta, \beta) = E^{(2)}_{[-n]} + 1 = 0, \]  

(3.14)

must be solved for \( \mu \). The second order energy eigenvalue is given by

\[
E^{(2)}_{[-n]} = \begin{cases} 
\frac{1}{2} p^+(+) + p^+(-) + p^-(+) + p^-(--) & n \geq 1 \\
\frac{1}{2} + \frac{1}{2} \left[ \frac{1}{2} \chi^2(n) + \frac{1}{2} \chi(n) \Delta \right] & n = 0
\end{cases}
\]

(3.15)

where \( p^+(\pm) \) and \( p^-(\pm) \) are given by

\[
p^+(\pm) = \frac{n \left\{ \beta^2(n + 1) + \left[ -\frac{\Delta}{2} - \chi(n) \right] \left[ -\frac{\Delta}{2} \pm \chi(n + 1) \right] \right\}^2}{2\chi^2(n + 1) + \chi(n) \Delta \left[ 2\chi^2(n + 1) \mp \chi(n + 1) \Delta \right]} \]

(3.16)

Equation (3.15) and (3.16) with \( \Delta = 0 \) recovers equations (18) and (19) from [55]. The solutions for the boundaries for \( n \geq 1, \) and \( \Delta \neq 0 \) are too complicated to be shown analytically. However, in the case \( n = 0, \) the expression in full dimensional form is

\[
\frac{\mu_0 - \omega}{\beta} = -\frac{1}{2} \left[ \Delta + z\kappa \beta + \sqrt{\left( \frac{\Delta - z\kappa}{\beta} \right)^2 + 4} \right].
\]

(3.17)

This expression is also recovered without using either the mean-field or the perturbation approximations, which lends further credence to this technique. This is discussed in the next section and displayed in equation (3.32).

Also, we find the solutions (which were not displayed analytically in [55]) of equation (3.14) for \( n > 0 \) and \( \Delta = 0, \) where \( \bar{\kappa} = z\kappa/\beta \) are given by
\[
\mu_n^\pm - \omega \beta = -\frac{\bar{\kappa}}{4} \pm \frac{1}{2} \sqrt{a(\bar{\kappa}, n) + b(\bar{\kappa}, n)} \\
\pm \frac{1}{2} \sqrt{2a(\bar{\kappa}, n) - b(\bar{\kappa}, n)} \mp \frac{\bar{\kappa}^3 - 16n\bar{\kappa} - 32\sqrt{n}}{4\sqrt{a(\bar{\kappa}, n) + b(\bar{\kappa}, n)}}
\]

(3.18)

where

\[
a(\bar{\kappa}, n) = \frac{\bar{\kappa}^2}{4} + \frac{8n}{3} \quad \text{(3.19a)}
\]

\[
b(\bar{\kappa}, n) = \frac{c(\bar{\kappa}, n)}{3\sqrt{2}} + \frac{4\sqrt{2}d(\bar{\kappa}, n)}{c(\bar{\kappa}, n)} \quad \text{(3.19b)}
\]

\[
c(\bar{\kappa}, n) = \frac{3}{16}c(\bar{\kappa}, n) + \sqrt{c(\bar{\kappa}, n)^2 - 6912d(\bar{\kappa}, n)^3} \quad \text{(3.19c)}
\]

\[
d(\bar{\kappa}, n) = \bar{\kappa}^2n - 2\bar{\kappa}\sqrt{n} + \frac{4n^2}{3} - 1 \quad \text{(3.19d)}
\]

\[
e(\bar{\kappa}, n) = -81\kappa^3\sqrt{n} + (288n^2 - 27)\kappa^2 - 144\kappa n^{3/2} - 128n^3 + 144n. \quad \text{(3.19e)}
\]

We introduce the function \( f(\bar{\kappa}, n) \), where

\[
f(\bar{\kappa}, n) = e(\bar{\kappa}, n)^2 - 6912d(\bar{\kappa}, n)^3
\]

\[
= (6561n - 6912n^3)\kappa^6 + 162\sqrt{n} (27 - 32n^2)\kappa^5
+ 27 (2048n^4 - 2016n^2 + 27)\kappa^4 + 1728n^{3/2} (28n^2 - 25)\kappa^3
- 864n (128n^4 - 64n^2 - 63)\kappa^2 + 13824\sqrt{n} (8n^4 - 11n^2 + 3)\kappa
- 6912 (n^2 - 1),
\]

the square root of which appears in equation (3.19c). The sign of this function determines whether \((\mu_n^+ - \omega)/\beta\) will be real or imaginary. The smallest value of \(\bar{\kappa}\) for which \(\mu_n^+ = \mu_n^-\), for \(n \geq 1\), is called the \textit{nose} of the lobe. We find empirically that \(f(\bar{\kappa}, n) = 0\) is equivalent to \(\mu_n^+ = \mu_n^-\), and as such this more simple expression can be used to determine the position of the nose of each lobe. As \(f(\bar{\kappa}, n)\) is a 6th order polynomial in \(\bar{\kappa}\), \(f(\bar{\kappa}, n) = 0\) does not
3. Phase diagram of the JCH in the ground state

<table>
<thead>
<tr>
<th>n</th>
<th>( \bar{\kappa} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 0.1595 = 10^{-0.7971} )</td>
</tr>
<tr>
<td>2</td>
<td>( 0.0124 = 10^{-1.904} )</td>
</tr>
<tr>
<td>3</td>
<td>( 0.0042 = 10^{-2.375} )</td>
</tr>
</tbody>
</table>

Table 3.1: The position of the noses (where the smallest value of \( \bar{\kappa} \) for which \( \mu_n^+ = \mu_n^- \), for \( n \geq 1 \), is called the nose of the lobe), for the first three lobes when \( \Delta = 0 \). These are also shown as red points in figure 3.2.

have general solutions for \( \bar{\kappa} \). However, numerically they can be determined: the first three noses are shown numerically in table 3.1, and graphically in figure 3.2. We have focused specifically on the region for which \((\mu_n^+ - \omega)/\beta\) is real for \( \kappa \) less than the first nose point. There are other regions for larger \( \kappa \) where there are real results, however we deem these non-physical for two reasons. Firstly, as they are far from the region when the superfluid order parameter \( \psi \) is zero, about which we are basing our perturbative analysis. Secondly, they are in the superfluid region, where chemical potential (the vertical axis of the plot) has no meaning (it takes no energy to add a photon to a superfluid), and as such are meaningless.

In figure 3.2 we plot the boundary \( \mu_0 \) as shown in equation (3.17), and the boundaries \( \mu_1^+, \mu_2^+ \) and \( \mu_3^+ \), for detuning \( \Delta/\beta = 0 \) (a) [as shown in equation (3.18)], \( \Delta/\beta = -2 \) (b), and \( \Delta/\beta = 2 \) (c). Figure 3.2(a) is equivalent to figure 2(b) of [55], but parts (b) and (c) are original work. For all three cases, there is a very good match between the numerically determined mean-field phase diagram and the perturbation theory mean-field boundaries.

The phase diagrams generated in this section are based on the mean-field approximation, which assumes an infinite number of cavities. In the next section we investigate phase diagrams based on a finite number of cavities, and in section 3.3 compare the two approaches.

3.2 Exact diagonalisation

Another way to calculate the phase diagram is by using exact diagonalisation of the Hamiltonian: this is used for a finite number of cavities. The key advantage of this
Phase diagram of the JCH in the ground state

\[ \log_{10} \left( \frac{z \kappa}{\beta} \right) \left( \mu - \omega \right) / \beta \]

\[ \langle \psi | g,0 \rangle - 3, -2, -1, 0, 1 \]

\[ \langle \psi | -,1 \rangle - 3, -2.5, -2, -1.5, -1, -0.5, 0 \]

\[ \langle \psi | 0 \rangle 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4 \]

Figure 3.2: Phase diagrams for (a) \( \Delta / \beta = 0 \), (b) \( \Delta / \beta = -2 \), (c) \( \Delta / \beta = 2 \). The white lines show the perturbation theory boundaries \( \mu_0 \), as shown in equation (3.17), and \( \mu_1^\pm, \mu_2^\pm \) and \( \mu_3^\pm \), as shown in equation (3.18) (\( \Delta / \beta = 0 \) only). These show the boundaries between the Mott-insulator phase and the superfluid phase. They are overlaid on the mean-field phase diagram, as first shown in figure (3.1) for \( \Delta / \beta = 0 \). The red points show the nose points for the first three lobes, as given in table 3.1. The match between the two approaches is excellent.

The approach over the mean-field approach is that the mean-field approximation, where each cavity is assumed identical to an infinite field of such cavities, is no longer taken. A new order parameter for showing the phases must be chosen, as that used for mean-field, \( \psi \) no longer exists, as it was only introduced in the mean-field approximation, equation (3.3). Instead we choose \( \langle L \rangle = \left( \sum_{i=1}^{N} a_i^\dagger a_i + \sigma_i^+ \sigma_i^- \right) \), the expectation value of the total number of excitations in the system. In general, \( \langle L \rangle \) is a real number. However, we now show that rather than varying continuously as \( \psi \) does in the mean-field case, this order parameter of minimum energy eigenstates takes only integer values: these form plateaux in the phase diagram. The plateaux are a fundamental consequence of the finite
The $N$ cavity bare basis of the JCH system consists of state vectors of the form $|s_1, n_1\rangle \otimes |s_2, n_2\rangle \otimes \cdots \otimes |s_N, n_N\rangle$, $s_i \in \{g, e\}$, $n_i \in \{0, 1, \ldots\}$. In principle, this basis is infinite in extent, because the number of photonic excitations per cavity is unbounded. By ordering the bare basis by the total number of excitations (either photonic or atomic) across all cavities, one may express the Hamiltonian of equation (2.9) in block diagonal form

$$
\mathcal{H} = \text{diag}[\mathcal{H}^{(0)}, \mathcal{H}^{(1)}, \mathcal{H}^{(2)}, \ldots],
$$

where $\mathcal{H}^{(l)}$ is the matrix corresponding to $l$ excitations. The size of each block is determined by the number of ways in which the excitations can be shared between the atomic and photonic degrees of freedom. We denote the number of states for $l$ excitations [equal to the size of the matrix $\mathcal{H}^{(l)}$] as $s$, where

$$
s = \sum_{i=0}^{\min(l, N)} \binom{N}{i} S_{l-i}^N.
$$

The above summation has two components. The first, $\binom{N}{i}$, is the total number of atomic excitations across the lattice (note that on each site the number of atomic excitations can only be zero or one). The second, $S_{l-i}^N$, represents the number of photonic excitations, and is the number of ways to share $l - i$ photons between $N$ cavities, e.g. in the case of sharing two photons among three cavities,

$$
S_2^3 = \text{length}[(2, 0, 0), (1, 1, 0), (0, 2, 0), (1, 0, 1), (0, 0, 2), (0, 1, 1)] = 6.
$$

To gain insight into the problem, we explicitly show $\mathcal{H}^{(0)}$ and $\mathcal{H}^{(1)}$ for a two-cavity ($N = 2$) system in the bare basis as follows:
\[ H^{(0)} = \begin{pmatrix} 0 \\ g,0 \otimes g,0 \end{pmatrix} \]  \hspace{1cm} (3.24a)

\[ H^{(1)} = \begin{pmatrix} \omega & \beta & -\kappa & 0 \\ \beta & \epsilon & 0 & 0 \\ -\kappa & 0 & \omega & \beta \\ 0 & 0 & \beta & \epsilon \end{pmatrix}, \begin{pmatrix} g,1 \otimes g,0 \\ e,0 \otimes g,0 \\ g,0 \otimes g,1 \\ g,0 \otimes e,0 \end{pmatrix} \]  \hspace{1cm} (3.24b)

where the (two-cavity) basis for \( H^{(0)} \) and \( H^{(1)} \) are shown as column vectors to the right of their respective Hamiltonians.

Note that \( \hat{L} \) is diagonal when represented in either the dressed or bare basis (but has different values in each). From [112], examining our Hamiltonian equation (2.9), we determine that \( \langle \hat{L} \rangle = -\partial E_g / \partial \mu \), where \( E_g \) is the ground state energy. Some preliminary analytics can simplify the calculation of \( \langle \hat{L} \rangle \) considerably; we show this now.

We begin by noting that the part of \( \hat{L} \) corresponding to exactly \( l \) excitations [by analogy to \( H^{(l)} \)], represented as \( \hat{L}^{(l)} \), has the form

\[ \hat{L}^{(l)} = lI. \]  \hspace{1cm} (3.25)

where \( I \) is the identity matrix. Again employing the Hellmann-Feynman theorem [42, 24], equation (2.14), restated as

\[ \frac{\partial E_\lambda}{\partial \lambda} = \langle \psi(\lambda) | \frac{\partial H_\lambda}{\partial \lambda} | \psi(\lambda) \rangle, \]  \hspace{1cm} (3.26)

we show that

\[ \frac{\partial E_g^{(l)}}{\partial \mu} = \langle \psi_g | \frac{\partial}{\partial \mu} (H^{(l)} - \mu \hat{L}) | \psi_g \rangle = -l = -\langle L \rangle, \]  \hspace{1cm} (3.27)

where \( E_g^{(l)} \) is the ground state energy, and \( | \psi_g \rangle \) is the corresponding eigenstate of \( H^{(l)} - \mu \hat{L}^{(l)} \). Since \( l \) is always a positive integer, we have shown that the phase diagram will always consist of plateaux, with boundaries set by the discrete intersection points.
So, if $M$ is a list of real numbers given by

$$M = \{ \min[\text{eigenvalues}(\mathcal{H}^{(0)} - \mu \hat{L}^{(0)})], \min[\text{eigenvalues}(\mathcal{H}^{(1)} - \mu \hat{L}^{(1)})], \ldots \},$$

(3.28)

and

$$f : \{0, 1, \ldots \} \rightarrow M,$$

(3.29)

then

$$\langle \hat{L} \rangle = f^{-1}[\min(M)].$$

(3.30)

In short, to find $\langle \hat{L} \rangle$, one needs to locate which block of the Hamiltonian the minimum eigenvalue of $(\mathcal{H} - \mu \hat{L})$ corresponds to. Obviously, $\langle \hat{L} \rangle$ can only have non-negative integer values, corresponding physically to the number of excitations in the system. This is
illustrated further in figure 3.3. In this figure, the smallest eigenvalue of $\mathcal{H}^{(0)}, \mathcal{H}^{(1)}, \ldots$ is plotted as a function of $(\mu - \omega)/\beta$ for $\kappa/\beta = 0$. For each value of $(\mu - \omega)/\beta$, $\langle \hat{L} \rangle$ is given by the negative slope of the smallest eigenvalue at that point.

In this section we show the quantum phase diagrams of the Hamiltonian of equation (2.9) for various topologies. Geometry is implemented through the adjacency matrix $A$.

We display the phase diagrams corresponding to two, three, four, and five cavities arranged in one dimension with periodic boundary conditions in figure 3.4. Each color corresponds to a different plateau, a constant state in excitation space - these are Mott-insulator phases. It is worth pointing out that (unlike the mean-field approximation), in our discrete model, no superfluid phase exists. However, as $\kappa$ increases, the width of each plateau in the chemical potential direction decreases. As the plateaux get infinitely thin in this direction, they show the signature of the transition to a superfluid phase.

In total, eleven topologies were examined. These are listed in the first column of table 3.3. The topologies of a square, triangle and six cavities with $z = 3$ could be considered special, as they can represent infinite square, triangular and hexagonal lattices respectively, as shown in table 3.2. However, no significant differences (with respect to matching of phase diagrams to mean-field) are found between these topologies and the rest.

For all topologies, a “pinch” effect is noted as $\kappa \to 0$ between $\langle \hat{L} \rangle = N$ and $\langle \hat{L} \rangle = 2N$, between $\langle \hat{L} \rangle = 2N$ and $\langle \hat{L} \rangle = 3N$, etc. That is, all fractional occupations (plateaux corresponding to heights that are not integer multiples of the number of cavities $N$) disappear as $\kappa \to 0$, this compares well with the mean-field solution. The point at which this pinching occurs is called the critical chemical potential $\mu_c$, as shown for the mean-field case in [33],

$$
\mu_c(n) = \omega + \chi(n) - \chi(n + 1),
$$

(3.31)

where $\chi(n)$ is defined in equation (2.7), and $\chi(0) = -\Delta/2$. The critical chemical potential is independent of the number or arrangement of cavities, and independent of whether or not the mean-field approximation is used, as expected from the $\kappa \to 0$ limit.
3. Phase diagram of the JCH in the ground state

Figure 3.4: Expectation value of the total number of excitations $\langle \hat{L} \rangle$ as a function of $(\mu - \omega)/\beta$ and $\kappa/\beta$, for two, three, four and five cavities in periodic boundary conditions, with $\Delta = 0$. Note that the top boundary in each plot is the limit of calculations. For $N = 2, 3, 4,$ and $5$, the Hamiltonian matrix used to create each plot is truncated at $l = 12, 9, 8$ and $5$, respectively.
Table 3.2: Certain infinite lattices may be simulated with a small number of cavities. An infinite square lattice can be modelled by four sites, each with four connections. An infinite triangular lattice can be modelled by three sites, each with six connections. An infinite hexagonal lattice can be modelled by six sites, each with three connections.
3. Phase diagram of the JCH in the ground state

<table>
<thead>
<tr>
<th>Geometry</th>
<th>$N$</th>
<th>$z$</th>
<th>$(\langle L \rangle)$</th>
<th>Associated ground eigenstate (dressed basis)</th>
</tr>
</thead>
<tbody>
<tr>
<td>arbitrary</td>
<td>$n$</td>
<td>-</td>
<td>0</td>
<td>$\frac{1}{n} P_n(g, 0) \otimes (-1)^n \otimes (-1)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>$n$</td>
<td>-</td>
<td>1</td>
<td>$\frac{1}{n} P_n(g, 0) \otimes (-1)^n \otimes (n-1)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>$n$</td>
<td>-</td>
<td>$n-1$</td>
<td>$\frac{1}{n} P_n(g, 0) \otimes (-1)^n \otimes (n-1)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>$n$</td>
<td>-</td>
<td>$n$</td>
<td>$\frac{1}{n} P_n(g, 0) \otimes (-1)^n \otimes (n-1)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>$\frac{1}{2} P_2(g, 0) \otimes (-1)^2 \otimes (-1)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>4</td>
<td>2</td>
<td>2</td>
<td>$\frac{1}{4} P_4(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{4} P_2(g, 0) \otimes (-1)^2 \otimes (0)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>6</td>
<td>2</td>
<td>2</td>
<td>$\frac{1}{6} P_6(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_4(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_2(g, 0) \otimes (-1)^2 \otimes (0)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>6</td>
<td>3</td>
<td>2</td>
<td>$\frac{1}{6} P_6(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_4(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_2(g, 0) \otimes (-1)^2 \otimes (0)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>6</td>
<td>4</td>
<td>2</td>
<td>$\frac{1}{6} P_6(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_4(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_2(g, 0) \otimes (-1)^2 \otimes (0)$</td>
</tr>
<tr>
<td>arbitrary</td>
<td>6</td>
<td>5</td>
<td>2</td>
<td>$\frac{1}{6} P_6(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_4(g, 0) \otimes (-1)^2 \otimes (0) + \frac{1}{6} P_2(g, 0) \otimes (-1)^2 \otimes (0)$</td>
</tr>
</tbody>
</table>

Table 3.3: Summary of information about the number of cavities $N$, and nearest neighbors $z$, excitation state $\langle L \rangle$ and associated ground eigenstate for eleven topologies up to $N = 6$ for the band $m = 0$. Eigenstates for higher bands $m$ are determined by replacing $|g, 0\rangle$ by $|-m\rangle$ and $|-1\rangle$ by $-m + 1\rangle$ in every instance. The first four rows are valid for any geometry.
Although in general, one cannot analytically determine the positions of all the boundaries, we find that for all topologies, assuming a uniform number of nearest neighbours, the first boundary (between $\langle \hat{L} \rangle = 0$ and $\langle \hat{L} \rangle = 1$) is described by the analytic equation

$$\frac{\mu - \omega}{\beta} = -\frac{1}{2} \left[ \frac{\Delta + z\kappa}{\beta} + \sqrt{\left( \frac{\Delta - z\kappa}{\beta} \right)^2 + 4} \right],$$

(3.32)

where $z$ is the number of nearest neighbors (the third column in table 3.3). This recovers the boundary generated in the perturbation theory section, equation (3.17). Equation (3.32) was determined by equating the smallest eigenvalue of $\mathcal{H}^{(1)}$ with zero (the only eigenvalue of $\mathcal{H}^{(0)}$). This has been compared numerically for $z = 1, 2, 3, 4,$ and $6$, and is in excellent agreement. One cannot expect analytic boundaries for generic $z$ between $\langle \hat{L} \rangle = 1$ and $\langle \hat{L} \rangle = 2$ or higher to exist, indeed none were determined. This is because they are truly in the realm of many-body physics (unlike the lower boundary). A higher boundary would be the solution of a commensurately higher order polynomial. In the simplest case, $N = 2$ and $l = 2$; from equation (3.22), $s = 8$, so an eighth order polynomial must be solved to determine the boundaries.

For each plateau, the ground eigenstate can be calculated (hence below we use “ground eigenstates” to refer to the different ground states for the different plateaux). These ground eigenstates are represented in the many cavity dressed state basis.

To easily represent this information, it is useful to define two operators: the translation operator $\hat{T}$ (which shifts all states to the right and moves the last state back to the beginning) and the permutation operator $\hat{P}_m$ (which is the sum over $\hat{T}_i$ applied to the state $m$ times)

$$\hat{T}|s_1, n_1\rangle \otimes \ldots \otimes |s_{N-1}, n_{N-1}\rangle \otimes |s_N, n_N\rangle = |s_N, n_N\rangle \otimes |s_1, n_1\rangle \otimes \ldots \otimes |s_{N-1}, n_{N-1}\rangle,$$

(3.33)
3. Phase diagram of the JCH in the ground state

Figure 3.5: The expectation value of the total number of excitations $\langle \hat{L} \rangle$ of two cavities with periodic boundary conditions in the ground state. The eigenstates of the four lowest plateaux are marked, (see table 3.3). The upper boundary marks the limit of calculations.

\[
\hat{P}_m |s_1, n_1 \rangle \otimes \ldots \otimes |s_N, n_N \rangle = \sum_{i=0}^{m-1} T^i |s_1, n_1 \rangle \otimes \ldots \otimes |s_N, n_N \rangle. \tag{3.34}
\]

The ground eigenstates for all eleven topologies, up to $\langle \hat{L} \rangle = N - 1$, i.e., total number of excitations equal to one less than the number of cavities, are displayed in table 3.3. Figure 3.5 shows a diagrammatic example of how the information from table 3.3 matches the plateaux in the two cavity phase diagram.

We now investigate eigenstates for higher numbers of excitations. Consider bands of $N$ plateaux, labeled by $m$, where

\[
mN \leq \langle \hat{L} \rangle \leq (m + 1)N - 1 \quad \forall m = 0, 1, \ldots \tag{3.35}
\]

One finds that the physics of each band has a repetitive structure, hence the introduction of this parameter. In table 3.3 only results for the band of plateaux corresponding to $m = 0$ are displayed, i.e. $\langle L \rangle = 0, 1, \ldots, N - 1$. While higher bands include many more possible states (e.g. $|-, 1 \rangle \otimes |+, 1 \rangle \otimes |-, 2 \rangle$), we find higher bands have a structure that is
easily related to $m = 0$. To obtain the general states for some other band $m$, one needs to replace $| -, 1 \rangle$ by $| -, m + 1 \rangle$, and $| g, 0 \rangle$ by $| -, m \rangle$, in every instance.

The differences between topologies are apparent when comparing, for example, the band $m = 0$, for $2 \leq \langle \hat{L} \rangle \leq N - 1$, two excitations in a square geometry compared with two excitations in a tetrahedron geometry. In the square case, there is a different coefficient for excitations adjacent as to excitations separated, compared with the tetrahedron case, where all terms have the same coefficient.

Three different topologies (pentagon, six cavities with $z = 3$, and six cavities with $z = 4$) have some coefficients displayed to three decimal places, these have been calculated to twelve decimal places. An exact form is not derived, as these numbers represent solutions of polynomials of order $\geq 50$, no exact form is necessarily expected.

We also examine the expectation value of the number of excitations of each cavity, $\langle \hat{L}_i \rangle$ and $\langle \hat{L}_i^2 \rangle$, and find that, independent of geometry,

$$\langle \hat{L}_i \rangle = \frac{\langle \hat{L} \rangle}{N}$$

$$\langle \hat{L}_i^2 \rangle = (m + 1)^2 \left( \frac{\langle \hat{L} \rangle - mN}{N} \right) + m^2 \left( 1 - \frac{\langle \hat{L} \rangle - mN}{N} \right), \quad (3.36)$$

so that the variance of $\hat{L}_i$ is

$$\text{var}(\hat{L}_i) = \sqrt{\langle \hat{L}_i^2 \rangle - \langle \hat{L}_i \rangle^2} = \sqrt{\frac{\langle \hat{L} \rangle - mN}{N} - \left( \frac{\langle \hat{L} \rangle - mN}{N} \right)^2}, \quad (3.37)$$

where the band $m$ is defined by equation (3.35), and both equations (3.36) and (3.37) are valid for $i = 1, \ldots, N$. From this, one can determine that if $\langle \hat{L} \rangle$ is an integer multiple of $N$, $\text{var}(\hat{L}_i) = 0$, as expected. Also, if we consider the thermodynamic limit, where both the
3. Phase diagram of the JCH in the ground state

Figure 3.6: These plots show $\langle \hat{L} \rangle$ as a function of $(\mu - \omega)/\beta$ and $\Delta/\beta$ for two cavities in periodic boundary conditions with (a) $\kappa = 0$ and (b) $\kappa = 10^{-1/2}\beta$. The upper boundary in both cases marks the limit of calculations. Note that only even plateaux are present in (a); this is because of the pinching effect as $\kappa \to 0$ - in this limit, plateaux corresponding to fractional occupation do not exist. The white dashed line marks $\Delta/\beta = 0$, and aids the eye in seeing that the boundaries above the first (second) are symmetric (asymmetric) in plot (a) [(b)].

While this paper primarily focuses on phase changes as a function of $\kappa$, one can also examine phase changes as a function of detuning $\Delta$ [7]. Indeed experimentally, shifts in $\Delta$ may prove to be more accessible (e.g. via the Stark shift on the embedded atoms), as $\kappa$ cannot be changed post-fabrication in many systems. In figure 3.6(a) we plot $\langle \hat{L} \rangle$ as a function of $\Delta/\beta$ and $(\mu - \omega)/\beta$ for $\kappa = 0$, and in figure 3.6(b) we do the same for $\kappa = 10^{-1/2}\beta$. There are fewer plateaux in (a) than there are in (b) because there are fewer plateaux (due to the pinching effect, discussed above) at $\kappa/\beta = 0$. Note the symmetry around $\Delta = 0$, in the second and subsequent boundaries of figure 3.6(a) (c.f. figure 3 of [33]), and the corresponding asymmetry in the third and subsequent boundaries of figure 3.6(b). This symmetry is perfect at $\kappa = 0$, and the asymmetry increases with increasing $\kappa$.
3.3 Comparing mean-field with exact diagonalisation

In this chapter, we have examined the phase diagram of the JCH model primarily using two different techniques: the mean-field approximation and exact diagonalisation. Here, we examine the similarities and differences between the results using these two techniques.

A mean-field phase diagram that is comparable with the phase diagrams of the previous section can be made \[33\]. An accurate comparison between the exact results of the previous section, with mean-field, is made when we consider topologies with \( z \) nearest neighbors with mean-field results for \( z \) nearest neighbors. In all eleven distinct topologies tested, a very accurate match is seen. One such result is displayed in figure 3.7. We find that the boundaries from equation (3.31) are preserved in the mean-field solutions.

In mean-field, the region with \( \psi = 0 \) corresponds to the various Mott-insulator lobes (e.g., \( |g, 0\rangle, |-, 1\rangle, |-, 2\rangle \) etc.), while \( \psi > 0 \) is the superfluid state. The bottom lobe is described as the zeroth lobe \( (|g, 0\rangle) \), the next lobe up as the first lobe \( (|-, 1\rangle) \), and so on. In figure 3.8(a), we examine the underside of the first lobe in mean-field with \( z = 2 \), and overlay the boundary between \( \langle \hat{L} \rangle = N - 1 \) and \( \langle \hat{L} \rangle = N \) for \( N = 2, 3, 4, 5, \) and 6.
Figure 3.8: The hatched region represents the $\psi = 0$ area of the mean-field approximation for two nearest neighbors. The lines (or markers, for distinction purposes only) represent the exact calculations. (a) shows the boundary between the zeroth and first lobe, and (b) shows the boundary between the first and second lobe. Note that as the number of cavities increases, the lines tend to hug the upper mean-field lobe. This indicates qualitatively that as $N \to \infty$, the exact calculations should approach the mean-field ($N = \infty$) limit.

cavities in periodic boundary conditions. In figure 3.8(b), we examine the underside of the second lobe in mean-field with $z = 2$, and plot the boundary between $\langle \hat{L} \rangle = 2N - 1$ and $\langle \hat{L} \rangle = 2N$ for $N = 2, 3, 4, 5$ cavities, also in periodic boundary conditions. One can clearly see that as the number of cavities increases, the boundaries approach the boundary of mean-field, and eventually may pinch off for each lobe entirely (so that plateaux of height $\langle \hat{L} \rangle / N = 1, 2, \ldots$ do not continue as $\kappa \to \infty$, but rather have finite size in this direction). These boundaries accord well with the structures observed by Rossini and Fazio (figure 3 of reference [83]), which were obtained independently by the density matrix renormalisation group procedure, which lends weight to both quantum treatments. Furthermore, as $N \to \infty$, our exact results slowly approach that of the mean-field, which have a more rounded cutoff for the Mott lobes than these finite cavity results.

Note that while equation (3.30) informs that the total number of excitations is integer, the mean-field Hamiltonian of equation (3.4) informs of the number of excitations per cavity. Accordingly, we will find equivalence when the number of excitations is a multiple of the number of cavities.
3.4 Disorder and effective model temperature

In this section, we modify the results found using the exact diagonalisation techniques, as in section 3.2, to investigate how the phase diagram changes with non-zero temperature. This is done in two ways. We first consider the modification of the chemical potential with small temperature increase (less than the scale for photon generation, $kT \ll \hbar \omega$) and hence this modifies the phase diagrams shown in section 3.2. We then examine fabrication disorder in the form of a normal distribution of photon energies for each cavity. We show that this fabrication disorder is qualitatively similar to effective temperature, providing a connection between disorder and an effective temperature in this analogue system.

3.4.1 Modification of chemical potential

Note that we set Boltzmann’s constant $k_B = 1$. We begin by differentiating the free energy $F = E - TS$ with respect to the total number of excitations $l$,

$$\frac{\partial F}{\partial l} = \frac{\partial E}{\partial l} - T \frac{\partial S}{\partial l} - S \frac{\partial T}{\partial l},$$  \hspace{1cm} (3.38)

recalling the definition of chemical potential in equation (2.13), and assuming that temperature does not depend on the number of excitations (i.e., $\partial T/\partial l = 0$, assuming that the temperature scale is too low to generate a photon, i.e., $kT \ll \hbar \omega$, for example $\omega \sim 10^{15}$ Hz, $\hbar \sim 10^{-34}$ J s implies $\hbar \omega \sim 10^{-16}$ J, hence $T \lesssim 10^5$ K, or in radio frequency $\omega \sim 10^9$ Hz, hence $T \lesssim 10^{-1}$ K), we get

$$\mu = \frac{\partial E}{\partial l} + T \frac{\partial S}{\partial l},$$  \hspace{1cm} (3.39)

this then gives an effective chemical potential

$$\mu' = \mu + T \frac{\partial S}{\partial l}.$$  \hspace{1cm} (3.40)

We calculate the entropy $S$ in the $\kappa \to 0$ limit in the following manner. Assume that the photon blockade is complete, i.e., $|-, 2, g, 0 \rangle \not\rightarrow |-, 1, -, 1 \rangle$, then we can consider each band
Phase diagram of the JCH in the ground state

[recall equation (3.35)] separately. More specifically, each band acts like a paramagnet [5]. Recall that a one-dimensional paramagnet is a line of spin states, where each spin can point up or down. Compare with our system, where each cavity can have either \(|g, 0\rangle\), or \(|-1, 1\rangle\) (for band \(m = 0\)). Strictly speaking, each state (as in table 3.3) is a pure state, and as such the entropy is zero. However, if we assume that the number of cavities \(N\) is very large, then the superposition states act like a mixed state, and we can define entropy as for a paramagnet (essentially the logarithm of the number of microstates) by

\[
S(l) = \ln \left( \frac{N}{l - mN} \right),
\]

(3.41)

for a completely mixed state. Note that this solution is only valid within each band, as such we can ignore the infinities that arise in \(\partial S/\partial l\) when \(l\) is an integer multiple of \(N\), as at these points the paramagnetic approximation does not apply. Recall that the phase diagram of \(\langle \hat{L} \rangle\) is concerned with finding the slope of the smallest energy eigenvalue with respect to \(\mu\), and that this slope is always an integer. The Hamiltonian of equation (2.9) is block diagonal; we know from earlier analysis that the ground state energy of each block \(\mathcal{H}^{(l)}\) has constant slope with respect to \(\mu\) of \(-l\). Consider figure 3.3, when temperature is included, each line will move, with respect to \((\mu - \omega) / \beta\) by some amount to the left or to the right. For each \(\mu\), we choose the smallest energy eigenvalue at that point, and take the negative slope at that point. For small finite temperatures, this is manifest as a “splitting” of the pinches, as seen in [25]. We plot this splitting between the zeroth and first lobes, and the first and second lobe, for \(N = 10, 100,\) and \(1000\) in figure 3.9(a).

3.4.2 Disorder

Fabrication of a system of photonic cavities will undoubtedly be subject to certain errors. Here we model uncertainty in the cavity frequency \(\omega\). We assume that each atom may be tuned individually to be resonant with its cavity, so that \(\Delta_i = 0 \forall i = 1, \ldots, N\) (e.g. via the Stark shift on the embedded atoms), and as such we model the Hamiltonian by
Figure 3.9: (a) shows how the boundaries between plateaux change (when $\kappa = 0$) for 10, 100, and 1000 cavities with increasing temperature in natural units. (b) shows how the boundaries between plateaux change (when $\kappa = 0$) for two, three, and four cavities with increasing disorder, measured in units of standard deviation $\varsigma$. Note that when $\varsigma = 0.4$, the difference between the top line of the bottom pinch, and the bottom line of the top pinch, is $(\mu - \omega)/\beta = 0.434$, 0.361, and 0.320 for two, three and four cavities, respectively. This gives some indication of a threshold of fabrication tolerance that will still allow observation of the Mott lobes.

$$\mathcal{H} = \sum_{j=1}^{N} \left[ (\omega_i + \delta_i)(\sigma^+_i \sigma^-_i + a_i^\dagger a_i) ight. \right.$$

$$+ \left. \beta_i(\sigma^+_i a_i + \sigma^-_i a_i^\dagger) \right] - \kappa \sum_{(i,j)} a_i^\dagger a_j,$$

where the set $\{\delta_1, \delta_2, \ldots, \delta_N\}$ is chosen from a normal distribution with zero mean and standard deviation $\varsigma$. For fixed number of cavities and fixed $\varsigma$, we calculate 1000 sets each of boundaries above $l = 0$ to below $l = 2N$, and take the mean of the results. Results are shown in figure 3.9(b).
3. Phase diagram of the JCH in the ground state

Figure 3.10: How $T^\ast$, the temperature at which the top boundary of the first group in figure 3.9(a) meets the boundary of the second group, changes as a function of the number of cavities.

3.4.3 Comparing disorder and chemical potential modification

One can see by comparing figures 3.9(a) and 3.9(b) that disorder and temperature produce qualitatively the same results. However, we have only calculated the disorder effects up to four cavities due to the limitations of computing resources, and the temperature analysis is only valid for large numbers of cavities. Hence the two techniques cannot be compared directly. If the exact diagonalisation technique could be extended to a larger number of cavities, it could be compared quantitatively with disorder, and one would expect rigorous matching of the standard deviation with the effective temperature $T$.

If one envisions figure 3.9(a) as temperature increases even further, there will be some temperature $T^\ast$ such that the top line from the bottom group (corresponding to $l = N-2$) will meet the bottom line of the top group (corresponding to $l = N+1$). We examine $T^\ast$ as a function of the number of cavities, and find that this is given by

$$T^\ast = (2 - \sqrt{2}) \left[ \frac{\Gamma(N-2) + \Gamma(N+2)}{-\Gamma(N-1) - \Gamma(N+1)} \right]^{-1},$$

where $\Gamma(l') = l' \frac{\partial S}{\partial l} \bigg|_{l=l'}$, this function is plotted in figure 3.10. $T^\ast$ appears to converge to a constant, non-zero temperature as $N \to \infty$, however further study is needed to determine
if this asymptote is correct. If $T^*$ converges to a non-zero temperature, then provided a very large system of JC cavities has temperature below $T^*$, the system can transition to the Mott-insulator phase.

### 3.5 Conclusions

In this chapter we have presented an extensive analysis of phase diagrams of the Jaynes-Cummings-Hubbard model using the exact diagonalisation technique - we studied the phase diagrams via the expectation value of the total number of excitations. We examined various topologies of small networks of cavities, and compared this work with the infinite cavity mean-field approximation, we found good agreement in all topologies. We also examined the mean-field phase diagrams using time independent perturbation theory. We studied the effective model temperature, and compared this qualitatively with disorder in the photon energy of the exact JCH, and also found good agreement. This implies that the way we have modelled disorder is a good analogy for modelling non-zero temperature in the system. The following chapter investigates an alternative way of presenting phase diagrams for the system, in particular suited to an ion trap system.
3. **Phase diagram of the JCH in the ground state**
A trapped ion is an ion that is cooled to the ground state of a trapping potential in a vacuum. They are isolated quantum systems and a range of quantum dynamics has been demonstrated with them (see the review article in reference [45]). It is proposed that an ion trap system, via a laser-driven ion chain in a linear Paul trap, can be used to embody the physics described by the JCH Hamiltonian [48]. Spontaneous emission from the ions can be neglected, if Raman transitions are used to couple two ground state hyperfine levels to the phononic degree of freedom.

The traditional JCH system (see section 2.3 for a more complete description) contains a number of photonic cavities, each containing a two-level system, where photons are exchanged between cavities. The ion trap system we consider in this chapter consists of a

Figure 4.1: An example ion trap system with three traps. The ions are represented by small blue circles, and the traps by the larger ovals. The traps are connected by coupling $\kappa$, and each ion is connected to its resident trap by coupling $\beta$. 
4. Phase diagrams of the JCH in an ion trap system

<table>
<thead>
<tr>
<th>JCH</th>
<th>ion trap</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>number of photons</td>
</tr>
<tr>
<td>$\omega$</td>
<td>photon energy</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>transition from ground</td>
</tr>
<tr>
<td>$\beta$</td>
<td>photon/atom coupling</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>cavity-cavity coupling</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>detuning between atom and cavity energy scales</td>
</tr>
</tbody>
</table>

Table 4.1: Physical interpretation for the parameters in the canonical JCH, and the ion trap system.

number of individually trapped ions, which experience phonon-phonon repulsion due to the ion-laser interaction. These ions can be in one of two states, and phonons are exchanged between traps due to the Coulomb interaction. As such, a few minor modifications are needed to explore the connections between the JCH and its ion trap equivalent: rather than photon hopping, there is phonon hopping, the cavity frequency varies between the individual traps, and when considering coupling between traps, all neighbours are considered with scaling of the form $1/r^3$, so that the coupling is long range, but not uniform to all traps. The Bogoliubov transformation changes the $a^+a$ term from globalised normal mode frequencies of the motional degrees of freedom of the ions to localised modes (to compare more formally with the JCH system) [48]. A schematic of the ion trap system is shown in figure 4.1. While the Hamiltonian for a canonical JCH system, and an ion trap system, are very similar mathematically, there are some differences in the physical interpretation of the variables. These differences are summarised in table 4.1.

In this chapter, the rotating wave approximation has been used (as it also has in [48]). This means that we assume that the Rabi frequency is much less than the phonon frequency, that is, $\beta\sqrt{n} \ll \omega$. If this approximation were not used, then extra terms would need to be added to the Hamiltonian: specifically, a term of the form $\beta(\sigma^+a^1 + \sigma^-a)$ to the Jaynes-Cummings Hamiltonian. This would then violate conservation of excitation number, and the techniques used in this chapter could no longer be used. Including this term is beyond the scope of this thesis.

To understand the connections between the ion trap and JCH models, we compare the
accessible phase diagrams. The methods of exciting the lattices are different in each case and we display both the phase diagram for the traditional JCH system, as well as the ion trap system. A key advantage that the ion trap has over a traditional JCH system is that the coupling between sites can be tuned during the experiment (either by changing the voltages on the confining electrodes or by squeezing the whole system): this contrasts a typical, (e.g. photonic crystal cavity array) JCH system where the hopping rates are defined at fabrication. As with the JCH, two phases are present in this system: a Mott-insulator phase and a superfluid phase. Note that as there are only a fixed number of excitations, this system can only approximate a superfluid phase. However, for brevity, the term “superfluid phase” will be used throughout this chapter.

The phase diagrams discussed in this chapter are analogous to the phase diagrams discussed in chapter 3, as they both clearly show the theoretical existence of different phases in the JCH system. In chapter 3 the phase diagrams were shown as a function of intercavity hopping and chemical potential. In this chapter we instead focus on a different method of displaying the phase transition involving a fixed number of excitations (which does not include chemical potential), in particular this method of manifesting the phase transition is amenable to experimental verification in ion traps, as introduced by Ivanov [48].

4.1 Calculating the phase diagram

Here we generate and display phase diagrams for both the canonical JCH and the ion trap system. In the phase diagrams of chapter 3, the total number of excitations was not fixed. As such, as one explored the phase diagram as shown in that chapter, the number of excitations could fluctuate. Here we seek to start with a fixed number of excitations, and investigate the change in uncertainty of the number of excitations in the first cavity, $\Delta L_1 = \Delta (a_1^\dagger a_1 + \sigma_1^+ \sigma_1^-)$, as a function of the coupling between cavities $\kappa/\beta$. Choosing a cavity other than the first one to display the uncertainty might provide quantitatively different results due to the hard wall boundary conditions, but qualitatively the results will be the same, as such the choice of cavity is arbitrary. The state that we are interested
4. Phase diagrams of the JCH in an ion trap system

in is the ground state of the system. In this way, we investigate the two phases present in
the JCH system: the Mott insulator phase and the superfluid phase.

We use the JCH Hamiltonian as first displayed in equation (2.9),

\[
H = \sum_{i=1}^{N} H_{i}^{JC} - \kappa \sum_{i,j=1}^{N} A_{i,j} a_i^\dagger a_j - \sum_{i=1}^{N} \mu_i (\sigma_i^+ \sigma_i^- + a_i^\dagger a_i),
\]  

(4.1)

where the adjacency matrix \( A \) describes the geometry of the system: in this chapter
we use hard wall boundary conditions, as given by equation (2.11). The rotating wave
approximation has been taken for this Hamiltonian, see [48]. This calculation uses the
separate blocks of the Hamiltonian \( H^{(l)} \) corresponding to \( l \) excitations [see equations (3.21)
and (3.24)]. For a set of variables \( \epsilon, \omega, \beta, \) and \( \kappa \), one determines the eigenvector of
\( H^{(l)} \) corresponding to the smallest eigenvalue. This state is then used to determine the
uncertainty in the number of excitations on the first cavity \( \Delta L_1 \).

We first show an example of how the uncertainty is calculated from the Hamiltonian for
the first non-trivial case. The cases \( l = 0 \) and \( l = 1 \) for all \( N \) are trivial because the
uncertainty of the minimum eigenstate does not depend on \( \kappa \). As such the first non-trivial
case is 2 cavities, \( N = 2 \), with 2 excitations, \( l = 2 \). The corresponding block of the
Hamiltonian is given by [as in equation (3.21)]

\[
H^{(2)} = \begin{pmatrix}
2\omega & \sqrt{2}\beta & 0 & 0 & \sqrt{2}\kappa & 0 & 0 & 0 \\
\sqrt{2}\beta & \epsilon + \omega & 0 & 0 & 0 & \kappa & 0 & 0 \\
0 & 0 & \epsilon + \omega & \beta & \beta & 0 & \kappa & 0 \\
0 & 0 & \beta & 2\epsilon & 0 & \beta & 0 & 0 \\
\sqrt{2}\kappa & 0 & \beta & 0 & 2\omega & \beta & 0 & \sqrt{2}\kappa \\
0 & \kappa & 0 & \beta & \beta & \epsilon + \omega & 0 & 0 \\
0 & 0 & \kappa & 0 & 0 & 0 & \epsilon + \omega & \sqrt{2}\beta \\
0 & 0 & 0 & \sqrt{2}\kappa & 0 & \sqrt{2}\beta & 2\omega & 0
\end{pmatrix},
\]  

(4.2)

where the order of the basis is given by
Also, the operator for the total number of excitations in the first cavity is given by

\[ L_1 = a_1^\dagger a_1 + \sigma_1^+ \sigma_1^- = \text{diag}(0, 0, 1, 1, 1, 1, 2, 2). \]  \hspace{1cm} (4.4)

As such, to calculate the relevant uncertainty, we use

\[ \Delta L_1 = \sqrt{\langle L_1^2 \rangle - \langle L_1 \rangle^2} \]  \hspace{1cm} (4.5)

to determine the final uncertainty. Throughout this chapter, we assume that \( \Delta = \omega - \epsilon = 0 \), as such the diagonal elements of \( \mathcal{H}^{(2)} \) in equation (4.2) are all equivalent, and can be set to zero. The only remaining parameters are \( \beta \) and \( \kappa \). When \( \kappa \ll \beta \), the smallest eigenvalue is \( -2\beta \), which corresponds to the smallest eigenvector \( |1\rangle \otimes |2\rangle \). Hence \( \langle L_1 \rangle = \langle L_1^2 \rangle = 0 \), and \( \Delta L_1 = 0 \). When \( \kappa \gg \beta \), the smallest eigenvalue is \( -2\kappa \), which corresponds to the smallest eigenvector \( \frac{1}{\sqrt{2}} |g, 0\rangle \otimes |g, 2\rangle + \frac{1}{\sqrt{2}} |g, 1\rangle \otimes |g, 1\rangle \). Hence \( \langle L_1 \rangle = 1 \) and \( \langle L_1^2 \rangle = 3/2 \), and \( \Delta L_1 = 1/\sqrt{2} \).

We now display and analyse the phase diagrams for 2, 3 and 4 cavities, both for the canonical JCH system and the ion trap system. Figure 4.2(a), corresponds to 2 cavities, \( N = 2 \), and shows two distinct phases: on the left and the right of the diagram. When the coupling between cavities is very small, \( \kappa \ll \beta \), the uncertainties asymptote to only two possible values: 0 and 0.5. This corresponds to either the lattice being occupied by a number of excitations which is an integer multiple of the number of cavities, or a half-
Figure 4.2: Phase diagram for 2 cavities (left) and 2 ions (right). The left figure shows the diagram for the JCH system, while the right shows that for the ion trap system (modified so that the coupling is proportional to the phonon energy, and (in general) all neighbours are included, with scaling like inverse distance cubed). When $\kappa/\beta \ll 1$, the Mott phase is realised, when $\kappa/\beta \gg 1$, the superfluid phase is realised. In between these two limits is the signature of the phase transition. The numbers inset in the JCH plot indicate the number of excitations in the system, these always (also for figure 4.3 and 4.4) increase consecutively with increasing uncertainty in excitation number when $\kappa/\beta \gg 1$. Note that while the left and right figure look qualitatively the same, there are quantitative differences in the shape of the phase transition region, as well as in the values of the asymptotes when $\kappa/\beta \gg 1$. These asymptotes are given by equation (4.6) for the JCH case.

integer number of cavities. One may also think of this as the excitations being evenly shared between the two cavities, or there being one “remainder” excitation which may hop between the two cavities. This limit corresponds to the Mott-insulator phase. When the coupling between cavities is large, $\kappa \gg \beta$, the uncertainty asymptotes to a different value for every value of $l$. As $l$ increases, in the large $\kappa$ limit the uncertainty in excitation number increases, as the excitations are free to roam the lattice. This corresponds to the superfluid phase. Shown in table 4.2 are the eigenstates corresponding to the minimum eigenvalues for $N = 2$ for $l = 0, 1$, and 2. This re-asserts that in the case $l = 0$ and $l = 1$, the ground state of the system is identical in the case $\kappa \ll \beta$ and $\kappa \gg \beta$, whereas for $l = 2$ this ground state changes as a function of $\kappa$.

The $N = 2$, $N = 3$ and $N = 4$ phase diagrams for the JCH system are shown in figures
Table 4.2: Eigenstates for Mott-insulator and superfluid states for a system of 2 cavities, for 0, 1 and 2 excitations in the JCH system.

<table>
<thead>
<tr>
<th>excitations ( l )</th>
<th>min. eigenstate ( \kappa \ll \beta ) (MI)</th>
<th>min. eigenstate ( \kappa \gg \beta ) (SF)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(</td>
<td>g, 0\rangle^\otimes 2 )</td>
</tr>
<tr>
<td>1</td>
<td>( \frac{1}{\sqrt{2}} \hat{P}_2</td>
<td>g, 0\rangle \otimes</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{1}{\sqrt{2}} \hat{P}_2</td>
<td>g, 0\rangle \otimes</td>
</tr>
</tbody>
</table>

Figure 4.3: Phase diagram for 3 cavities (left) and 3 ions (right). Note that the difference between the JCH and ion trap phase diagrams is more pronounced than the 2 cavity case, figure 4.2. Also, the asymptotes on the left are more complicated for the ion trap than for the JCH case (some degeneracies have been broken due to the unusual coupling between ions). In the JCH case, the two asymptotes on the left correspond to the number of excitations being a multiple of 3 (asymptotes to 0) or a multiple of 3 plus or minus 1. In the ion trap case, an inset has been shown for the left asymptotes.

4.2(a), 4.3(a) and 4.4(a). In each case, in the limit that \( \kappa \ll \beta \), there is always an asymptote at 0. This always corresponds to there being an integer number of excitations per cavity. For the case \( N = 3 \), there is only one other asymptote - corresponding to an excess of 1 or 2 excitations per cavity. For the case \( N = 4 \), there are two other asymptotes, the first corresponds to one extra or one fewer excitation per cavity \( (l = 1, 3, 5, or 7 in the figure) \) and the second to 2 excess excitations per cavity \( (l = 2 or 6 in the figure) \). In all cases, \( N = 2, 3 \) and 4, in the limit that \( \kappa \gg \beta \), there is a separate asymptote for each value of \( l \). These asymptotes have a general formula for \( N = 2 \), but for higher values of \( N \) no general formula exists, due to the complicated nature of the higher polynomials. The
4. Phase diagrams of the JCH in an ion trap system

Figure 4.4: Phase diagram for 4 cavities (left) and 4 ions (right). Note that the difference between the JCH and ion trap phase diagrams is more pronounced than the 2 and 3 cavity cases, figures 4.2 and 4.3. In the JCH case, the three asymptotes on the left correspond to the number of excitations being a multiple of 4 (asymptotes to 0), a multiple of 4 plus or minus 1, and a multiple of 4 plus or minus 2 (asymptotes to 1/2).

asymptotes when $\kappa \gg \beta$ for $N = 2$ are given by

$$\lim_{\kappa/\beta \to \infty} \Delta L_1 = \frac{\sqrt{I}}{2}. \quad (4.6)$$

Also shown, in figures 4.2(b), 4.3(b) and 4.4(b), are results labelled as “ion trap”. The only difference between these calculations and the pure JCH case is the coupling between cavities $\kappa$ and the cavity frequency $\omega$. The following formulas are taken from the work of Mering [68]. The inter-cavity coupling is given by

$$\kappa_{i,j} = \frac{\kappa}{(i - j)^3} \quad (4.7)$$

as in equation (56) of [68], see also figure 4.5. Note that this is no longer merely nearest neighbour coupling, but instead every cavity can couple to every other cavity, albeit with a reduced coupling strength that goes like the distance between the sites cubed. The phonon frequency is given by
Figure 4.5: Coupling between 4 cavities, for (a) the standard JCH case (nearest neighbour coupling only is considered), and (b) the ion trap case, where all orders of next-nearest neighbour coupling are included, with a scaling of distance between cavities cubed, as in equation (4.7).

![Coupling Diagram](image)

\[ \omega_i = \kappa \left[ 2\zeta(3) + \frac{1}{2} \psi(2, i + 1) + \frac{1}{2} \psi(2, N - i) \right] \]  

(4.8)

as in equation (57) of [68], but generalised for a finite number of cavities [which we derived from equation (55)]. The function \( \zeta(s) \) is the Riemann zeta function, and \( \psi(2, s) \) is the second polygamma function (equivalent to the second derivative of the \( \Gamma \) function).

The phase diagrams corresponding to the ion trap case are more complicated than the canonical JCH case due to the more complicated forms for \( \kappa_{i,j} \) and \( \omega_i \) (though this difference is only significant for \( N \geq 3 \)). Despite the asymptotes being in slightly different locations in the phase diagram of the ion trap system, they still increase monotonically in the limit that \( \kappa \gg \beta \), and they still exist in the limit that \( \kappa \ll \beta \). As such, regardless of whether the JCH case or the ion trap is chosen, both cases display two clear phases - Mott-insulator when \( \kappa \ll \beta \) and superfluid when \( \kappa \gg \beta \). These calculations hence inform a possible experimental approach for observing these two phases.

We expect one may be able to realise the two phases, Mott-insulator and superfluid, via the following experimental approach. Firstly, prepare a system of \( N \) weakly coupled individually micro-trapped ion traps containing \( n \) phonons (i.e. \( n \)-phonon Fock state via resonant sideband excitation\(^*\)). Let the system relax to the ground state. Measure the

\(^*\)Resonant sideband excitation is an experimental method of changing the state of a quantum system. For example, assume a \( \Lambda \) type three state system consisting of the two ground states as \( |g, 0\rangle \) and \( |g, 1\rangle \).
fluctuations in the number of excitations, then compress the system a little, effectively increasing the coupling $\kappa$ to $\kappa + \delta\kappa$ and the microtrap frequency $\omega_i$ to $\omega_i + \delta\omega_i$. Continue this process until a new asymptote has been reached. Note that of scientific interest is to map out the entire phase diagram, not just the asymptotes. Increase the number of phonons in system by one, and start the process again.

4.2 Conclusions

In this chapter we have shown how to generate phase diagrams as a function of intercavity coupling $\kappa$, for a fixed number of excitations. These phase diagrams are shown for both the canonical JCH system, and the ion trap system. As such, if one were in the possession of a sufficiently controllable ion trap system, one could experimentally verify that two separate phases, a Mott-insulator and a superfluid phase, exist in this system. One would have to both have the capacity to manipulate the coupling between ions, as well as read out expectation value of the number of excitations and the square of this quantity, and hence the uncertainty of this quantity. As such this is opening the JCH system to a new experimentally realisable medium. Both this chapter and the previous explore phase diagrams, the following chapters will explore the behaviour of the JCH under time evolution.

and the excited state as $|e, 0\rangle$: two photon pumping can convert the system from a $|g, 0\rangle$ state to a $|g, 1\rangle$ state via the $|e, 0\rangle$ state.
In this chapter, we explore the dynamics of single excitations (where an excitation can be either photonic or atomic or an arbitrary superposition) in the linear JCH system, which describes a coupled cavity waveguide. We use direct, analytic diagonalisation of the Hamiltonian to study cases where inter-cavity coupling is either uniform or varies parabolically along the chain. Two initial states are investigated: excitations located in a single cavity, or one excitation as a Gaussian pulse spread over many cavities. We predict unusual behaviour of this system in the time domain, including slower than expected propagation of the excitation, and also splitting of the excitation into two distinct pulses, which travel at distinct speeds. In certain limits, we show that the JCH system mimics two Heisenberg spin chains. The work discussed in this chapter has been published in reference [65].

5.1 Introduction

Here we investigate the time evolution of a one dimensional coupled cavity waveguide [4] described by the Jaynes-Cummings-Hubbard (JCH) model [33], and introduced in chapter 2. In the single excitation subspace (section 2.3.2) we diagonalise the JCH Hamiltonian exactly and consider the dependence of this system on three parameters: atom-cavity detuning $\Delta$, atom-photon coupling $\beta$ and coupling between cavities $\kappa$. We then investigate limits in which localised and delocalised behaviour can be seen. In this chapter, we refer to the propagation of photonic or atomic excitations as the photonic and atomic compo-
nents, or modes, respectively (in the atomic case, the atoms remain stationary whilst the excitation passes through). In particular we focus on three limits. Firstly, the limit where the atom-cavity detuning is zero, $\Delta = 0$ and the coupling strength between cavities is much less than the photonic cavity-atomic coupling $\kappa \ll \beta$. In this limit, the propagation dynamics of the atomic and photonic components are identical; we find they propagate as a pulse travelling back and forth along the line of cavities. Secondly, we study the limit where $\Delta = 0$ and photon hopping dominates all other parameters of the system, $\kappa \gg \beta$. In this limit, the atomic component does not move, while the photonic component propagates. Thirdly, we study the limit where the atom-cavity detuning is much larger than all other energy scales of the system. In this limit the atomic and photonic modes travel at two different speeds. In these three limits we compare the behaviour with that of two uncoupled Heisenberg spin chains [7, 67, 84], in the one-excitation case. Solitonic behaviour has not been predicted in this system, unlike the 1D coupled cavity wave guide realisations of the Dicke model [78] and the XXZ model in the presence of a tilted magnetic field [63].

We discuss the JCH model and the uniform coupling case in section 5.2. We then continue with dispersion-free pulses using parabolic coupling, section 5.3, and initial Gaussian pulses, section 5.4. In section 5.5 we discuss the limit of large atom-cavity detuning, in this limit the atomic and photonic modes travel at two distinct speeds.

### 5.2 Uniform coupling

We re-state the one excitation JCH Hamiltonian, equation (2.18), from subsection 2.3.2 for ease of viewing:

$$
\mathcal{H}_{\text{1exc}}^{\text{JCH}} = \frac{\Delta}{2} I_N \otimes Z + \beta I_N \otimes X - \kappa A \otimes \frac{I_2 + Z}{2},
$$  \hspace{1cm} (5.1)

where the $2N$ basis vectors are given by $|Q\rangle \otimes |g, 1\rangle$ and $|Q\rangle \otimes |e, 0\rangle$, $Q = 1, \ldots, N$. As this Hamiltonian is represented as a matrix composed of the tensor product of $2 \times 2$ matrices by $N \times N$ matrices, and two out of three of these $N \times N$ matrices are the identity
matrix, then by diagonalising the adjacency matrix $A$ [equation (2.10)] the whole JCH Hamiltonian restricted to one excitation can be diagonalised. $A$ cannot be diagonalised for an arbitrary geometry, (though some attempts have been made, for example in the infinite cavity limit [68]) however the 1D uniform coupling chain with hard wall boundary conditions is diagonalisable. The eigenvectors of the $A$ matrix given in equation (2.11) are standard [6, 20].

$$|k\rangle_{\text{mom.}} = \frac{\sqrt{2}(-1)^k \sin \left( \frac{Nk\pi}{N+1} \right)}{\sqrt{N+1} \sin \left( \frac{k\pi}{N+1} \right)} \sum_{Q=1}^{N} \sin \left( \frac{Qk\pi}{N+1} \right) |Q\rangle,$$  \hspace{1cm} (5.2)

where $k = 1, \ldots, N$.

We now proceed to obtain the energy eigenstates and energy eigenvalues for the entire one excitation subspace. For a linear chain of cavities the Hamiltonian $H_{\text{JCH}}^{1\text{exc}}$ can be expressed by the $2N$ basis vectors $\{|k\rangle_{\text{mom.}} \otimes |g, 1\rangle, |k\rangle_{\text{mom.}} \otimes |e, 0\rangle\}$, $k = 1, \ldots, N$ as a block diagonal matrix, in which the $k$th block appears as

$$H_{\text{JCH}}^{1\text{exc}}(k) = \begin{pmatrix} \Delta/2 + 2\kappa \cos \left( \frac{k\pi}{N+1} \right) & \beta \\ \beta & -\Delta/2 \end{pmatrix}. \hspace{1cm} (5.3)$$

The eigenvalues of the full Hamiltonian, from equation (2.18), are

$$E_{\pm}^k = \kappa \cos \left( \frac{k\pi}{N+1} \right) \pm \sqrt{\left[ \frac{\Delta}{2} + \kappa \cos \left( \frac{k\pi}{N+1} \right) \right]^2 + \beta^2}, \hspace{1cm} (5.4)$$

where the second term of this appears very similar to the Rabi frequency $\chi(1)$, equation (2.7), with the detuning $\Delta$ shifted by the cosine term (similarly derived in [81]).

These eigenvalues have corresponding eigenvectors

$$|\pm, k\rangle_{\text{mom.}} = \frac{(\Delta + 2E_{\pm}^k) |g, 1\rangle + 2\beta |e, 0\rangle}{\sqrt{(\Delta + 2E_{\pm}^k)^2 + 4\beta^2}} \otimes |k\rangle_{\text{mom.}}, \hspace{1cm} (5.5)$$

which are generated by diagonalising equation (5.3). For example, for a two cavity system, $N = 2$, the $|\pm, 1\rangle_{\text{mom.}}$ momentum eigenstate is given by
5. Time evolution of the 1D JCH Hamiltonian

\[ |\pm, 1\rangle_{\text{mom.}} = \left\{ \frac{(\Delta + 2E_1^\pm)|g, 1\rangle + 2\beta|e, 0\rangle}{\sqrt{(\Delta + 2E_1^\pm)^2 + 4\beta^2}} \right\} \otimes \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \]

(5.6a)

\[ = -\frac{1}{\sqrt{2}} \left\{ \frac{(\Delta + 2E_1^\pm)|g, 1\rangle + 2\beta|e, 0\rangle}{\sqrt{(\Delta + 2E_1^\pm)^2 + 4\beta^2}} \right\} \otimes |g, 0\rangle \\
+ |g, 0\rangle \otimes \left\{ \frac{(\Delta + 2E_1^\pm)|g, 1\rangle + 2\beta|e, 0\rangle}{\sqrt{(\Delta + 2E_1^\pm)^2 + 4\beta^2}} \right\} \right\}.

(5.6b)

Equation (5.5), \(|\pm, k\rangle_{\text{mom.}}\) is an exact diagonalisation of the linearly-coupled JCH system in the one excitation subspace, with momentum \(k\). Hence, it is possible to determine analytically, for an arbitrary number of cavities \(N\), the time-evolution of an arbitrary one excitation initial state. In the case with two cavities, i.e. \(N = 2\), and in appropriate limits to each case, this evolution recovers equations (22), (28) and (29) of Ogden et al. [73].

Specifically, we are interested in plotting the expectation value of both the photonic and atomic excitations in cavity \(j\), by examining the photonic and atomic number operators \(a_j^\dagger a_j\) and \(\sigma_j^+ \sigma_j^-\) respectively.

As a demonstration of the dynamics of the system when on resonance (i.e. \(\Delta = 0\)), we consider evolution of an excitation initially located in the first cavity in a line of 100 cavities, in an equal superposition of atomic and photonic modes, i.e.

\[ |\psi(t = 0)\rangle = |1\rangle \otimes (|g, 1\rangle + |e, 0\rangle)/\sqrt{2}, \]

(5.7)

which corresponds to the single cavity energy eigenstate \(|+, 1\rangle\) from equation (2.5) in the case \(\Delta = 0\). As such, there will be no evolution within a cavity, but only evolution between cavities. The state in equation (5.7) also constitutes one of the simplest states to realise experimentally, as the JC resonance can be driven directly by a transverse field. We solve the evolution analytically, using the usual Schrödinger equation, \(i\partial_t |\psi\rangle = H|\psi\rangle\) (with \(\hbar = 1\)). The solution is not shown as it is too cumbersome to display. The dispersion and other effects discussed in this chapter stem directly from the strong atom-photon
5. Time evolution of the 1D JCH Hamiltonian

Figure 5.1: Space-time diagrams for evolution of an excitation \((|1\rangle \otimes (|g,1\rangle + |e,0\rangle)/\sqrt{2})\) along a chain of 100 JC cavities for three different parameter regimes. In each case, we plot the probability of occupation of a particular cavity (vertical axis) as a function of time (horizontal axis) for the system initialised in an even superposition of the atomic and photonic mode of the first cavity. The upper three plots show the population of the atomic components whereas the lower three plots are the photonic components. The ratio of cavity-cavity coupling to atom-photon coupling varies from left to right, with (a) and (b) \(\kappa/\beta = 10^{-3}\), (c) and (d) \(\kappa/\beta = 10\) and (e) and (f) \(\kappa/\beta = 10^3\). In plots (a), (b) and (f), the dashed lines represent \(Q_{\Lambda}\), as given in equation (5.11).

interaction via the JC Hamiltonian. If we were to consider a system with vanishing coupling to the atoms \((\beta = 0)\), we regain the conventional photon propagation results [90, 91, 62] in which a Gaussian wave propagates smoothly.

We are ultimately interested in the behaviour of the system when various energies dominate, such as the atom-photon coupling \(\beta\) or the cavity-cavity coupling \(\kappa\). For this reason, we will now consider the system in several different limits. When \(\kappa/\beta \ll 1\) and \(\Delta = 0\), the atomic and photonic modes have identical propagation dynamics. The case \(\kappa/\beta = 10^{-3}\) is shown in figure 5.1(a) and (b). We may understand the equal propagation because the atom-photon coupling \(\beta\) is much stronger than the cavity-cavity coupling \(\kappa\), hence the excitation is free to form the single cavity eigenstate between inter-cavity hops. By shifting to the interaction picture [70], that is \(|\chi\rangle = e^{i\beta I \otimes X_t} |\psi\rangle\), the Hamiltonian equation (2.18), or (5.1) becomes
where the fast rotating terms have been ignored. It is useful at this point to compare with the Hamiltonian that describes the well-known Heisenberg spin chain [25, 94].

\[ H^\text{Heis} = -J \sum_{n=1}^{N} S_n S_{n+1} = -J \sum_{n=1}^{N} \left[ \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) + S_n^z S_{n+1}^z \right], \quad (5.9) \]

where \( S_n = \{ S_n^x, S_n^y, S_n^z \} \) are the Pauli operators acting on the \( n \)th site, and the raising and lowering operators on the \( n \)th site are given by \( S_n^\pm = S_n^x \pm iS_n^y \). The single site basis of this system consists of spins pointing up and down along the direction of the \( z \) axis, \( \{|\uparrow\rangle, |\downarrow\rangle\} \).

The \( N \) site basis comprises of a tensor product of \( N \) such bases. This Hamiltonian also conserves the total spin in the \( z \) direction. So, if we limit the \( N \) site basis to having only one \(|\uparrow\rangle\), and the rest \(|\downarrow\rangle\), then the Hamiltonian can be represented in this restricted subspace as

\[ H^\text{Heis} = -\frac{J}{2} A. \quad (5.10) \]

We ignore contributions from the \( S^z \) term, which is largely a phase factor apart from a minor shift at the ends of the chain, which is inconsequential for long chains. The basis vectors are now \(|1\rangle, |2\rangle, \ldots, |N\rangle\), and \(|Q\rangle\) represents \(|\uparrow\rangle\) at site \( Q \) and \(|\downarrow\rangle\) at every other site, and \( A \) is the adjacency matrix, in general given by equation (2.10), a particular example is given in equation (2.11). The initial state \(|1\rangle\) will evolve along the chain (with momentum only in the direction away from the wall, due to the hard wall boundary conditions) with an approximate speed \( J \) (the rate at which the front of the excitation wave travels across the chain), according the to triangle wave

\[ Q_\Lambda = \frac{N - 1}{\pi} \arcsin \left\{ \sin \left[ \pi \left( \frac{Jt}{N} - \frac{1}{2} \right) \right] \right\} + \frac{N + 1}{2}. \quad (5.11) \]

We find that the speed \( J \) as described above is given by the derivative of equation (5.11), i.e. \( J = |\partial_t Q_\Lambda| \), (defined at all points apart from the instant at which the “bounce” of
the excitation from the walls occurs.

By comparing equation (5.10) with equation (5.8), we see that the JCH Hamiltonian in the regime $\Delta = 0$, $\kappa \ll \beta$, mimics two Heisenberg spin chains, in each of the photonic and the atomic states [52]. In both cases, $J = \kappa$ (the approximate excitation speed).

Next we consider an alternative limit, where the coupling between cavities dominates the evolution, $\kappa/\beta \gg 1$. In this regime, the atomic mode does not propagate at all, while the photonic mode propagates at twice the speed of the previous case. This is because the atom-photon coupling is effectively zero compared to the much faster inter-cavity coupling rate, freezing the atomic excitation. The case $\kappa/\beta = 10^3$ is shown in figure 5.1(e) and (f).

In this limit, the Hamiltonian trivially reduces to

$$H = -\kappa A \otimes \frac{I_2 + Z}{2},$$  \hspace{1cm} (5.12)

by setting $\Delta = 0$ and $\beta = 0$. As such, the photonic excitation travels with speed $2\kappa$, and the atomic excitation does not move at all. We can think of this limit as that of a pure photon gas, albeit with only one photon, which is equivalent to a single-excitation spin chain.

When $\Delta = 0$, and $\kappa$ and $\beta$ are of the same order of magnitude, the evolution of the state equation (5.7) now experiences a large amount of dispersion: the full JCH nature of the evolution is now expressed, and the Hamiltonian no longer approximates two Heisenberg spin chains (as it does in the $\kappa/\beta \ll 1$ and $\kappa/\beta \gg 1$ limits). As the atom-cavity coupling $\beta$ and the cavity-cavity coupling $\kappa$ are of the same order, there is no opportunity for the excitation to form any single cavity eigenstates, instead the excitation is relatively free to roam between photonic and atomic modes, as well as between cavities. The example $\kappa/\beta = 10$ is shown in figure 5.1(c) and (d).

To more clearly see this interplay between JC and photon dominated regimes, we consider the dispersion of the wave packet as it travels along the chain. Figure 5.2 shows how the dispersion of a pulse changes with $\kappa/\beta$. We define the position operators
5. Time evolution of the 1D JCH Hamiltonian

Figure 5.2: Dispersion of the wave packet, $\Delta Q$, at a fixed point in time, as a function of $\kappa/\beta$, with atom-cavity detuning $\Delta = 0$ and number of cavities $N = 100$. The solid (dashed) line shows $\Delta Q_{\text{JCH}}^{\text{atomic}}$ ($\Delta Q_{\text{JCH}}^{\text{photonic}}$). The dotted (dot-dashed) line shows $\Delta Q_{\text{Heis}}^{\text{atomic}}$ with $J = 2\kappa$ ($J = \kappa$). The dispersion is measured at a time $T = N/4\kappa$, at which point the packet is ‘freely’ evolving along the chain. This point is chosen such that the effects of the hard-wall boundaries can be ignored for both large and small $\kappa$. At the left of the plot, $\kappa/\beta \ll 1$, and the JCH chain mimics two identical Heisenberg spin chains, an example is shown of this localised behaviour in figure 5.1(a) and (b), where $\kappa/\beta = 10^{-3}$. The corresponding spatial profile of the pulse at $T = N/4\kappa$ is shown in the left inset (the solid line shows the photonic profile and the dashed line shows the atomic profile, in this case they are coincident). At the right of the plot, $\kappa/\beta \gg 1$, and the photonic mode of the JCH chain mimics a Heisenberg spin chain, while the atomic mode does not propagate at all. An example of this type of localised behaviour is shown in figure 5.1(e) and (f), where $\kappa/\beta = 10^3$, the corresponding profile of the pulse at $T = N/4\kappa$ is shown in the right inset. In the middle of the plot a travelling excitation shows a large amount of dispersion, an example of this delocalised behaviour is shown in figure 5.1(c) and (d), where $\kappa/\beta = 10$, and the corresponding profile at $T = N/4\kappa$ is shown in the middle inset. The horizontal lines show the dispersion $\Delta Q_{\text{Heis}}^{\text{Heis}}$ of a Heisenberg spin chain with 100 spins after the initial state $|1\rangle$ evolves until the front of the excitation is half way (dotted line) and quarter way (dot-dashed line) along the excitation chain. The exact correspondence between the Heisenberg and JCH systems is seen in these asymptotic limits.
\[ Q_{\text{photonic}} \equiv \text{diag}(1, 0, 2, 0, \ldots, N, 0) = \sum_{Q=1}^{N} Q(|Q\rangle \otimes |g, 1\rangle)(\langle Q| \otimes \langle g, 1|) \]
\[ Q_{\text{atomic}} \equiv \text{diag}(0, 1, 0, 2, \ldots, 0, N) = \sum_{Q=1}^{N} Q(|Q\rangle \otimes |e, 0\rangle)(\langle Q| \otimes \langle e, 0|) \] (5.13)

in the basis \( \{|Q\rangle \otimes |g, 1\rangle, |Q\rangle \otimes |e, 0\rangle\} \), \( Q = 1, \ldots, N \). The definitions of equation (5.13) assume that when calculating expectation values for photonic (atomic) position, the photonic (atomic) states are selected from the wave function and normalised as a single vector of length \( N \). Imagine measuring two characteristics on each of an infinite set of identically prepared 1D JCH systems. The first quality is the atomic/photonic nature of the excitation. The second quality is position. Averaging the position reading of all photonic (atomic) systems gives the expectation value of the photonic (atomic) position, as given in equation (5.13).

Note that these position operators cannot be used reliably to represent the position of atomic and photonic excitations in the 1D one excitation JCH system. Consider the state \( |1\rangle \otimes |g, 1\rangle \). The expectation value of photonic position yields

\[ \langle Q_{\text{photonic}} \rangle = (\langle 1| \otimes \langle g, 1| 1 \rangle \otimes |g, 1\rangle)(\langle 1| \otimes \langle g, 1| 1 \rangle \otimes g, 1\rangle) = 1, \] (5.14)

which is correct, however the expectation value of atomic position yields

\[ \langle Q_{\text{atomic}} \rangle = (\langle 1| \otimes \langle g, 1| 1 \rangle \otimes |e, 0\rangle)(\langle 1| \otimes \langle e, 0| 1 \rangle \otimes g, 1\rangle) = 0, \] (5.15)

which is not correct and has no physical meaning. As such, these position operators may only be used when the probability of the excitation being atomic is equal to the probability of the excitation being photonic. In the simulations used in this chapter, we find that this is always the case. We know of no more general position operators (the atomic/photonic nature of the excitation cannot be traced out).

The dispersion for photonic and atomic modes is given by the standard deviation of the
position operator $\Delta Q$

$$(\Delta Q_{\text{type}})^2 = \langle Q^2_{\text{type}} \rangle - \langle Q_{\text{type}} \rangle^2.$$  

Looking at figure 5.2, we see the link between the two limits $\kappa/\beta \ll 1$ and $\kappa/\beta \gg 1$ for $\Delta = 0$. The solid (dashed) line shows $\Delta Q_{\text{atomic}}^{\text{JCH}}$ ($\Delta Q_{\text{photonic}}^{\text{JCH}}$). In these two limits, the JCH chain mimics two Heisenberg spin chains, while in the middle range, the full JCH dynamics are realised. With increasing $\kappa/\beta$, the photonic (atomic) dispersion of a pulse is constant (constant) when $\kappa/\beta \ll 1$, increases for moderate values of $\kappa/\beta$, then becomes constant (zero) when $\kappa/\beta \gg 1$. Dispersion is measured at the time $T = N/4\kappa$ for a system with $N = 100$ cavities initially in the state given by equation (5.7) (i.e. $|1\rangle \otimes |+,1\rangle$ with $\Delta = 0$). The horizontal lines drawn on the figure show the dispersion $\Delta Q_{\text{Heis}}$, where

$$Q_{\text{Heis}} = \text{diag}(1,2,\ldots,N) = \sum_{Q=1}^{N} Q|Q\rangle\langle Q|$$  

of a Heisenberg spin chain with 100 spins and initial state $|1\rangle$ for $J = \kappa$ (dotted line) and $J = 2\kappa$ (dot-dashed line) along the excitation chain. The $J = \kappa$ Heisenberg dispersion line matches both the photonic and atomic dispersion in the limit when $\kappa/\beta \ll 1$. The $J = 2\kappa$ Heisenberg dispersion line matches the photonic dispersion in the limit when $\kappa/\beta \gg 1$, while the atomic dispersion in this limit tends to zero (as the atomic mode no longer propagates).

The left inset of figure 5.2 and figure 5.1(a) and (b) correspond to the example $\kappa/\beta = 10^{-3}$. The inset shows the pulse profile at the time $T = N/4\kappa$ [with pulse approximately a quarter along the chain, $Q_{\lambda} = N/4$, and solid (dashed) line representing the photonic (atomic) profile], while part (a) and (b) shows that the evolution of the atomic and photonic modes are identical. The middle inset of figure 5.2 and figure 5.1(c) and (d) correspond to the example $\kappa/\beta = 10$. The inset shows the high dispersion of the pulse profile at the time $T = N/4\kappa$ (the dashed line shows atomic profile), and part (b) shows the high dispersion evolution. The right inset of figure 5.2 and figure 5.1(e) and (f) correspond to the example $\kappa/\beta = 10^3$. The inset shows the pulse profile at $T = N/4\kappa$, note that the photonic profile
Figure 5.3: Evolution of a Heisenberg spin chain Hamiltonian [equation (5.10)], with $J = 1$.

(a) Evolution of $|1\rangle$ under uniform coupling, note that at first the excitation travels fairly neatly, but both within a single pass, as well as during the reflection, the excitation pulse spreads out. Note the faint lines which are parallel but displaced from the wavefront. These lines are due to the nature of the Heisenberg Hamiltonian. (b) Evolution of $|1\rangle$ under parabolic coupling, note that the evolution is smooth and repetitive, the excitation travels sinusoidally from one end of the line of spins to the other end and back again, without spreading out. (c) Evolution of a Gaussian pulse as in equation (5.25), with $Q_c = 50$, $s = 10$, $k = \pi/2$, with uniform coupling. Note that the evolution is dispersion-free.

is approximately half way along the chain ($Q = N/2$), while the dashed line shows the atomic profile, which does not propagate. The atomic and photonic modes remain in superposition, despite the fact that the atomic mode does not propagate and the photonic mode does.

Consider the profile (probability distribution at an instant in time) of a single excitation as it travels along the chain. In figure 5.3(a), we display the expectation value of the evolution of a single up spin (initially at $|1\rangle$) for a Heisenberg spin chain with uniform coupling $J$ between each of the 100 sites. One sees that the pulse is initially well-formed, but later suffers from increasing dispersion of the excitation, both when travelling through the chain, and also when reflecting from the end of the chain. Regardless, the speed of the pulse is given by $J$, at least for the first reflection, where the wave speed can be realistically interpreted. Figure 5.4(a) is a different way of showing the same evolution, by plotting the expectation value and uncertainty of the operator $Q^{\text{Heis}} = \text{diag}(1, 2, \ldots, N)$.
Figure 5.4: Evolution of a Heisenberg spin chain Hamiltonian [equation (5.10)], with \( J = 1 \). The solid lines display the expectation value of the position \( \langle Q \rangle \), the dashed lines show the dispersion \( \Delta Q \). (a) Evolution of \(|1\rangle\) under uniform coupling, \( \Delta Q \) increases with time, this indicates increasing dispersion as time progresses. (b) Evolution of \(|1\rangle\) under parabolic coupling, here \( \Delta Q \) does not increase with time, as such this indicates dispersion-free evolution. (c) Evolution of a Gaussian pulse as in equation (5.25), with \( Q_c = 50, s = 10, k = \pi/2 \), with uniform coupling. As in (b), there is no overall increase in dispersion, as such this pulse is also dispersion-free.

highlighting the spread of the pulse with time. While the physics of Heisenberg spin chains is well studied [25, 94], it is useful to contrast this behaviour with the next regime we will examine.

5.3 Parabolic coupling

One way to control the dispersion of the pulse is to define a non-uniform distribution of couplings between cavities. One such possibility is to choose a regime of parabolic couplings [3, 20], where the coupling between cavity \( i \) and cavity \( i+1 \) is given by \( \sqrt{i(N - i)} \), so that the adjacency matrix becomes

\[
A_{ij} = \begin{cases} 
\sqrt{j(N - j)} & i - j = 1 \\
\sqrt{i(N - i)} & j - i = 1 \\
0 & \text{otherwise}
\end{cases} \quad (5.18)
\]
Figure 5.5: Parabolic coupling between neighbouring cavities in a one dimensional chain of 100 JC cavities, the implications of which are explored in section 5.3. The coupling is no longer uniform between cavities, as in the section 5.2, but instead varies as in equation (5.18), so that the strongest coupling is experienced between cavities in the centre of the chain.

Thus the couplings will be symmetric around the central cavity (or between the two central cavities), with strongest coupling at the centre of the chain and weakest coupling at the ends, see figure 5.5. A spin chain of length $N$ with this coupling can be mapped to a single spin $(N-1)/2$ particle, placed in a magnetic field in the $x$ direction. This system provides the physical insight for why this coupling is dispersion-free [3]. The eigenvalues of this matrix are $E_k = N - 1 - 2k$ and the eigenvectors are given analytically by

$$|k\rangle_{\text{mom.}} = \sum_{Q=1}^{N} \sqrt{\frac{(1-N)_k(N-1)!}{(-1)^k(2^{N-1})(2Q-1)!(N-Q)!}} K_k(Q-1, \frac{1}{2}, N-1)|Q\rangle,$$  

(5.19)

where the Pochhammer symbol $(N)_k$ is a generalisation of the factorial function, it is defined as

$$(N)_k = (N)(N+1)\ldots(N+k-1), \quad k = 1, 2, 3, \ldots$$  

(5.20)

and the Krawtchouk polynomial $K$ [8, 2] is related to the hypergeometric function $F$ by

$$K_k(l, p, N) = {}_2F_1 \left( -\frac{k}{N}; \frac{1}{p^{-1}} \right).$$  

(5.21)

The eigenvectors of equation (5.19) are the harmonic oscillator solutions: the first three...
of these \((k = 0, 1, 2)\) for 100 cavity system, \(N = 100\), are shown in figure 5.6.

Now we examine the behaviour of the JCH chain under this parabolic coupling scheme. We find that, again in the basis given by \(\{ |k\rangle_{\text{mom}} \otimes |g, 1\rangle, |k\rangle_{\text{mom}} \otimes |e, 0\rangle \}\), the Hamiltonian is a block diagonal matrix, with the \(k\)th block appearing as

\[
H_{1\text{exc}}(k) = \begin{pmatrix}
\Delta / 2 & -\kappa (N - 1 - 2k) & \beta \\
-\kappa (N - 1 - 2k) & \beta & -\Delta / 2 \\
\beta & -\Delta / 2 & -\Delta / 2
\end{pmatrix}.
\]

(5.22)

The eigenvalues of the full Hamiltonian (2.18) in the parabolic coupling case are

\[
E_{k}^{\pm} = \frac{1}{2} \left\{ \kappa (2k - N + 1) \pm \sqrt{[\Delta + \kappa (2k - N + 1)]^2 + 4\beta^2} \right\}
\]

(5.23)

and the eigenvectors are

\[
|\pm, k\rangle_{\text{mom.}} = \frac{1}{\sqrt{(\Delta + 2E_{k}^{\pm})^2 + 4\beta^2}} \left( \Delta + 2E_{k}^{\pm} \right) |g, 1\rangle + 2\beta |e, 0\rangle \otimes |k\rangle_{\text{mom.}}.
\]

(5.24)

The example of the \(|\pm, 1\rangle_{\text{mom.}}\) eigenstate for a 2 cavity system is identical to the example shown in the previous section, equation (5.6), with equation (5.23) used for the energy \(E_{k}^{\pm}\). We find the matching that occurs in limiting cases for the parabolic JCH system, occurs in exactly the same way as the uniform coupling case. That is, when \(\Delta = 0\) and \(\kappa \ll \beta\), \(J = \kappa\) for both the atomic and photonic parts. When \(\Delta = 0\) and \(\kappa \gg \beta\), \(J = 2\kappa\)
Figure 5.7: Space-time diagrams for evolution of an excitation \(|1⟩ \otimes (|g, 1⟩ + |e, 0⟩)/\sqrt{2}\) along a chain of 100 JC cavities with parabolic inter-cavity coupling profile. The upper plots show the population of the atomic components whereas the lower plots are the photonic components. The ratio of cavity-cavity coupling to atom-photon coupling varies from left to right, with (a) and (b) \(\kappa/\beta = 10^{-4}\), (c) and (d) \(\kappa/\beta = 10^0\), (e) and (f) \(\kappa/\beta = 10^3\). In plots (a), (b) and (f), the white dashed lines represent \(\langle Q(t)⟩\), as given in equation (5.28). The effect of the parabolic coupling is to constrain the pulse.

for the photonic mode and the atomic mode does not propagate. Figures 5.7 and 5.8 show very similar results to figures 5.1 and 5.2, with only one significant difference (apart from the dispersion-free pulses), that the uncertainty in position for moderate values of \(\kappa/\beta\) is much larger than the uniform coupling case.

5.4 Gaussian pulses

As an alternative to modifying the coupling profile, we can consider uniform coupling and a Gaussian wave packet as our initial state. In this case, the momentum distribution of the pulse is well defined (and narrow) which allows the excitation to travel down the chain with minimal increase in dispersion [91, 90]. We therefore choose an appropriate initial state

\[
|\psi(k, s, Q_c)(t = 0)⟩ = \mathcal{N} \sum_{Q=1}^{N} e^{-\frac{(Q - Q_c)^2}{2s^2}} e^{-ikQ} |Q⟩, \quad (5.25)
\]
for a Heisenberg spin chain, or

$$|\psi^{(k,s,Q_c)}(t=0)\rangle = \mathcal{N} \sum_{Q=1}^{N} e^{-\frac{(Q-Q_c)^2}{2s^2}} e^{-ikQ}|Q\rangle \otimes (|g,1\rangle + |e,0\rangle)/\sqrt{2}, \quad (5.26)$$

for a JCH chain, where $\mathcal{N}$ is the normalisation, $k$ is the wave number, $Q_c$ is the centre of the pulse, $s$ is the width of the pulse, and $Q$ denotes cavity number, with $Q = 1, \ldots, N$.

We choose $Q_c = N/2$, $s = N/10$, such that the pulse is initiated at the centre of the chain with a width approximately 2/10 times the length of the chain. The value $k = \pi/2 + n\pi$, where $n$ is an integer, produces dispersion-free evolution of the pulse.

Figure 5.9 shows the evolution of a Gaussian pulse for three different values of $\kappa/\beta$, in analogy to figures 5.1 and 5.7. The white dashed lines correspond to a triangle wave similar to equation (5.11), but with a phase shift by $\pi/2$. The phase shift is necessary as we have initiated the Gaussian pulse in the centre of the chain, to avoid boundary effects.
Figure 5.9: Space-time diagrams for evolution of an Gaussian pulse along a chain of 100 JC cavities with a uniform inter-cavity coupling profile. The upper plots show the population of the atomic components whereas the lower plots are the photonic components. The ratio of cavity-cavity coupling to atom-photon coupling varies from left to right, with (a) and (b) $\kappa/\beta = 10^{-2}$, (c) and (d) $\kappa/\beta = 10^0$, (e) and (f) $\kappa/\beta = 10^3$. In plots (a), (b) and (f), the white dashed lines represent $Q_G^{\text{Gaussian}}$, as given in equation (5.27). The effect of the Gaussian pulse is to have chosen a narrow momentum distribution, which allows the excitation to propagate freely in the system.

Figure 5.10 shows the dispersion of the pulse as a function of $\kappa/\beta$, in analogy to figure 5.2 and 5.8. Note how this figure is much simpler than the earlier two, as the dispersion is a constant throughout the evolution of the pulse, provided the pulse is not interacting with the boundaries. As such, only one horizontal line to indicate dispersion of a corresponding

\[ Q_G^{\text{Gaussian}} = \frac{N - 1}{\pi} \arcsin \left[ \sin \left( \frac{J \pi t}{N} \right) \right] + \frac{N + 1}{2}. \]  

(5.27)
5. Time evolution of the 1D JCH Hamiltonian

Figure 5.10: Dispersion of a Gaussian wave packet, $\Delta Q$, at a fixed point in time, as a function of $\kappa/\beta$, at $\Delta = 0$. The dispersion is measured at time $T = N/8\kappa$, at which point the packet is ‘freely’ evolving along the chain. The initial state of the Gaussian is given by equation (5.26), with centre of the pulse at $Q_c = N/2$, width of the pulse $s = N/10$, wave number $k = \pi/2$, and number of cavities $N = 100$. The width of the pulse is small enough such that the boundaries do not have an effect on $\Delta Q$ for the value of $T = N/8\kappa$ in the limits $\kappa/\beta \ll 1$ and $\kappa/\beta \gg 1$. At the left of the plot, $\kappa/\beta \ll 1$, and the JCH chain mimics two identical Heisenberg spin chains, an example is shown of this localised behaviour in figure 5.9(a) and (b), where $\kappa/\beta = 10^{-2}$. The corresponding spatial profile of the pulse is shown in the left inset, (the solid line shows the photonic profile and the dashed line shows the atomic profile, in this case they are coincident). At the right of the plot $\kappa/\beta \gg 1$, and the photonic mode of the JCH chain mimics a Heisenberg spin chain, while the atomic mode does not propagate at all. An example of this type of localised behaviour is shown in figure 5.9(e) and (f), where $\kappa/\beta = 10^3$, the corresponding profile of the pulse at $T = N/8\kappa$ is shown in the right inset. In the middle of the plot a travelling excitation shows a large amount of dispersion, an example of this delocalised behaviour is shown in figure 5.9(c) and (d), where $\kappa/\beta = 10$, and the corresponding profile at $T = N/8\kappa$ is shown in the middle inset. The horizontal line shows the dispersion $\Delta Q_{\text{Heis}}$ of a freely evolving pulse [this value does not change, provided the pulse is not interacting with the boundary, as is evidenced by figure 5.4(c)].

Heisenberg spin chain is necessary. Also, the dispersion of the photonic mode is equal to the dispersion of the atomic mode.

By comparing figure 5.3(a) (uniform coupling) with 5.3(b) (parabolic coupling) and figure 5.3(c) (uniform coupling, Gaussian pulse) we can indeed see that the pulse in the uniform chain has more dispersion than that of the parabolic chain and the uniform chain with an initial Gaussian pulse, the dispersion is manifest as a number of faint lines paral-
Figure 5.11: The pulse profile for various points in time as a function of cavity number, for evolution of a Heisenberg spin chain. (a) Evolution of $|1\rangle$ with uniform coupling between spins. (b) Evolution of $|1\rangle$ with parabolic coupling between spins. (c) Evolution of a Gaussian pulse, as given in equation (5.25) with uniform coupling between spins. In the first uniform case, the profile is initially given by a Kronecker delta function, but later spreads into a function with one primary peak and a number of smaller trailing peaks. In the parabolic case, at each end of the chain, the pulse is given by a Kronecker delta function, while in the middle of the chain the pulse approximates a Gaussian. In the uniform coupling case with an initial Gaussian pulse, it evolves along the chain with fixed profile, and at the ends of the chain interferes and changes direction.

Hence the period of oscillation is $2\pi/J$, which does not depend on the number of cavities $N$. For the coupling profile, we find that the pulse (while more dispersed) is approximately Gaussian shaped in space. This can be seen by examining figure 5.11(b), which shows the pulse profile at fixed instants in time. In comparison, figure 5.11(a) has much higher dispersion, while figure 5.11(c) also has low dispersion, which is largely constant and only reduces slightly as the pulse is reflected at the boundaries of the chain.
5.5 Large detuning limit

We now consider the case where the magnitude of the detuning is much larger than the other energy scales of the system, that is, \( \kappa, \beta \ll |\Delta| \). The effect of increasing detuning is to decrease the atom-photon coupling, thereby approximating a Bose-Hubbard system. We are therefore interested in any non-trivial effects which appear in this limit.

We now shift again to an interaction picture, where states of the system \( |\psi\rangle \) are transformed to

\[
|\xi\rangle = e^{i(\Delta I \otimes Z/2 + \beta I \otimes X)t} |\psi\rangle. 
\]  

(5.29)

Under this shift, the Hamiltonian becomes

\[
H = -\kappa A \otimes \left[ \frac{I + Z}{2} \left( 1 - \frac{2\beta^2}{\Delta^2 + 4\beta^2} \right) + \frac{I - Z}{2} \frac{2\beta^2}{\Delta^2 + 4\beta^2} + \frac{\Delta \beta}{\Delta^2 + 4\beta^2} X \right]. 
\]  

(5.30)

In this equation, the coefficient of \((I+Z)/2\) is related to the speed of the atomic component, and the coefficient of \((I-Z)/2\) is related to the speed of the photonic component. We will discuss the effect of the \(X\) term shortly.

To explore the dynamics of this system, we again start with the equal superposition initial state as given in equation (5.7) (note that this is no longer a single cavity eigenstate, as was the case when \( \Delta = 0 \)). For example, the uniform coupling case with \( \Delta = 10^3 \beta, \kappa = \beta \) is shown in figure 5.12(a). By again comparing to the Heisenberg spin chain Hamiltonian, equation (5.10), we see now that the photonic excitation corresponds to a Heisenberg spin chain with speed \( J = 2\kappa \left[ 1 - 2\beta^2/(4\beta^2 + \Delta^2) \right] \), and the atomic excitation corresponds to a Heisenberg spin chain with speed \( J = 2\kappa \beta^2/(4\beta^2 + \Delta^2) \). In this regime, the atomic and photonic excitations travel at two completely different speeds: the photonic mode travels much faster than the atomic mode, although the integrity of each mode is preserved.

We also can see in figure 5.12 that this splitting of the system into two separate modes happens for both parabolic coupling (b) and an initial Gaussian pulse (c). This splitting is an observation which can be predicted directly from the \( \kappa A \) independent form of the
Figure 5.12: These plots show the evolution of the state $|1\rangle \otimes (|e, 0\rangle + |g, 1\rangle)$ (a) and (b) and a Gaussian pulse (c) in a one-dimensional JCH system consisting of 100 cavities, with $\kappa = \beta$ and $\Delta/\beta = 10^3$. Note the time scales are different in each case. (a) Evolution in a uniform chain, where the dashed lines are a triangle wave giving approximate evolution of the wavefront, as given in equation (5.11). (b) Evolution in a parabolically coupled chain, where the dashed lines are as given in equation (5.28). (c) Evolution in a uniformly coupled chain, with an initial Gaussian pulse, as given in equation (5.26). The dashed lines show the expectation value of position, as given in equation (5.27).
in which we see that it is an effective JC type coupling between neighboring atoms and photons. The effect of this term on the propagating atom and photon chains will be zero at first order as it couples between chains. The second order effect is not zero, as

\[ [X_{j,j+1}, X_{j+1,j+2}] = -(\sigma_j^+ \sigma_{j+2}^- - \sigma_j^+ \sigma_j^- + a_j^+ a_{j+2} - a_{j+2}^+ a_j), \] (5.32)

giving an effective next-nearest-neighbor coupling (assuming the one excitation subspace).

The strength of this correction is given by the square of the \( A \otimes X \) coefficient in equation (5.30) and therefore vanishes as the detuning is increased. In the limit where mixing effects are visible due to this additional term, we also observe asymmetric behaviour with respect to the sign of the detuning, similar to that seen previously in a two cavity system [47]. It should be noted that here, we always initialise the system in an equal superposition of atomic and photonic states, whereas in previous work [47], the detuning asymmetry is accentuated by an initial state which is always an eigenstate of the JC Hamiltonian.

### 5.6 Conclusions

In conclusion, we find that when limited to the one excitation subspace, one can analytically solve for the evolution of the excitation pulse. As such, we extend previous work on the topic [47, 73] from \( N = 2 \) to the many-cavity regime. We observe both localised and delocalised behaviour in this system, which points to a complex interplay between atomic and photonic degrees of freedom, even in the single excitation limit.

We consider three natural limits, and show that the behaviour of the atomic and photonic modes of the JCH chain can be mapped to two independent Heisenberg spin chains. In the limit when the detuning is zero and the inter-cavity coupling is much smaller than the atom-photon coupling, we find that the system is mapped to two Heisenberg spin chains both with \( J = \kappa \). When the detuning is zero but atom-photon coupling is much smaller than inter-cavity coupling, the photonic mode propagates with approximate speed \( J = 2\kappa \).
and the atomic mode does not.

In the limit when the detuning is much larger than both the inter-cavity coupling and the atom-photon coupling, the system is mapped to two Heisenberg spin chains, with $J = 2\kappa[1 - 2\kappa\beta^2/(\Delta^2 + 4\beta^2)]$ for the photonic mode, and $J = 2\kappa\beta^2/(\Delta^2 + 4\beta^2)$ for the atomic mode. We also derive similar analytic solutions for the case of a parabolic variation in inter-cavity coupling, resulting in a Gaussian like wave packet propagation along the chain, as well as an initial Gaussian pulse in a uniform coupled chain.

This theoretical work will potentially be of importance to some of the first experiments done with coupled cavity systems. This chapter has shown that it is possible to predict the time evolution of an arbitrary initial state, with an arbitrary number of cavities: and hence will be very useful in any initial time dependent coupled cavity experiments. The following two chapters focus on extensions to this work: chapter 6 investigates virtual waveguides and beamsplitters in the 1D JCH system, created via the introduction of a time dependent JCH Hamiltonian, and chapter 7 investigates the use of matrix product states for exploring multiple excitations in the 1D JCH system.
5. Time evolution of the 1D JCH Hamiltonian
This chapter will consider complex propagation effects in the one dimensional JCH system through the external control of the detuning profile. A useful way of viewing such propagation in the spatial-temporal plane is in terms of a structure analogous to a waveguide [56] in two spatial dimensions. We term this picture a *virtual waveguide*, and subsequently a *virtual beamsplitter*. This is different to the work of, for example [10], where the physical waveguide is two-dimensional and hence fixed post-fabrication, as in figure 6.1(a). A virtual waveguide has only one spatial dimension, the second dimension is given by time, as shown in figure 6.1(b), as such virtual waveguides may be changed at will. The virtual waveguide is constructed by modifying the detuning profile in a particular way along the chain of cavities. By making the detuning profile a sufficiently deep Gaussian well, the excitation is trapped, and in this way we control the position of the excitation. When

![Figure 6.1](image)

*Figure 6.1: Shows the difference between a normal waveguide (a) and the virtual waveguide (b).*
6. Virtual Waveguides and Beamsplitters in a 1D JCH System

the Gaussian well is moved in time, a complete isomorphism (space-space to space-time) with normal waveguides is made. When two virtual waveguides are brought together, by analogy with normal waveguides, they produce a virtual beamsplitter.

Section 6.1 describes the conversion of the usual one excitation JCH Hamiltonian, describing \( N \) cavities, to a set of equations describing an infinite number of cavities - a continuum model. Section 6.2 describes single virtual waveguides, section 6.3 describes two virtual waveguides and how these can form virtual beamsplitters.

6.1 Conversion from discrete to continuum model

Taking the limit in which there are an infinite number of cavities, a continuum model, is useful because we will have a coupled pair of partial differential equations to solve, which is much less computationally expensive to evolve than a time dependent Hamiltonian for a large number of cavities \( N \), yet still captures the essential physics of the problem.

Recall the one excitation, one-dimensional Jaynes-Cummings-Hubbard (JCH) Hamiltonian, first described in section 2.3.2 [65], equation (2.18), but now with a factor of \( 1/\Delta x \) in the inter-cavity coupling term and a time-varying detuning \( \Delta(t) \)

\[
H_{\text{JCH}}^{1\text{exc}} = \frac{\Delta(t)}{2} I_N \otimes Z + \beta I_N \otimes X - \frac{\kappa}{\Delta x} A \otimes \frac{I_2 + Z}{2}. \tag{6.1}
\]

The inter-cavity coupling term now makes explicit the \( 1/\Delta x \) dependence of \( \kappa \) – the distance between cavities is inversely proportional to the strength of coupling between cavities. This is made explicit as it will be useful in the conversion to a continuum model. In equation (6.1) the detuning \( \Delta(t) \) is the same for every cavity. However, to create a detuning profile, we must allow this to vary with cavity number, equation (6.1) becomes

\[
H_{\text{JCH}}^{1\text{exc}} = \sum_{Q=1}^{N} \frac{\Delta_Q(t)}{2} \text{diag}(e_Q) \otimes Z + \beta I_N \otimes X - \frac{\kappa}{\Delta x} A \otimes \frac{I_2 + Z}{2}, \tag{6.2}
\]

where
\[ e_Q = \{0, 0, \ldots, 0, 1, 0, 0, \ldots, 0\}. \]  
(6.3)

The time dependent Schrödinger equation in general is given by

\[ \mathcal{H}\psi = i\hbar \frac{\partial}{\partial t}\psi, \]  
(6.4)

throughout the rest of this chapter we set \( \hbar = 1 \). In the limit of a the continuum model, the Hamiltonian (6.2) will now be represented by what are effectively infinite dimensional matrices, hence effectively continuous wave functions will be utilised. As such the original discrete wave function will turn into the continuous variant

\[
\begin{pmatrix}
\langle \psi|(|1 \otimes |g, 1) \\
\langle \psi|(|1 \otimes |e, 0) \\
\langle \psi|(|2 \otimes |g, 1) \\
\langle \psi|(|2 \otimes |e, 0) \\
\vdots \\
\langle \psi|(|N \otimes |g, 1) \\
\langle \psi|(|N \otimes |e, 0)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\vdots \\
\psi_p(x - \Delta x, t) \\
\psi_a(x - \Delta x, t) \\
\psi_p(x, t) \\
\psi_p(x, t) \\
\psi_p(x + \Delta x, t) \\
\psi_a(x + \Delta x, t) \\
\vdots
\end{pmatrix},
\]  
(6.5)

where \( \psi_p(x, t) \) and \( \psi_a(x, t) \) are continuous complex functions that represent the wave functions of the photonic and atomic excitations respectively. We take the limit that \( \Delta x \) is small, where these cavities are infinitesimally close to each other. The normalisation condition in the discrete case is \( \langle \psi|\psi \rangle = 1 \) and in the continuous case is

\[ \int_{-\infty}^{\infty} |\psi_p(x, t)|^2 + |\psi_a(x, t)|^2 dx = 1 \quad \forall t. \]  
(6.6)

Let us now consider how each of the terms in equation (6.2) affects our new continuous wave functions. Firstly, \( I_N \) is the identity matrix acting on \( N \) cavities, and as such will transform into an identity operator, i.e.
6. Virtual Waveguides and Beamsplitters in a 1D JCH System

\[ I_N : (\psi_p, \psi_a) \rightarrow (\psi_p, \psi_a). \]  
\[ (6.7) \]

Recall that in general the adjacency matrix \( A \) is given by equation (2.10), and we consider the specific case of a 1D chain, as given in equation (2.11). Also note that \( A \) acts only on the photonic part of the equation. Let us investigate what happens in the continuum cavity limit:

\[
\frac{1}{\Delta x} A |\psi\rangle = \begin{pmatrix}
\ddots & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
\ddots & \ddots & \ddots \\
0 & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
\psi_p(x - \Delta x, t) \\
\psi_p(x, t) \\
\psi_p(x + \Delta x, t) \\
\vdots
\end{pmatrix}
\]
\[ = \frac{1}{\Delta x} \begin{pmatrix}
\psi_p(x - 2\Delta x, t) + \psi_p(x, t) \\
\psi_p(x - \Delta x, t) + \psi_p(x + \Delta x, t) \\
\psi_p(x, t) + \psi_p(x + 2\Delta x, t) \\
\vdots
\end{pmatrix}. \]  
\[ (6.8) \]

Taking a line from the matrix equation above, we have

\[
\frac{1}{\Delta x} A \psi_p(x, t) = \frac{\psi_p(x - \Delta x, t) + \psi_p(x + \Delta x, t)}{\Delta x}. \]  
\[ (6.9) \]

Recall the definition of the second order derivative of a continuous function:

\[
\frac{\partial^2 f(x)}{\partial x^2} = \lim_{\Delta x \to 0} \left[ \frac{f(x + \Delta x) + f(x - \Delta x) - 2f(x)}{\Delta x} \right]. \]  
\[ (6.10) \]

Hence the matrix \( A/\Delta x \), up to a constant, represents the differential operator \( \partial^2/\partial x^2 \). That is,
\[
\frac{1}{\Delta x} A : \psi_p \rightarrow \left( \frac{\partial^2}{\partial x^2} + 2 \right) \psi_p, \quad (6.11)
\]

for the purposes of our qualitative examinations of this system, we choose to ignore the second term above, so that

\[
\frac{1}{\Delta x} A : \psi_p \rightarrow \frac{\partial^2}{\partial x^2} \psi_p. \quad (6.12)
\]

This cannot be justified in general, but in the limits we investigate in this chapter ($\beta \gg \kappa$), this is a perfectly valid approximation.

Finally, the $2 \times 2$ Pauli operators act as

\[
\begin{align*}
X &: (\psi_p, \psi_a) \rightarrow (\psi_a, \psi_p) \\
Z &: (\psi_p, \psi_a) \rightarrow (\psi_p, -\psi_a) \\
\frac{I_2 + Z}{2} &: (\psi_p, \psi_a) \rightarrow (\psi_p, 0)
\end{align*}
\]

and the detuning term becomes

\[
\sum_{Q=1}^{N} \frac{\Delta Q(t)}{2} \text{diag}(\epsilon_Q \otimes Z) : (\psi_p, \psi_a) \rightarrow \frac{\Delta(x, t)}{2} (\psi_p, -\psi_a) \quad (6.14)
\]

where $\Delta(x, t)$ is the continuum limit of the discrete detuning $\Delta_Q(t)$. As such the Schrödinger equation (6.4) for the 1D, one excitation JCH Hamiltonian (6.2) in the continuum limit is given by

\[
\begin{align*}
\frac{i}{\partial t} \psi_p &= \frac{\Delta(x, t)}{2} \psi_p + \beta \psi_a - \kappa \frac{\partial^2}{\partial x^2} \psi_p \quad (6.15a) \\
\frac{i}{\partial t} \psi_a &= -\frac{\Delta(x, t)}{2} \psi_a + \beta \psi_p. \quad (6.15b)
\end{align*}
\]

The detuning profile $\Delta(x, t)$ is now allowed to vary with both cavity space $x$ and time $t$. 
In the limit that \( \kappa \gg \beta \), these equations decouple (by effectively setting \( \beta \) to zero). The atomic excitation no longer evolves (this behaviour is also seen in section 5.2), and the photonic excitation now evolves according to the equation

\[
i \frac{\partial}{\partial t} \psi_p = \Delta(x,t) - \frac{\kappa}{2} \frac{\partial^2}{\partial x^2} \psi_p. \tag{6.16}
\]

If \( \Delta(x,t) = 0 \), this is the freely evolving particle equation (Schrödinger equation with no potential).

In the limit that \( \beta \gg \kappa \) (also discussed in section 5.2), the equations also decouple. The equations become identical (because of the rapid conversion of atomic excitation to photonic excitation, and vice versa), hence the atomic and photonic evolution are identical, as such the subscript of \( \psi \) may be dropped. The \( \kappa \) term remains, despite \( \beta \gg \kappa \), as this facilitates the hopping between cavities. The equation describing this evolution is

\[
i \frac{\partial}{\partial t} \psi = \Delta(x,t) - \frac{\kappa}{2} \frac{\partial^2}{\partial x^2} \psi. \tag{6.17}
\]

The primary difference between equation (6.16) and (6.17) is the factor of two in the final term. This is effectively due to the excitation being shared between two modes in the \( \beta \ll \kappa \) case. The excitation travels at half the speed when \( \kappa \ll \beta \) as to when \( \kappa \gg \beta \) (this is also seen in chapter 5, section 5.2). We use equation (6.17) for the remainder of this chapter.

We choose a Gaussian well as a suitable detuning profile in which to trap single excitations. The general form is given by

\[
\Delta(x,t) = -d \sum_{i=1}^{i_{\text{max}}} \exp\left\{-[x - c_i(t)]^2/(2s^2)\right\} \tag{6.18}
\]

where the number of detuning centres \( i_{\text{max}} \) determines the number of virtual waveguides, and the moving detuning centre(s) are given by \( c_i(t) \). The depth of the potential is \( d \) and the width of the potential is \( s \) (these are both assumed identical for all waveguides).

In each case explored, we assume that the excitation is initially of the Gaussian form.
\[ \psi(x, t = 0) = \frac{1}{\pi^{1/4}\sqrt{w}} e^{i k x} \exp[-(x - x_0)^2/(2w^2)] \]  

(6.19)

where \( w \) is the width of the excitation, \( x_0 \) is the centre of the excitation, \( k \) is the initial momentum, and the wave function has been normalised such that \( \int \vert \psi(x, t) \vert^2 dx = 1 \). We then solve numerically for \( \psi(x, t) \) and display \( \vert \psi(x, t) \vert^2 \). The cavity direction \( x \) is assumed to have periodic boundary conditions. This excitation is usually chosen to initially coincide with the detuning centre, that is, \( x_0 = c_i(0) \) for some \( i \). Particular attention must be paid to the initial position \( x_0 \) and the momentum \( k \), these can be set arbitrarily, and are usually chosen to match the initial position and velocity of the detuning centre.

### 6.2 Single virtual waveguides

Firstly we examine a single virtual waveguide. In each case, we use equation (6.18) with \( i_{\text{max}} = 1 \). We also examine the single waveguide fidelity, a measure of the extent to which the Gaussian wavepacket maintains its shape, which is given by the overlap between the wave function at \( t = 0 \), \( \psi(x, t = 0) \), and at the final time \( t_f \) but shifted back to the original location, \( \psi^*[x - c_1(0) + c_1(t_f), t = t_f] \). It is given by

\[
F = \left| \int_{-\infty}^{\infty} \psi(x, t = 0) \psi^*[x - c_1(0) + c_1(t_f), t = t_f] dx \right|^2,
\]

(6.20)

note that \( 0 \leq F \leq 1 \), when \( F = 1 \) the excitation is perfectly guided.

#### 6.2.1 Stationary virtual waveguide

We first show that the excitation can be confined by a Gaussian detuning profile. In this section the waveguide function is independent of time: the centre of the waveguide remains at the position of the excitation,

\[ c_1(t) = x_0, \]

(6.21)
6. Virtual Waveguides and Beamsplitters in a 1D JCH System

Figure 6.2: The three simulations in (a) show how an excitation can be confined inside a virtual waveguide. (b) The initial states for each of the three simulations, the vertical lines centred around each Gaussian show $c_1(0)$ and $c_1(0)\pm 2w$. In both (a) and (b), (i) represents $d = 0$ (ii) $d = 5$, and (iii) $d = 10$. As the depth of the Gaussian potential increases, as shown in (b) the excitation is increasingly well confined, as shown in (a), when $d = 10$ (iii) the excitation does not spread at all. (c) shows how the fidelity, equation (6.20), of the waveguide increases with $d$, the vertical lines indicate the 3 examples shown in (a) and (b). Note that the fidelity $F$ reaches some maximum at around $d = 25$, perhaps the decline in $F$ after this point is due to breathing modes or the finite size in the cavity direction. In all cases, $s = 1$, $w = 1$, $\kappa = 4$.

and the initial momentum of the excitation is zero, $k = 0$. In figure 6.2(a) (time evolution) and (b) (initial state and potential), the series of plots show three examples with this starting configuration: as the depth of the potential increases [(i) $d = 0$, (ii) $d = 5$, (iii) $d = 10$], the excitation is increasingly confined. Figure 6.2(c) shows that the fidelity, equation (6.20), increases with increasing depth, from $d = 0$ to $d = 20$. The fidelity decreases again after $d \approx 25$, this is perhaps due to breathing modes or the finite size of the simulation in the cavity direction. Regardless, this is a good indicator that the system can indeed form virtual waveguides, indicating the usefulness of the virtual waveguide picture.
6.2.2 Straight virtual waveguide

The next obvious step is to investigate how the excitation may move at constant velocity within this virtual waveguide picture. That is, the centre of the waveguide $c_1(t)$ is given by

$$c_1(t) = x_0 + vt.$$  \hfill (6.22)

One might expect some maximum velocity $v_{\text{max}}$ beyond which the waveguide cannot guide the excitation. However, the initial excitation is prepared as a Gaussian state, equation (6.19), with initial momentum $k$. There is no mathematical restriction on making $k$ as large as one likes - the only restriction here is experimental. As such, $v_{\text{max}}$ is a function of experimental parameters of the system. Mathematically, provided that $v = \kappa k$, the excitation may be guided up to arbitrarily fast speeds, and the fidelity will be independent of $v$.

6.2.3 Virtual waveguide with corner

We now investigate a single virtual waveguide with what would be dubbed in the normal waveguide case a “corner”. The centre of the waveguide is given by

$$c_1(t) = \sqrt{r + m^2(t - t_f/2)^2} + m(t - t_f/2)$$ \hfill (6.23)
Figure 6.4: The waveguide can be made to change the direction of the excitation. The horizontal axis of (b) shows the hardness of the corner in the single waveguide, \( r \), while the vertical axis shows the fidelity of the waveguide, equation (6.20), where \( c_1(t) \) is given by equation (6.23). The white lines show the deepest point of the Gaussian as a function of time, \( c_1(t) \), and the black lines show \( c_1(t) \pm 2w \). As the hardness of the corner softens, the fidelity of the waveguide improves. The vertical lines in (b) indicate the three simulations shown in (a): (i) \( r = 0 \), (ii) \( r = 4 \), and (iii) \( r = 8 \). In all cases, \( m = 4.5 \), \( \kappa = 4 \), and \( t_f = 1 \).

where \( r \) indicates the sharpness of the corner, \( m \) indicates the slope of the waveguide after changing direction, and \( t_f \) is the final time for which we calculate the waveguide. As such the excitation is initially at position

\[
x_0 = c_1(0) = \sqrt{r + (mt_f/2)^2} - mt_f/2.
\]

(6.24)

and the initial momentum of the excitation is zero, \( k = 0 \). Equation (6.23) is also shown graphically in figure 6.3.

Three cases of evolution using equation (6.23) are shown in figure 6.4(a), as \( r \) increases [(i) \( r = 0 \), (ii) \( r = 4 \), (iii) \( r = 8 \)], the waveguide has greater ability to guide the excitation around the corner. Figure 6.4(b) shows how the fidelity, equation (6.20), increases with increasing \( r \), which shows that a virtual waveguide can be made to change the direction of an excitation.
6.3 Two virtual waveguides

Now that one virtual waveguide has been shown to successfully trap and move a single excitation, we show how two virtual waveguides can perform a virtual beamsplitting function on a single excitation. In the following cases we take $i_{\text{max}} = 2$ from equation (6.18).

6.3.1 Virtual beamsplitter with parallel component

We firstly examine a virtual beamsplitter with a parallel component. The centre of the potentials of the left and right waveguides are given by the piecewise continuous function

\[
  c_{\text{right}}(t) = -c_{\text{left}}(t) = \\
  \begin{cases} 
  \sqrt{r + (mt + c - \frac{c}{4})^2} - mt + c + \frac{c}{4} & t < t_f/2 \\
  \sqrt{r + [-m(t - t_f) + c - \frac{c}{4}]^2} & t \geq t_f/2 \\
  +m(t - t_f) + c + \frac{c}{4} \end{cases} 
\]  

(6.25)

where $m$ is the slope and $c$ is the separation between the parallel components of the waveguide, and $r$ is the hardness of the corner. The position of the excitation is initially in the left waveguide, such that

\[
x_0 = c_{\text{left}}(0) = -\left[\sqrt{r + (c - x_l/4)^2} + c + x_l/4\right] 
\]

(6.26)
6. Virtual Waveguides and Beamsplitters in a 1D JCH System

Figure 6.6: When two virtual waveguides form a beamsplitter with a parallel component, typical oscillation behaviour of the photon between the waveguides is observed. The black lines show the deepest point of the Gaussians, \( c_{\text{right}}(t) \) and \( c_{\text{left}}(t) \), as shown in equation \((6.25)\), and the dashed lines show \( c_{\text{right}}(t) \pm 2w \) and \( c_{\text{left}}(t) \pm 2w \). In this evolution, \( \kappa = 4 \), \( r = 0.5 \), \( c = 0.5 \), \( m = 1.5 \), \( w = 1 \), \( s = 1 \), \( d = 10 \).

and the initial momentum is the slope of the left waveguide at time \( t = 0 \), divided by the inter-cavity coupling \( \kappa \), that is

\[
  k = \left. \frac{1}{\kappa} \frac{\partial c_{\text{left}}}{\partial t} \right|_{t=0} = \frac{1}{\kappa} \left[ \frac{-m(x_l/4 - c)}{\sqrt{(x_l/4 - c)^2 + r}} + m \right].
\]

Equation \((6.25)\) is shown graphically in figure 6.5. The results of the simulation are shown in figure 6.6. Note that the excitation, after initially starting in the left waveguide, jumps back and forth between waveguides, before leaving primarily through the left waveguide. This behaviour is important to note, as it informs one of the limits of the beamsplitter in the next section.

6.3.2 50/50 virtual beamsplitter

In this case, we describe two virtual waveguides, performing a beamsplitting type function. The two waveguides behave symmetrically, where

\[
  c_{\text{right}}(t) = -c_{\text{left}}(t) = \sqrt{r + (vt - x_l/2)^2}
\]

(6.28)
and $r$ is a similar measure of the sharpness of the corner as in equation (6.25), $\pm v$ is the initial velocity of the waveguides (set to $\pm \kappa k$), and $x_l$ is the limit in the cavity direction. The initial excitation is placed in the left waveguide, such that

$$x_0 = c_{\text{left}}(0) = -\sqrt{r + (x_l/2)^2}, \quad (6.29)$$

and equation (6.28) is shown graphically in figure 6.7.

The results are shown in figure 6.8. The horizontal axis in (a) shows the momentum $k$, which is both proportional to the velocity of the left waveguide initially (and the negative velocity of the right waveguide), as well as being the initial momentum of the excitation.

Let us first consider the fidelity of the excitation being in the left waveguide, $F_{\text{left}}$, after the excitation has been evolved for $t_f = x_l/(k\kappa)$ [as in equation (6.20)], as shown in figure 6.8(a). When $k$ is small, the waveguides are approaching an almost parallel state. As such, the excitation behaves similarly to the behaviour seen in figure 6.6, where the excitation may jump back and forth between waveguides multiple times. So, there is a large amount of variation for a small change in $k$. When $k$ is large, the waveguides are very sharply crossed - it is energetically favourable for the excitation to quickly jump from the left waveguide to the right waveguide, rather than to turn a very sharp corner to stay in the left waveguide. As such, the fidelity drops to zero (all excitation going into the right waveguide) for large $k$. An example of this is shown in figure 6.8(c).

We now consider the sum of the fidelity for the excitation to be in the left waveguide plus the excitation to be in the right waveguide, $F_{\text{tot}}$, that is,
6. Virtual Waveguides and Beamsplitters in a 1D JCH System

\[ F_{\text{tot}} = F_{\text{left}} + F_{\text{right}} \]
\[
\left| \int_{-\infty}^{\infty} \psi(x, t = 0)\psi^* [x - c_{\text{left}}(0) + c_{\text{left}}(t_f), t = t_f] dx \right|^2 +
\left| \int_{-\infty}^{\infty} \psi(x, t = 0)\psi^* [x - c_{\text{right}}(0) + c_{\text{right}}(t_f), t = t_f] dx \right|^2,
\]

note that \(0 \leq F_{\text{tot}} \leq 1\). In figure 6.8(a), \(F_{\text{tot}}\) is close to one for small \(k\), as the excitation is trapped by one or the other waveguides (determined by examining \(F_{\text{left}}\) and \(F_{\text{right}}\)). \(F_{\text{tot}}\) is also close to one when \(k\) is large: the excitation is entirely trapped by the right waveguide. For moderate values of \(k\), \(F_{\text{tot}}\) is less than 1.

When the excitation, after travelling through the beamsplitter, has achieved a 50/50 split between the two arms, a beamsplitter has been achieved. This is indicated by horizontal and vertical lines in figure 6.8(a), when \(F_{\text{left}} = F_{\text{right}}\), where \(F_{\text{left}}\) is slightly less than 0.5, due to the finite size of the simulations. An example is shown in figure 6.8(b).

6.4 Conclusions

This chapter has shown that a photonic or atomic Gaussian excitation in a very large number of 1D JCH chain can be trapped, and moved by a single virtual waveguide. Consequently a second virtual waveguide may be introduced and a virtual beamsplitter realised. This virtual waveguide is useful because it is analogous to the conventional devices of linear optics, which are enormously useful in many optical devices today. The advantage of the virtual waveguide over the canonical waveguide is that because one dimension is that the temporal dimension can be changed at will. In the next chapter, we investigate matrix product states, which can be used to explore the 1D JCH system with multiple excitations.
Figure 6.8: The excitation is initiated in the left waveguide and then evolved for some time $t_f = x_l / (k \kappa)$ (a) Fidelity of excitation in the left and right waveguides $F_{\text{left}}$ and $F_{\text{right}}$, and also the summation of these, $F_{\text{tot}} = F_{\text{left}} + F_{\text{right}}$, as a function of the log of the wavenumber $k$. (b) An example of the evolution when $k = 10^{-0.7258}$ (corresponding to $F_{\text{left}} = F_{\text{right}}$, indicated by horizontal and vertical lines) - this shows a 50/50 beamsplitter. (c) An example of the evolution when $k = 10^1$, an example where the excitation travels straight from the left to the right waveguide. Note the different time-scales in (b) and (c). The black lines in (b) and (c) show the deepest point of the two Gaussians as a function of time, $c_{\text{left}}(t)$ and $c_{\text{right}}(t)$, as shown in equation (6.28), and the dashed lines show $c_{\text{left}}(t) \pm 2w$ and $c_{\text{left}}(t) \pm 2w$. In all cases, $s = 1$, $w = 1$, $r = 1$, $\kappa = 2$, $d = 10$. 
6. **Virtual Waveguides and Beamsplitters in a 1D JCH System**
In this chapter we show that matrix product states (MPS) are a useful framework for exploring JCH physics. In particular they are a powerful technique to explore the physics of multiple excitations in the JCH model in one spatial dimension. This chapter reviews the MPS formalism based on references [106, 107, 108] and describes the application to the JCH model.

Matrix product states are a way of representing a quantum mechanical wave function for a many body system under an entanglement truncation scheme [106]. For a one-dimensional system (where a number of identical systems are arranged in a line), this is a very efficient method of approximately representing a state, and usually the amount by which entanglement is truncated is only very small. Time evolution on an MPS can be carried out where the computational cost grows linearly with the number of systems [107]. It is also efficient to determine the expectation value of an operator, especially a single-site operator [106].

Section 7.1 reviews graphical representations of tensors as well as multiplication style operations between tensors. Section 7.2 shows how to represent an arbitrary wave function as an MPS, and then shows some examples. Section 7.3 demonstrates the efficient method that may be used for finding the expectation value of an operator when a wave function is represented as an MPS, and section 7.4 shows how to perform time evolution using MPS. Finally, in section 7.5 MPS results for the JCH model are shown and discussed.
7. Investigating 1D JCH systems using MPS

7.1 Graphical Representation of Tensors and Tensor Operations

A tensor is a mathematical object: in this context, a grid-like method of storing a sequence of numbers or functions. Specifically, a 0-tensor is more commonly known as a scalar, a 1-tensor as a vector, and a 2-tensor as a matrix. There is no common name for a \( n \)-dimensional tensor, or \( n \)-tensor, where \( n \geq 3 \).

A tensor network is a set of tensors in an arrangement whereby they can be multiplied together. An MPS is a tensor network. The normal algebraic notation of representing a tensor network is not always intuitive: instead we review the graphical method for representing tensors and tensor networks.

Some conventional algebraic representations are, for example, \( x \) for a 0-tensor, \( v_i \) for a 1-tensor, \( A_{ij} \) for a 2-tensor, or \( T_{ijk} \) for a 3-tensor. However, these representations becomes cumbersome when the number of dimensions \( n \) is large. A graphical representation of a \( n \)-tensor is a circle with \( n \) “legs”. In table 7.1 we show in a succinct form both algebraic and graphical representations of tensors of order 0, 1, 2, 3 and \( n \). It is also important to label the sizes (the \( i \)th leg is in general labelled by \( |i| \)) of the \( n \) indices associated with each \( n \)-tensor.

<table>
<thead>
<tr>
<th>Tensor</th>
<th>Common name</th>
<th>Algebraic rep.</th>
<th>Dimensions</th>
<th>Graphical rep.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-tensor</td>
<td>scalar</td>
<td>( x )</td>
<td>-</td>
<td>( x )</td>
</tr>
<tr>
<td>1-tensor</td>
<td>vector</td>
<td>( v_i )</td>
<td>( i = 1, 2, \ldots,</td>
<td>i</td>
</tr>
<tr>
<td>2-tensor</td>
<td>matrix</td>
<td>( A_{ij} )</td>
<td>( i = 1, 2, \ldots,</td>
<td>i</td>
</tr>
<tr>
<td>3-tensor</td>
<td>-</td>
<td>( T_{ijk} )</td>
<td>( i = 1, 2, \ldots,</td>
<td>i</td>
</tr>
<tr>
<td>( n )-tensor</td>
<td>-</td>
<td>( T_{a_1a_2\ldots a_n} )</td>
<td>( a_i = 1, 2, \ldots,</td>
<td>a_i</td>
</tr>
</tbody>
</table>

Table 7.1: Graphical and algebraic representations of tensors.

One of the simplest tensor operations is to flatten a tensor: flatten requires only a single tensor, and reduces an \( n \)-tensor to an \( m \)-tensor, where \( m < n \). This rearranges the elements
held inside the tensor into a new order. For example, a matrix may be flattened into a
vector by systematically rearranging the grid of numbers into a column of numbers. One
way of doing this is to stack each column from the matrix into one long vector. Flattening
a matrix into a vector is represented graphically by

\[
\begin{array}{c}
A \quad |i| \\
|j| \\
\end{array}
= \quad \begin{array}{c}
v \quad |ij| \\
\end{array}
\]

Multiplying an \( n \)-tensor by an \( m \)-tensor is possible, provided that certain conditions have
been met. The case \( n = m = 2 \) is the usual matrix multiplication. In algebraic notation
matrix multiplication between the \( f \times g \) matrix \( A \) and the \( g \times h \) matrix \( B \) is

\[
M = AB, \quad M_{ij} = \sum_{k=1}^{[k]} A_{ik} B_{kj}, \quad i = 1, 2, \ldots, [i], \quad j = 1, 2, \ldots, [j].
\] (7.1)

For this operation to be valid, the size of the second dimension of the first matrix must
equal the size of the first dimension of the second matrix. Matrix multiplication is repre-
sented graphically as

\[
\begin{array}{c}
A \quad |i| \\
\quad |k| \\
|j| \\
\end{array}
\begin{array}{c}
B \quad |i| \\
\quad |j| \\
\end{array}
= \begin{array}{c}
M \quad |i| \\
\quad |j| \\
\end{array}
\]

where the multiplication process is achieved graphically by contracting the appropriate
legs (labelled as \(|k|\)) together. The condition for valid tensor multiplication in general is
that for any two legs to be contracted together, they must have equal dimension. The
order of the resultant tensor is determined by the number of free legs. The graphical
representation of matrix multiplication may be expanded to an arbitrary tensor network.
A more complicated example of tensor multiplication, this time involving two 3-tensors,
\( A \) and \( C \), and two 2-tensors, \( B \) and \( D \), is given algebraically by
7. Investigating 1D JCH systems using MPS

\[
\sum_{m=1}^{\bar{m}} \sum_{l=1}^{\bar{l}} \sum_{k=1}^{\bar{k}} \sum_{j=1}^{\bar{j}} A_{ijk} B_{jl} C_{klm} D_{mn} = E_{in} \quad (7.2)
\]

\[i = 1, \ldots, |i|, \quad n = 1, \ldots, |n|\]

which is represented graphically by

This graphical notation has been introduced as it significantly simplifies the representation of MPS states, as well as finding expectation values and time evolution. We now investigate representing a wave function as an MPS.

7.2 Representing a wave function as an MPS

Here we describe how a many-body wave function may be represented as a matrix product state. Consider the wave function of \(N\) \(d\)-dimensional states

\[
|\psi\rangle = \sum_{i_1=1}^{d} \cdots \sum_{i_n=1}^{d} c_{i_1 \ldots i_n} |i_1\rangle \otimes \cdots \otimes |i_N\rangle, \quad (7.3)
\]

where \(|i_N\rangle = |1\rangle, |2\rangle, \ldots |d\rangle\). The tensor \(c_{i_1 i_2 \ldots i_N}\) is a set of \(d^N\) complex numbers. It can be represented algebraically as

\[
c_{i_1 i_2 \ldots i_N} = \sum_{\alpha_1, \ldots, \alpha_{N-1}}^{\chi} \Gamma_{\alpha_1}^{[i_1]} \lambda_{\alpha_1}^{[1]} \Gamma_{\alpha_1 \alpha_2}^{[i_2]} \lambda_{\alpha_2}^{[2]} \cdots \Gamma_{\alpha_{N-1}}^{[N]|i_N} \quad (7.4)
\]

where the tensors \(\Gamma^{[i]}\) represent the state of the \(i\)th site, and the matrices \(\lambda^{[i]}\) represent the entanglement between the left (sites 1 to \(i\)) and right (sites \(i+1\) to \(N\)) segments of
the chain. The tensor $c_{i_1i_2...i_N}$ is shown graphically as

$$
\begin{align*}
\Gamma^{[1]} & \quad \chi \quad \Gamma^{[2]} \quad \chi \quad \cdots \quad \chi \\
\quad d & \quad \quad d & \quad \quad d \\
\end{align*}
$$

The positive integer parameter $\chi$ quantifies the amount of entanglement that can be represented in the system: it is called the Schmidt rank or Schmidt number [70]. To fully represent a completely arbitrary state, $\chi$ must be a very large number. The approximation of the MPS state comes in by truncating $\chi$. This is discussed further in section 7.5.

In the case of a pure state of only 2 sites, there is effectively only one class of entanglement, called concurrence [114]. For the pure state of 3 sites, there are two unique classes of entanglement which can be differentiated by the 3-tangle [23]. For the pure state of 4 sites it is still unknown how many unique classes of entanglement there are [105, 57, 58, 75, 76]. Finally, for the pure state of 5 or more sites there are an infinite number of classes of entanglement, which are all valid, and all unique. The entanglement parameter $\chi$, the Schmidt rank, is the one used for MPS as it conveniently parametrises the entanglement between neighbouring sites of a one dimensional many-body quantum system, which arises because MPS is a Schmidt decomposition of a full wave function [106].

### 7.2.1 Examples of wave functions represented using MPS

Here we show some examples to demonstrate how to represent some common states using MPS. These examples utilise some important JCH states, to further enhance the connection between MPS and JCH. For all examples, we assume that the basis on each site is truncated to only three possible states: $|g, 0\rangle$, $|e, 0\rangle$, and $|g, 1\rangle$. We will show that the entanglement parameter $\chi$ is 1 for a product state and 2 for a GHZ state.

#### Product state

A product state is any state that is not an entangled state: a trivial example of a product state is $|0\rangle \otimes |0\rangle \otimes \ldots \otimes |0\rangle = |0\rangle^\otimes N$ for $N$ sites. A state where the first cavity is in the
7. Investigating 1D JCH systems using MPS

positive dressed state for zero detuning $\Delta = 0$, that is $|+, 1\rangle$, and the rest of the cavities are unexcited is

$$\frac{|\epsilon, 0\rangle + |g, 1\rangle}{\sqrt{2}} \otimes |g, 0\rangle \otimes (N-1).$$ (7.5)

This state is used extensively as an initial state in chapter 5 on time evolution.

The $N$-tensor $c$ from equation (7.4) representing the state (7.5) has two non-zero values: $c_{21...1} = c_{31...1} = 1/\sqrt{2}$. This can be represented as an MPS by

$$\Gamma_{1, |g, 0\rangle} = \left(0\right), \Gamma_{1, |e, 0\rangle} = \Gamma_{1, |g, 1\rangle} = \left(1/ \sqrt{2}\right)$$ (7.6a)

$$\Gamma_{i, |g, 0\rangle} = \left(1\right), \Gamma_{i, |e, 0\rangle} = \Gamma_{i, |g, 1\rangle} = \left(0\right), i = 2, \ldots, N$$ (7.6b)

$$\lambda_1 = \left(1\right), i = 1, \ldots, N - 1$$ (7.6c)

One can check that this MPS indeed recovers the product state shown above, by multiplying through the $\Gamma$ and $\lambda$ tensors until the $c$ tensor described above is recovered. Also note that the entanglement parameter is $\chi = 1$ for all $N$ (because $\lambda_i$ is a $1 \times 1$ matrix). This is the smallest non-zero value of $\chi$, which is the smallest amount of entanglement, consistent with a product state having no entanglement.

GHZ state

The GHZ state is represented as $(|00\ldots 0\rangle + |11\ldots 1\rangle)/\sqrt{2}$. One example of a JCH GHZ state, where the state is in a superposition of two states: every site in the ground state, and every site in the one photon state, is

$$\frac{1}{\sqrt{2}} (|g, 0\rangle \otimes N + |g, 1\rangle \otimes N).$$ (7.7)
The $N$-tensor $c$ from equation (7.4) has only 2 non-zero values: $c_{11..1} = c_{33..3} = 1$. For $N$ sites this is represented by an MPS as

$$
\Gamma_{i,|g,0\rangle} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_{i,|e,0\rangle} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_{i,|g,1\rangle} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad i = 2, \ldots, N-1
$$

(7.8a)

$$
\Gamma_{i,|g,0\rangle} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_{i,|e,0\rangle} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_{i,|g,1\rangle} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad i = 2, \ldots, N-1
$$

(7.8b)

$$
\Gamma_{N,|g,0\rangle} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_{N,|e,0\rangle} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Gamma_{N,|g,1\rangle} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
$$

(7.8c)

$$
\lambda_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad i = 1, \ldots, N
$$

(7.8d)

As such $\chi = 2$ for all $N$ (because $\lambda_i$ is a $2\times2$ matrix), corresponding to a small but non-zero amount of entanglement.

### 7.3 Efficient calculation of the expectation value of an operator using MPS

Finding the expectation value of some operator $s$, that is, $\langle s \rangle = \langle \psi | s | \psi \rangle$, is a fundamental mathematical operation required for many aspects of quantum mechanics. This operation is highly efficient when we assume a single site operator: that is, assume that the operator $s$ is a single site operator acting on site number $i$, that is, $I^\otimes(i-1) \otimes s \otimes I^\otimes(N-i)$. Using MPS in one dimension, one can calculate this scalar quantity very efficiently. In general it is represented graphically by
The algebraic representation in this case is significantly more complicated than the graphical representation, and does not show any new information, so will not be shown here. The above tensor network is a graphical representation of \( \langle I \otimes (i-1) \otimes s \otimes I \otimes (N-i) \rangle \), the expectation value of the operator \( s \) acting on the \( i \)th site. Note that there are no free legs, and as such the above tensor network represents a scalar quantity. In the above form, this tensor network must be contracted over \( 3N - 1 \) different legs. The computational difficulty in contracting this tensor network to a scalar is proportional to the number of legs which must be contracted. It is possible to show (but will not be shown here) that for an MPS in the canonical form \([106]\), the above tensor network is exactly equivalent to

which requires only 8 leg contractions - this is a great increase in computational efficiency, especially for long chains. This idea is easily extended to operators which act on two (or more) separate sites, where the number of leg contractions required to calculate the expectation value increases with the number of vacant sites between the two sites of interest.
7.4 Time evolution using MPS

In this section we show how time evolution can be performed efficiently on an MPS. Time evolution is efficient provided that the Hamiltonian can be separated into a sum over single site Hamiltonians $H^{(1)}_n$, and joint nearest-neighbour Hamiltonians $H^{(2)}_{n,n+1}$, i.e.

$$H = \sum_{n=1}^{N} H^{(1)}_n + \sum_{n=1}^{N-1} H^{(2)}_{n,n+1}. \quad (7.9)$$

For example, the JCH Hamiltonian, equation (2.9), in one spatial dimension with hard wall boundary conditions can be written this way. Here, the single site Hamiltonian is the JC Hamiltonian, equation (2.1), minus the chemical potential term,

$$H^{(1)}_n = H^{JC}_n - \mu (a_n^\dagger a_n + \sigma_n^+ \sigma_n^-), \quad (7.10)$$

and the nearest-neighbour Hamiltonian is the inter-cavity coupling,

$$H^{(2)}_{n,n+1} = -\kappa (a_n^\dagger a_{n+1} + a_n a_{n+1}^\dagger). \quad (7.11)$$

We now rearrange the terms of the Hamiltonian to suit time evolution of an MPS. Equation (7.9) can be rewritten as

$$H = \sum_{n=1}^{N} H'_n \quad (7.12)$$

where $H'_n$ is composed of the Hamiltonian of site $n$, site $n+1$, and the joint Hamiltonian which acts on both site $n$ and site $n+1$, with special scaling for the ends of the chain, i.e.

$$H'_n = \begin{cases} H^{(1)}_1 + \frac{H^{(1)}_2}{2} + H^{(2)}_{n,n+1} & n = 1 \\ \frac{H^{(1)}_n + H^{(1)}_{n+1}}{2} + H^{(2)}_{n,n+1} & n = 2, \ldots, N - 1 \\ \frac{H^{(1)}_{N-1}}{2} + H^{(1)}_N + H^{(2)}_{n,n+1} & n = N. \end{cases} \quad (7.13)$$

We now rearrange the normal time evolution operator (assuming that the Hamiltonian is
in such a way as to suit the MPS explicitly. We do this by utilising the first order Suzuki-Trotter expansion \([93, 97, 98]\)

\[
\exp(A + B) = \lim_{m \to \infty} (\exp(A/m) \exp(B/m))^m
\]

and hence we have the approximation

\[
\exp(A + B) \approx (\exp(A/m) \exp(B/m))^m.
\]

So, in the case \(m = 1\), the time evolution operator \(G(t)\), equation (7.14), becomes

\[
G(t) = \exp(-it\mathcal{H}) = \exp\left[-it \left( \sum_{n \text{ odd}} \mathcal{H}'_n + \sum_{n \text{ even}} \mathcal{H}'_n \right) \right] \quad (7.17a)
\]

\[
\approx \prod_{n \text{ odd}} \exp(-it\mathcal{H}'_n) \prod_{n \text{ even}} \exp(-it\mathcal{H}'_n) \quad (7.17b)
\]

\[
= \prod_{n \text{ odd}} G_n \prod_{n \text{ even}} G_n, \quad (7.17c)
\]

where \(G_n = e^{-it\mathcal{H}'_n}\). The time evolved state \(|\psi(t + \delta t)\rangle\) is given by \(G(\delta t)|\psi(t)\rangle\). Assuming that \(m = 1\), this can now be performed in two steps: an even step, the result of applying \(\prod_{n \text{ even}} G_n\), and an odd step, the result of applying \(\prod_{n \text{ odd}} G_n\). In our code we utilise the fourth order Suzuki-Trotter expansion, this means that the even and odd steps (with different sizes of \(\delta t\)) are repeated sequentially 18 times per time step. We use the graphical representation to show the even step for \(m = 1\) first,
where this diagram assumes that \( N \) is odd. At this point, we no longer have a tensor network in the MPS form, consisting of \( \lambda \)s and \( \Gamma \)s. We must return this tensor network to MPS form, ready for the odd step. To do this, we firstly contract parts of the tensor network to form a tensor network composed of \((N-1)/2\) tensors labelled \( \Theta \), and one \( \Gamma \) and one \( \lambda \) tensor. Each \( \Theta \) is the result of contracting two \( \Gamma \)s, a \( \lambda \) and a \( G \) into a 4-tensor, and then flattening the result into a 2-tensor. The result is a collection of tensors:

We then perform a singular value decomposition* on the \( \Theta \) tensors to turn them into three separate tensors, so that ultimately the entire tensor network will again be in MPS form.

The singular value decomposition is performed on each \( \Theta \) tensor as follows:

where the central three tensors are the result of the singular value decomposition, and the two outer \( \lambda \) tensors needed for normalisation. As such we return to the MPS form, and are now ready to perform the odd step.

---

*The singular value decomposition decomposes a single matrix \( X \) into three matrices such that \( X = USV^\dagger \), where \( S \) is a diagonal matrix containing only real elements, and \( U \) and \( V \) are unitary matrices.
and corresponding singular value decomposition. After this has taken place we are now left with a new wave function $|\psi(t = t + \delta t)\rangle$. Continuing this process of applying even and odd steps successively according to the Suzuki-Trotter expansion for each time step, produces the time evolved state at some arbitrary time $t$.

### 7.4.1 Finding the ground state

MPS may also be used for finding the ground state of a system. The ground state is obtained by evolving an arbitrary state in imaginary time for a sufficiently long period of time. By making the time imaginary, the exponential in the time evolution operator becomes real rather than imaginary. Consider a quantum system (without loss of generality) that has only two states: the ground state $|0\rangle$ with energy zero and the first excited state $|1\rangle$ with energy $E_1$. An arbitrary superposition of these is

$$|\psi\rangle = \sin \theta |0\rangle + e^{i\phi} \cos \theta |1\rangle$$  \hspace{1cm} (7.18)

We then time evolve the system in imaginary time $\tau = it$.

$$|\psi(t = -i\tau)\rangle = e^{-iHt}|\psi\rangle = e^{-H\tau}|\psi\rangle = \sin \theta |0\rangle + e^{-E_1\tau}e^{i\phi} \cos \theta |1\rangle$$  \hspace{1cm} (7.19)

As such, in the limit as $\tau \to \infty$

$$\lim_{\tau \to \infty} |\psi(\tau)\rangle = \sin \theta |0\rangle$$  \hspace{1cm} (7.20)
which after appropriate normalisation to remove the factor of $\sin \theta$, is the ground state. This can be extended to systems with more than 2 states, and where the ground state energy is not zero (as all excited states will decay faster than the ground state). Unfortunately, MPS is not a good method for obtaining a phase diagram of the JCH system, because as one approaches the phase boundaries, the code runs increasingly slowly. However, MPS is an excellent method performing time evolution and the expectation value of single-site operators. As such, we show results for the JCH model below.

### 7.5 MPS results with the JCH model

Using MPS to represent a wave function, evaluate expectation values, and perform time evolution, is ideally suited to a one-dimensional JCH system. We now discuss examples for one, two and three excitations in this system. The purpose of this is not to do an exhaustive study of the behaviour of multiple excitations in the JCH system, but rather to show that MPS can be a useful tool for such an investigation. We discuss the minimum value of $\chi$ needed for a good approximation to each system, according to the number of excitations in the examples shown\(^\dagger\). We also show how, when colliding two excitations,

---

\(^\dagger\)The MPS code is written such that only $\chi \geq 2$ is valid.
7. Investigating 1D JCH systems using MPS

Figure 7.2: Time evolution of the initial two excitation state $|+, 1\rangle \otimes |g, 0\rangle_{18} \otimes |+, 1\rangle$, for (a) $\chi = 2$ and (b) $\chi = 3$, in both cases $\kappa/\beta = 0.01$. In this regime the atomic and photonic evolution is identical and hence only one of these is shown. Note that when the time is less than about $10/\kappa$, evolution in (a) and (b) are identical - as it is effectively two single excitations which are not interacting, and are not entangled. After this point however the evolution is different in the two plots. Note that around the (imaginary) central horizontal line, the evolution is (a) asymmetric and (b) symmetric. This is another indicator that (b) is physical and (a) is not.

the population of the $|g, 2\rangle$ state (two photons in one cavity) in the system changes as a function of $\Delta/\beta$, according to the phase of the system.

Firstly, we explore the evolution of a single excitation: the initial state $|+, 1\rangle \otimes |g, 0\rangle_{19}$ for a twenty cavity system is evolved and shown in figure 7.1. In this example, the single excitation starts in the first cavity, then evolves along the line of cavities and eventually reflected off the opposite end. This is very similar to the evolution shown in figure 5.1(a) and (b) of chapter 5 except that this evolution is performed for only 20 cavities, and was used as a test of MPS, whereas the calculation in chapter 5 was performed for 100 cavities. Note that in this case, (and in both of the following examples for 2 and 3 excitations), $\kappa/\beta = 0.1$, in this regime (the regime of $\kappa/\beta \ll 1$, as discussed in chapter 5) the atomic and photonic evolution is identical and hence in figure 7.1 only one of these evolutions is shown. Note that in this case, (and in both of the following examples for 2 and 3 excitations), $\kappa/\beta = 0.1$, in this regime (the regime of $\kappa/\beta \ll 1$, as discussed in chapter 5) the atomic and photonic evolution is identical and hence in figure 7.1 only one of these evolutions is shown.

In this example, a $\chi$ of 2 is sufficient to provide a good approximation: increasing $\chi$ to 3 or more does not improve the approximation. Differences between evolutions generated with different $\chi$ can be explored by $D_{m,n}$, the mod square of the difference in photonic
Figure 7.3: The difference between the evolutions for a two excitation example as shown in figure 7.2 for $D_{3,2}$ (solid), and $D_{4,3}$ (dashed). The difference $D_{m,n}$ is shown in equation (7.21). The evolution is identical until a time of about $10/k$, when the two excitations collide (see also figure 7.2). Note that evolution for $\chi = 4$ has not been shown in figure 7.2, as it is identical to that of $\chi = 3$.

expectation values (photonic is chosen arbitrarily over atomic, as they are equivalent in the examples shown) for the evolution with a $\chi$ of $m$ and a $\chi$ of $n$. $D_{m,n}$ is

$$D_{m,n} = \left| \left\langle \sum_{i=1}^{N} a_i^\dagger a_i|\chi=m\rangle - \left\langle \sum_{i=1}^{N} a_i^\dagger a_i|\chi=n\rangle \right\rangle \right|^2.$$  \hfill (7.21)

Note that $D_{m,n} = D_{n,m}$. For the initial state $|+,1\rangle \otimes |g,0\rangle^{\otimes 19}$, $D(t)_{m,2} = 0$, for all $m \geq 3$: a $\chi$ of 2 is sufficient to describe the evolution of the system.

An example of two excitation evolution, where the state is initialised with a positive dressed start in the first and last cavities, and the ground state in every other cavity, i.e. $|+,1\rangle \otimes |g,0\rangle^{\otimes 18} \otimes |+,1\rangle$, is displayed in figure 7.2. Two excitations, initiated as positive dressed states on either end of the chain, approach each other until colliding at about a time of $10/k$. Figure 7.2(a) shows evolution with $\chi = 2$ and 7.2(b), $\chi = 3$. Figure 7.3 shows the difference between evolutions $D_{3,2}$ and $D_{4,3}$, as shown in equation (7.21). One can see, either by comparing figure 7.2 (a) and (b), or by considering $D_{3,2}$ in figure 7.3, that the evolution of the two plots is the same until about a time of $10/k$, when the two excitations collide. This equivalence of the results shows that the dynamics are effectively the product of two single-particle states, which is described effectively by $\chi = 2$. 

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Figure 7.4: Time evolution of the initial three excitation state $|+, 1\rangle \otimes |g, 0\rangle \otimes |+, 1\rangle \otimes |g, 0\rangle \otimes |+, 1\rangle$, for (a) $\chi = 2$ and (b) $\chi = 3$ (c) $\chi = 4$. Note that $\kappa/\beta = 0.01$; in this regime the atomic and photonic evolution is identical and hence only one of these is shown. Note that when the time is less than about $6/\kappa$, evolution between the three plots is identical - as it is effectively three single excitations which are not interacting. After this point however the evolution is different in the three plots.

as discussed previously. Also note that the evolution up to a time of $10/\kappa$ of the excitation that is initially in the first cavity is identical to the evolution shown in the single excitation evolution of figure 7.1. For this evolution, initiated as a product state, $D(t)_{m,3} = 0$, for all $m \geq 4$: a $\chi$ of 3 is sufficient to describe the evolution of the system.

Three excitation evolution for the initial state $|+, 1\rangle \otimes |g, 0\rangle \otimes |+, 1\rangle \otimes |g, 0\rangle \otimes |+, 1\rangle$, for a 21 cavity system (changed from the 20 cavity systems of the previous two examples to aid symmetry) is shown in figure 7.4. Three excitations evolve separately: two beginning
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Figure 7.5: The difference between the evolutions for a 3 excitation example as shown in figure 7.4 for $D_{3,2}$ (solid), $D_{4,3}$ (dashed), and $D_{5,4}$ (dot-dashed). The difference $D_{m,n}$ is shown in equation (7.21). The evolution in all three cases is identical until the excitations collide at about $6/\kappa$. Further, the evolution for $\chi = 3$ and $\chi = 4$ is identical until three excitation evolution becomes important at about $17/\kappa$. Note that evolution for $\chi = 5$ has not been shown in figure 7.4, as it is identical to that of $\chi = 4$.

from either end of the chain, and one from the centre of the chain, eventually colliding at a time of about $6/\kappa$. Part (a) of the figure displays evolution using $\chi = 2$, part (b) $\chi = 3$, and part (c) $\chi = 4$. Figure 7.5 shows the difference between evolutions $D_{3,2}$, $D_{4,3}$ and $D_{5,4}$, as shown in equation (7.21). One can see, either by comparing figure 7.4 (a), (b) and (c), or by considering figure 7.5 that the evolution is identical for the three plots regardless of $\chi$ until about a time of $6/\kappa$, the time at which the excitations collide. By considering $D_{4,3}$ in figure 7.5, it appears as though true 3 excitation behaviour doesn’t occur until a time of about $17/\kappa$, perhaps 3 excitations do not exist on the same site before then due to the blockade effect. For this evolution, initiated as a product state, $D(t)_{m,4} = 0$, for all $m \geq 5$: a $\chi$ of 4 is sufficient to describe the evolution of the system.

We have shown above three examples of JCH evolution, for one, two and three excitations using MPS. We find that for the initial product states used, a $\chi$ equivalent to the number of excitations is sufficient to simulate the evolution.

We also consider how the interaction between two colliding excitations changes by increasing the detuning $\Delta/\beta$ away from the photonic blockade regime. We show two examples in figure 7.6(a) and (b) of evolution from the initial state $|+\rangle \otimes |g,0\rangle \otimes |+\rangle$ with $\kappa/\beta = 0.01$. Parts (a) and (b) are each separately the result of a single simulation, the five
plots show the expectation values of the five operators: $1 - |g, 0⟩⟨g, 0|$, $|e, 0⟩⟨e, 0|$, $|g, 1⟩⟨g, 1|$, $|e, 1⟩⟨e, 1|$ and $|g, 2⟩⟨g, 2|$ for each site. The entanglement parameter $\chi$ is set to 3, which we know to be sufficient due to our earlier work as shown in figures 7.2 and 7.3. Figure 7.6(a) has $\Delta/\beta = 0$, which is in the photonic blockade regime, and (b) has $\Delta/\beta = 35$, which is not in the photonic blockade regime. When $\Delta/\beta = 0$, the positive dressed state $|+, 1⟩$ is an equal superposition of atomic and photonic excitations, $(|g, 1⟩ + |e, 0⟩)/\sqrt{2}$; when $\Delta/\beta = 35$, the positive dressed state $|+, 1⟩$ is approximately a photonic excitation, $|g, 1⟩$: these changes in the initial state of the excitation are reflected in the plots. Figure 7.6(c) shows the maximum quantity in the $|g, 2⟩$ state (summed over all 20 cavities) as a function of the detuning $\Delta/\beta$. The quantity shown on the vertical axis is given by the maximum value in time of the sum over the expectation value of the $|g, 2⟩$ states in all 20 cavities:

$$\max \left( \sum_{Q=1}^{N=20} ⟨\psi(t)|I^\otimes(Q-1) \otimes |g, 2⟩⟨g, 2| \otimes I^\otimes(N-Q)|\psi(t)⟩|t = 0, \delta t, 2\delta t, \ldots, t_{\max} \right). \quad (7.22)$$

Figure 7.6(c) shows that in the photonic blockade regime, when $\Delta/\beta$ is small, the two excitations cannot interact, and as such the system never experiences two photons in one cavity. As $\Delta/\beta$ increases, the system leaves the photonic blockade regime, where the two excitations may interact, and $|g, 2⟩$ is occupied.

### 7.6 Conclusions

Matrix product states are an efficient way of representing a wave function of a one-dimensional system: in particular this is amenable to the JCH system in one dimension. MPS can not only represent a wave function efficiently, but also find expectation values, perform time evolution, and find the ground state. Further study of the behaviour of two or more excitations in a one-dimensional JCH system should prove a fruitful area of study, one that MPS would be ideally suited to, as demonstrated by the successful application of time evolution to two and three excitations in figures 7.2, 7.4, and 7.6. In particular,
figure 7.6 shows how the behaviour of two excitations colliding changes as a function of the detuning. Another possibility is to investigate systems with time dependent potentials, which could actively control the location of one or more excitations - an alternative method to the infinite cavity case explored in chapter 6.
Figure 7.6: Evolution of the initial state $|+,1\rangle \otimes |g,0\rangle^{\otimes 18} \otimes |+,1\rangle$ for (a) $\Delta/\beta = 0$ and (b) $\Delta/\beta = 35$. Part (a) [(b)] is the result of a single simulation, the five plots show the expectation values of the five operators: $1 - |g,0\rangle\langle g,0|$, $|e,0\rangle\langle e,0|$, $|g,1\rangle\langle g,1|$, $|e,1\rangle\langle e,1|$ and $|g,2\rangle\langle g,2|$ for each site. In the case $\Delta/\beta = 0$, (a), the parameters place the system in the photonic blockade regime, as such two photons do not enter the same cavity when the two excitations meet (there are no excitations in the $|g,2\rangle$ state). In the case $\Delta/\beta = 35$, (b), the parameters place the system outside the photonic blockade regime, as such the two excitations do enter the same cavity when they meet, that is, the $|g,2\rangle$ state, albeit briefly, is occupied. (c) shows that as $\Delta/\beta$ increases and the system leaves the photonic blockade regime, the fraction of the excitations that achieve the $|g,2\rangle$ state (two photons in one cavity) increases. The vertical axis on this plot shows the maximum quantity in the $|g,2\rangle$ state, as shown in equation (7.22).
This thesis has investigated a variety of implications of the Jaynes-Cummings-Hubbard (JCH) model. The JCH model hides an astounding variety of physical effects. Here, we have studied phase diagrams and a theoretical investigation of a possible experimental verification of these, time evolution of a 1D JCH for both uniform detuning as well as a Gaussian detuning profile, and also investigated time evolution using matrix product states. Quantum phase transitions in the related Bose-Hubbard model have been predicted by Fisher et al. [25] and demonstrated by Greiner et al. [35]. We anticipate that our theoretical work will lead to future experimental verification of properties of the JCH, some examples of the many promising experimental systems have been discussed in section 2.4.

The phase diagram of the JCH in the ground state consists of two types of phases: Mott-insulator phases and superfluid phases. These phases are investigated in chapter 3 using both exact diagonalisation and perturbation theory techniques in this thesis: these methods are compared to the existing work performed using the mean-field approximation. In chapter 4 we focus on a different, but related form of phase diagram, which with a sufficiently controllable ion trap system (based on phonons rather than photons) be made manifest.

Time evolution of the 1D JCH system, even in the restriction of one excitation, shows a rich variety of physical properties, as explored in chapter 5. In certain limits, the evolution of the 1D JCH chain can be mapped to evolution of a 1D Heisenberg spin chain. Time evolution may also be explored using matrix product states, and this method is compared in chapter 7 with the analytic techniques of chapter 5.
Coupled cavity arrays can be used to realise all of the physics of planar waveguides, we have shown this by demonstrating the fundamental elements of virtual waveguides and virtual beamsplitters in the one excitation limit in chapter 6. Virtual waveguides are made by constructing a Gaussian detuning profile along a chain of JC cavities. This can confine and move a single excitation, which is analogous to a normal two dimensional waveguide, but instead this has only one spatial dimension and one time dimension. Subsequently, virtual beamsplitters may be made by bringing a second virtual waveguide into the vicinity of the first, so that the two waveguides may couple together. These virtual waveguides and virtual beamsplitters are easily modifiable, as the second dimension is time and hence can be manipulated easily, unlike normal waveguides and beamsplitters which are more difficult to modify post-fabrication.

This thesis has shown a variety of results related to the phase diagram and time dynamics of the JCH system. The results of this thesis point to the potential for useful further work on this system. In particular the investigation of two or more excitations in the JCH system will certainly lead to a variety of new effects, already work has been done in this direction by Wong et al. [113]. Two useful methods to investigate multiple excitations are using matrix product states, as outlined in chapter 7, and using the Bethe Ansatz [12]. Investigations using these two methods also leads to the possibility of exploring the statistics of the excitations by realising a two excitation Hong-Ou-Mandel interferometer [43], as well as colliding two excitations, to perform the action of quantum gates. A different avenue of research would be to use the 1D JCH system to investigate the event horizons of black and white holes, as done in reference [79], where excitations travelling at different speeds in a 1D system mimic the behaviour at an event horizon.

A variety of aspects of the JCH model have been investigated in this thesis, and it will continue to be an important area of research in the future. In particular, the phenomena of phase changes of light and time dynamics of few photon systems in the JCH system will be important for a variety of quantum emulators.
References


8. REFERENCES


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