

# **PHASE TRANSITION IN JAYNES-CUMMINGS- HUBBARD MODEL**

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## **CERTIFICATE**

This is to certify that the project work entitled “**Phase Transition in Jaynes – Cummings - Hubbard Model**” is the bonafide work done by **Mr. Muhammed Kutty P.V.**, under my guidance, in partial fulfillment of the requirements for the degree of Master of Philosophy in Physics for the year 2010 – 2011, at the Department of Theoretical Physics, University of Madras, Maraimalai Campus, Chennai – 600025.

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بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

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# Chapter 1

## Introduction:

Phase transitions play an essential role in nature. The universe itself is thought to have passed through several phase transitions as the high temperature plasma formed by the Big Bang cooled to form the world as we see it today. Normally, phase transition occur upon variation of an external control parameter. They occur at finite temperature where the macroscopic order is destroyed by thermal fluctuations.

During recent years, a different kind of phase transition namely, quantum phase transition [1] have attracted the attention of researchers. A non-thermal control parameter such as pressure or magnetic field is varied to access the transition point. Thus, the order is destroyed solely due to quantum fluctuations which are rooted in the Heisenberg uncertainty principle.

Some of the systems, exhibiting quantum phase transitions, which are of recent interest are heavy fermions in Kondo lattices, multi component systems of ultra-cold atoms in optical lattices, the ensemble of two-level atoms interacting with a bosonic mode described by the Dicke model and more recently, the Jaynes–Cummings–Hubbard (JCH) model. In the current thesis we study the Jaynes-Cummings-Hubbard model which is a combination of the two well-known systems (*i*) the Jaynes–Cummings (JC) model and (*ii*) the Bose–Hubbard (BH) model.

(*i*) The JC model describes the coupling of a single two-level system to a bosonic mode. The Hamiltonian describing this model is given by the expression:

$$\hat{H}^{JC} = \omega \sum_j \hat{a}_j^\dagger \hat{a}_j + \Delta \sum_j \hat{\sigma}_j^\dagger \hat{\sigma}_j^- + g \sum_j (\hat{\sigma}_j^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{\sigma}_j^-) \quad (1.1)$$

where,  $\hat{a}^\dagger, (\hat{a})$  is the photonic creation (annihilation) operator and  $\hat{\sigma}^+, (\hat{\sigma}^-)$  is the spin raising (lowering) operator. In Eq. (1.1),  $\omega$  is the cavity resonance frequency,  $\Delta$  is the transition energy of an atom and  $g$  denotes the cavity - mediated atom-photon coupling.

(*ii*) The Bose–Hubbard model describes the interaction and tunneling of bosons on a lattice. The Hamiltonian which describe the system is:

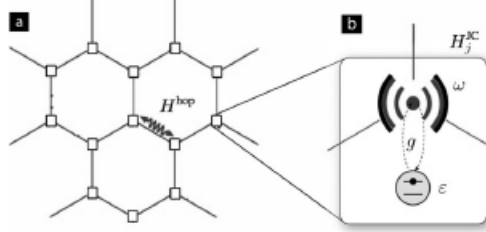


Figure 1.1: Schematic of the Jaynes-Cummings lattice system, consisting of an array of electromagnetic resonators [see (a)], with a coupling between nearest neighbor lattice sites due to photon hopping. Each resonator is coherently coupled to a two-level system shown in (b)

$$H^{BH} = -t \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) + \frac{U}{2} \sum_j \hat{n}_j (\hat{n}_j - 1) \quad (1.2)$$

where,  $\hat{b}^\dagger, (\hat{b})$  is the bosonic creation (annihilation) operator which satisfy the commutation relation  $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$  and  $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$  is the boson number operator. The factor  $t$  is the hopping amplitude. The notation  $\langle i, j \rangle$  implies that the summation is done over  $i$  and  $j$  with the condition that  $i \neq j$ .

The BH model is an extension of the Hubbard model. The Hubbard model, is the simplest model of interacting particles in a lattice, with only two terms in the Hamiltonian; a kinetic term allowing for tunneling (hopping) of particles between sites of the lattice of fermions and a potential term consisting of an on-site interaction. The Hubbard model is a good approximation for particles in a periodic potential at sufficiently low temperatures. When the lattice sites consists of bosons, it is called the Bose-Hubbard model. Recently, the BH model has been used to describe the behavior of ultracold atoms trapped in optical lattices. A combination of these two models (JC and BH) gives the JCH model described by the Hamiltonian

$$\hat{H} = \hat{H}^{JC} + \hat{H}^{hop} \quad (1.3)$$

where  $\hat{H}^{JC}$  is given in Eq. (1.1) and the kinetic term describing the hopping of the photon is

$$\hat{H}^{hop} = \sum_d t_d \sum_j (\hat{a}_j^\dagger \hat{a}_{j+d} + \hat{a}_{j+d}^\dagger \hat{a}_j) \quad (1.4)$$

The Jaynes-Cummings-Hubbard (JCH) model corresponds to a fundamental configuration exhibiting the quantum phase transition of light. In such a model, single two-level atoms are embedded in each cavity, and the dipole interaction leads to dynamics involving photonic and atomic degrees of freedom.

In this thesis we, first focus on various properties of the JCH model and provide two different approximation schemes namely the effective-strong coupling approximation and the fermionic approximation. Under these approximation schemes we obtain the analytical results for the critical hopping amplitude leading to the Mott-insulator [1,2] to the Superfluid [1] transition. Mott insulator is a class of materials that are conductors according to the conventional band theories, but were found to be insulators when measured at low temperatures. Superfluidity is a state of matter in which the matter behaves like a fluid without viscosity and with infinite thermal conductivity. In this work, we show that in the strong interaction limit, and near commensurate filling, approximate analytic solutions of the JCH can be found if there is translational invariance, that is, for an infinite homogenous system or periodic boundary conditions. These solutions give a good analytic approximation to the full ground-state phase diagram. We also apply both the approximation schemes to the simple nearest neighbor JCH model describing an array of coupled cavities and to the special case of a linear ion chain.

The outline of the present thesis is as follows: In the second chapter, the main features of the JCH model have been explained, along with certain other related quantities which have to be used in the subsequent chapters. First of all the eigen values and the eigen vectors of the Hamiltonian is found. Then the action of the photonic creation and annihilation operators  $\hat{a}^\dagger$  and  $\hat{a}$  over the eigen states of the JCH Hamiltonian is explained in detail. Then, the tools for evaluating the phase boundaries of the MI to SF transition are briefly discussed. The general expressions for the chemical potential is also given which is used to calculate the phase boundary. The hopping term of the JCH Hamiltonian is uncoupled in real space to yield a mean-field Hamiltonian which can be diagonalized leading to a easy calculation of the phase boundaries.

The third chapter is devoted to introducing two different approximation schemes both of which give analytic results for the critical hopping amplitude for the Mott-insulator to Superfluid transition. The first scheme is the effective strong-coupling model. The energy of the ground state is  $N = nL$  and there are no first order contributions arising from the perturbation theory. So the Hilbert space per site is one dimensional, consisting of the single state  $|-\rangle$ . The hopping operator is replaced by the spin operators and hopping term is converted in to a nearest neighbour spin -spin interaction. Thus the Hamiltonian is written in terms of the spin operators and this enables us compute the chemical potential easily. The second approximation, namely, the Fermionic approximation, the spin operators are replaced with fermionic operators and a Fourier transformation of the resulting Hamiltonian gives a simple expression in the momentum space which enables a easy calculation of the chemical potential.

The fourth chapter includes the application of both the approximation schemes to two different systems: (i) the JCHM with positive effective-mass and nearest-neighbor hopping and (ii) the linear ion chain. Here the analytic results obtained are compared with the numerical results obtained from density-matrix renormalization group and the mean-field calculations.

We present our conclusions in the final chapter



## Chapter 2

# The Jaynes-Cummings-Hubbard Model

In this chapter, we review certain features of the Jaynes-Cummings-Hubbard model described by the Hamiltonian (1.3). We also write down the dressed basis from the knowledge of the bare basis by solving the eigen value equation. Finally, we convert the JCH Hamiltonian into a local Hamiltonian incorporating the effects of interaction through a mean-field.

When the hopping amplitude is zero in equation (1.3), the Hamiltonian expression can be diagonalized easily, since the sites become independent. Solving the Schrodinger equation,

$$\hat{H}\psi = E\psi, \quad (2.1)$$

where,  $\psi$  is the column matrix  $\begin{bmatrix} |\uparrow, n-1\rangle \\ |\downarrow, n\rangle \end{bmatrix}$ . The state vectors  $|\uparrow, n-1\rangle$  and  $|\downarrow, n\rangle$  are the bare basis, in which the first part describes the state of the atom and the second part describes the number of photonic excitations. To construct the dressed basis, we find the elements of the matrix,

$$\hat{H} = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix}. \quad (2.2)$$

The elements of the matrix (2.2) are found [3] to be:

$$h_{11} = \langle \uparrow, n-1 | H | \uparrow, n-1 \rangle = (n-1)\omega + \Delta$$

$$h_{12} = \langle \uparrow, n-1 | H | \downarrow, n \rangle = g\sqrt{n},$$

$$h_{21} = \langle \downarrow, n | H | \uparrow, n-1 \rangle = g\sqrt{n} \text{ and}$$

$$h_{22} = \langle \downarrow, n | H | \downarrow, n \rangle = n\omega.$$

Solving the matrix (2.2) for the eigen vectors we obtain the elements of the dressed basis

$$|\pm, n\rangle = \frac{[\chi_n \mp (\omega - \Delta)] |\uparrow, n-1\rangle \pm 2g\sqrt{n} |\downarrow, n\rangle}{\sqrt{2}\sqrt{\chi_n^2 \mp (\omega - \Delta)\chi_n}}, \quad (2.3)$$

$$\equiv \alpha_n^\pm |\uparrow, n-1\rangle \pm \beta_n^\pm |\downarrow, n\rangle, \quad (2.4)$$

where,

$$\alpha_n^\pm = \frac{[\chi_n \mp (\omega - \Delta)]}{\sqrt{2}\sqrt{\chi_n^2 \mp (\omega - \Delta)\chi_n}},$$

$$\beta_n^\pm = \frac{2g\sqrt{n}}{\sqrt{2}\sqrt{\chi_n^2 \mp (\omega - \Delta)\chi_n}}, \text{ and}$$

$$\chi_n = \sqrt{(\Delta - \omega)^2 + 4ng^2}.$$

From (2.3) we can observe that the atomic and the field modes are entangled with each other and they are known as the polaritonic states. The eigenvalues of the polaritonic states are

$$E_n^\pm = n\omega + \frac{\Delta - \omega}{2} \pm \frac{1}{2}\chi_n. \quad (2.5)$$

It can be seen here that for  $n = 0$ , the ground state is degenerate and given by  $|- , 0\rangle = |\downarrow, 0\rangle$  with  $E_0 = 0$ . In the limit of strong interaction, that is for  $g \gg |\Delta - \omega|$ , the energy gap  $\Delta E_n = E_n^+ - E_n^- = \chi_n \sim 2g\sqrt{n}$  is very large compared with any other energy scale in the system. Thus, the excited state  $|+, n\rangle$  do not contribute to the ground state.

Now in the following discussions, it would be useful to consider the action of a single bosonic creation or annihilation operator on a given JC eigenstate  $|\pm, n\rangle$ . For convenience, we first define certain quantities [4] which would be very useful:

$$A_n^\pm = \begin{cases} \sqrt{n}\alpha_n^\pm \beta_{n+1}^\mp \pm \sqrt{n+1}\beta_n^\pm \alpha_{n+1}^\mp, & n > 0 \\ \alpha_1^\mp, & n = 0 \end{cases} \quad (2.6)$$

$$B_n^\pm = \begin{cases} \sqrt{n}\alpha_n^\pm \beta_{n+1}^\pm \mp \sqrt{n+1}\beta_n^\pm \alpha_{n+1}^\pm, & n > 0 \\ -\alpha_1^\pm, & n = 0 \end{cases} \quad (2.7)$$

$$C_n^\pm = \begin{cases} \sqrt{n-1}\alpha_n^\pm \beta_{n-1}^\mp \pm \sqrt{n}\beta_n^\pm \alpha_{n-1}^\mp, & n > 1 \\ 0, & n \leq 1 \end{cases} \quad (2.8)$$

$$D_n^\pm = \begin{cases} \sqrt{n-1}\alpha_n^\pm \beta_{n-1}^\pm \mp \sqrt{n}\beta_n^\pm \alpha_{n-1}^\pm, & n > 1 \\ \pm \beta_1^\pm \delta_{n,1}, & n \leq 1 \end{cases} \quad (2.9)$$

The action of the creation and annihilation operator on the dressed states is computed below:

$$\begin{aligned} \hat{a}^\dagger |+, n\rangle &= \hat{a}^\dagger \left[ \frac{(\chi_n - \epsilon) |\uparrow, n-1\rangle + 2g\sqrt{n} |\downarrow, n\rangle}{\sqrt{2}\sqrt{\chi_n^2 - \epsilon\chi_n}} \right], \\ &= \frac{(\chi_n - \epsilon)\sqrt{n} |\uparrow, n\rangle + 2g\sqrt{n(n+1)} |\downarrow, n+1\rangle}{\sqrt{2}\sqrt{\chi_n^2 - \epsilon\chi_n}}, \end{aligned} \quad (2.10)$$

where,  $\Delta - \omega = \epsilon$ .

$$\begin{aligned}\hat{a}^\dagger |-, n\rangle &= \hat{a}^\dagger \left[ \frac{(\chi_n + \epsilon)|\uparrow, n-1\rangle - 2g\sqrt{n}|\downarrow, n\rangle}{\sqrt{2}\sqrt{\chi_n^2 + \epsilon\chi_n}} \right], \\ &= \frac{(\chi_n + \epsilon)\sqrt{n}|\uparrow, n\rangle - 2g\sqrt{n(n+1)}|\downarrow, n+1\rangle}{\sqrt{2}\sqrt{\chi_n^2 + \epsilon\chi_n}}.\end{aligned}\quad (2.11)$$

Combining equations (2.10) and (2.11), we obtain the action of the creation operator on the dressed basis vectors

$$\hat{a}^\dagger |\pm, n\rangle = \frac{(\chi_n \mp \epsilon)\sqrt{n}|\uparrow, n\rangle \pm 2g\sqrt{n(n+1)}|\downarrow, n+1\rangle}{\sqrt{2}\sqrt{\chi_n^2 \mp \epsilon\chi_n}}. \quad (2.12)$$

In a similar manner, from the action of the annihilation operator on the dressed basis vectors, we get

$$\begin{aligned}\hat{a} |+, n\rangle &= \hat{a} \left[ \frac{(\chi_n - \epsilon)|\uparrow, n-1\rangle + 2g\sqrt{n}|\downarrow, n\rangle}{\sqrt{2}\sqrt{\chi_n^2 - \epsilon\chi_n}} \right], \\ &= \frac{(\chi_n - \epsilon)\sqrt{n-1}|\uparrow, n-2\rangle + 2gn|\downarrow, n-1\rangle}{\sqrt{2}\sqrt{\chi_n^2 - \epsilon\chi_n}},\end{aligned}\quad (2.13)$$

$$\begin{aligned}\hat{a} |-, n\rangle &= \hat{a} \left[ \frac{(\chi_n + \epsilon)|\uparrow, n-1\rangle - 2g\sqrt{n}|\downarrow, n\rangle}{\sqrt{2}\sqrt{\chi_n^2 + \epsilon\chi_n}} \right], \\ &= \frac{(\chi_n + \epsilon)\sqrt{n-1}|\uparrow, n-2\rangle - 2gn|\downarrow, n-1\rangle}{\sqrt{2}\sqrt{\chi_n^2 + \epsilon\chi_n}}.\end{aligned}\quad (2.14)$$

On combining the equations (2.13) and (2.14) the action of the annihilation operator on the dressed basis is as follows:

$$\hat{a} |\pm, n\rangle = \frac{(\chi_n \mp \epsilon)\sqrt{n-1}|\uparrow, n-2\rangle \pm 2gn|\downarrow, n-1\rangle}{\sqrt{2}\sqrt{\chi_n^2 \mp \epsilon\chi_n}}. \quad (2.15)$$

Making use of equations (2.6), (2.7), (2.8) and (2.9); the operations  $\hat{a}^\dagger |\pm, n\rangle$  and  $\hat{a} |\pm, n\rangle$  can be written as

$$\hat{a}^\dagger |\pm, n\rangle = A_n^\pm |+, n+1\rangle + B_n^\pm |-, n+1\rangle, \quad (2.16)$$

$$\hat{a} |\pm, n\rangle = C_n^\pm |+, n-1\rangle + D_n^\pm |-, n-1\rangle \quad (2.17)$$

respectively, which are derived by re-expressing, the equations (2.6), (2.7), (2.8) and (2.9). The coefficients  $A_n^\pm$  and  $B_n^\pm$  re-expressed considering only the  $n > 0$  case is

$$\begin{aligned}A_n^\pm &= \frac{2g\sqrt{n(n+1)}(\chi_n \mp \epsilon) \pm 2g\sqrt{n(n+1)}(\chi_{n+1} + \epsilon)}{\sqrt{2}\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{2}\sqrt{\chi_{n+1}^2 + \epsilon\chi_{n+1}}}, \\ &= \frac{g\sqrt{n(n+1)}[\chi_n \pm \chi_{n+1}]}{\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{\chi_{n+1}^2 + \epsilon\chi_{n+1}}},\end{aligned}$$

$$\begin{aligned}
B_n^\pm &= \frac{2g\sqrt{n(n+1)}(\chi_n \mp \epsilon) \mp 2g\sqrt{n(n+1)}(\chi_{n+1} - \epsilon)}{\sqrt{2}\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{2}\sqrt{\chi_{n+1}^2 - \epsilon\chi_{n+1}}}, \\
&= \frac{g\sqrt{n(n+1)}[\chi_n \mp \chi_{n+1}]}{\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{\chi_{n+1}^2 - \epsilon\chi_{n+1}}}.
\end{aligned}$$

Taking into account the  $n > 1$  case, the coefficients  $C_n^\pm$  and  $D_n^\pm$  are re-expressed as

$$\begin{aligned}
C_n^\pm &= \frac{2g(n-1)(\chi_n \mp \epsilon) \pm 2gn(\chi_{n-1} + \epsilon)}{\sqrt{2}\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{2}\sqrt{\chi_{n-1}^2 - \epsilon\chi_{n-1}}}, \\
&= \frac{g[(n-1)\chi_n \pm n\chi_{n-1} \pm \epsilon]}{\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{\chi_{n-1}^2 - \epsilon\chi_{n-1}}},
\end{aligned}$$

$$\begin{aligned}
D_n^\pm &= \frac{2g(n-1)(\chi_n \mp \epsilon) \mp 2gn(\chi_{n-1} - \epsilon)}{\sqrt{2}\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{2}\sqrt{\chi_{n-1}^2 - \epsilon\chi_{n-1}}}, \\
&= \frac{g[(n-1)\chi_n \mp n\chi_{n-1} \mp \epsilon]}{\sqrt{\chi_n^2 \mp \epsilon\chi_n}\sqrt{\chi_{n-1}^2 - \epsilon\chi_{n-1}}},
\end{aligned}$$

From equation (2.3), the states are written as follows:

$$|+, n+1\rangle = \frac{(\chi_{n+1} - \epsilon)|\uparrow, n\rangle + 2g\sqrt{n+1}|\downarrow, n+1\rangle}{\sqrt{2}\sqrt{\chi_{n+1}^2 - \epsilon\chi_{n+1}}}, \quad (2.18)$$

$$|-, n+1\rangle = \frac{(\chi_{n+1} + \epsilon)|\uparrow, n\rangle - 2g\sqrt{n+1}|\downarrow, n+1\rangle}{\sqrt{2}\sqrt{\chi_{n+1}^2 + \epsilon\chi_{n+1}}}. \quad (2.19)$$

Note here that  $\chi_{n+1}^2 = \epsilon^2 + 4(n+1)g^2$  and  $\sqrt{\chi_{n-1}^2 - \epsilon^2} = 2g\sqrt{n-1}$ .

In order to calculate the phase boundaries of the Mott-insulating lobes for the JCH model we will consider the system as comprising a fixed number of excitations, since the total number of excitations,

$$\hat{N} = \sum_j (\hat{a}_j^\dagger \hat{a}_j + \hat{\sigma}_j^+ \hat{\sigma}_j^-) \quad (2.20)$$

in the system commutes with the full Hamiltonian; (1.3) i.e.  $[\hat{N}, \hat{H}] = 0$ . We use the idea that the boundary of the  $n$ th lobe can be determined by calculating the total energy  $E(N)$  for  $N = nL - 1, N = nL$  and  $N = nL + 1$  excitations in

the system which have  $L$  sites in it. Denoting the upper boundary of the  $n$ th Mott lobe with  $\mu_n^+$  and the lower boundary with  $\mu_n^-$ , we can write:

$$\mu_n^\pm = \pm[E(nL \pm 1) - E(nL)]. \quad (2.21)$$

For  $t_d = 0$ ,  $\mu_n^\pm$  can be calculated without much difficulty. It should be noted here that  $n$  is the the number of polaritons on a single site,  $N$ , the number of polaritons on the entire lattice, and  $L$ , the number of lattice sites available. It can be seen that, for a commensurate number of excitations, due to the non-linear dependence of the single site energy  $E_n^-$  on  $n$ , the excitations will distribute equally over the entire lattice. Then the ground state is give by  $\vec{n} = (n, n, n, \dots, n)$ . Now, when adding a single excitation to the whole system, the ground state is given by  $\{n + 1, n, n, \dots, n\}$ , and when removing a single excitation from the whole system, the ground state is given by  $\{n - 1, n, n, \dots, n\}$ . Note that since we are interested only in the energy of the system which is homogenous, the degeneracy of the state has been ignored. Under these conditions, the energies can be written as:

$$E(nL - 1) = (L - 1)E_n^- + E_{n-1}^-, \quad (2.22)$$

$$E(nL) = LE_n^-, \quad (2.23)$$

$$E(nL + 1) = (L - 1)E_n^- + E_{n+1}^-. \quad (2.24)$$

The chemical potential  $\mu_n^+$  is given by:

$$\mu_n^+ = E_{n+1}^- - E_n^-, \quad (2.25)$$

which corresponds to:

$$\mu_n^+ = \omega - \frac{\chi_{n+1}}{2} + (1 - \delta_{n,0})\frac{\chi_n}{2} + \delta_{n,0}\frac{\Delta - \omega}{2}, \quad (2.26)$$

for any  $n$ . Noting here that  $\mu_n^+$  can also be written as:

$$\mu_n^+ = \omega - \frac{\chi_{n+1}}{2} + \frac{\chi_n}{2}. \quad (2.27)$$

In a similar manner, the expressions for  $\mu_n^-$  can be written as:

$$\mu_n^- = E_n^- - E_{n-1}^-, \quad (2.28)$$

which means that:

$$\mu_n^- = \omega - \frac{\chi_n}{2} + (1 - \delta_{n,1})\frac{\chi_{n-1}}{2} + \delta_{n,1}\frac{\Delta - \omega}{2}, \quad (2.29)$$

for  $n > 0$ .

For a commensurate number of excitations, the system exhibit particle-hole gaps. Since  $\mu_{n+1}^- = \mu_n^+$ , the chemical potential for non-commensurate total

number of excitations between  $N = nL$  and  $N = (n + 1)L$  is the same. This corresponds to a critical point [4]. If there is non-zero tunneling, the critical points extend to critical regions.

The next aim is to obtain a phase diagram for this phase transition using some numerical methods. The simplest available one is the so called mean-field theory. For the effective implementation of the mean-field theory, an order parameter  $\Psi$ . This order parameter is chosen to be homogenous and real valued in our case. The hopping term can be decoupled using a transformation involving the order parameter, as shown below:

$$\hat{a}_j^\dagger \hat{a}_l \mapsto \Psi(\hat{a}_j^\dagger + \hat{a}_l). \quad (2.30)$$

Using the transformaton (2.30), we get

$$\sum_j (\hat{a}_j^\dagger \hat{a}_{j+d} + \hat{a}_{j+d}^\dagger \hat{a}_j) = \sum_j \left[ (\Psi(\hat{a}_j^\dagger + \hat{a}_{j+d}) - |\Psi|^2 + \Psi(\hat{a}_{j+d}^\dagger + \hat{a}_j) - |\Psi|^2) \right]. \quad (2.31)$$

Substituting (2.31) in the Hamiltonian (1.3), we observe that it uncouples in the real space as a local Hamiltonian.

$$\hat{H}^{MF} = (\omega - \mu)\hat{a}^\dagger \hat{a} + (\Delta - \mu)\hat{\sigma}^+ \hat{\sigma}^- + g(\hat{a}^\dagger \hat{\sigma}^- + \hat{a} \hat{\sigma}^+) - 2\tilde{J}\Psi(\hat{a}^\dagger + \hat{a}) + 2\tilde{J}|\Psi|^2, \quad (2.32)$$

where  $\hat{H}^{MF} = \hat{H}^{JCH} - \mu\hat{N}$  and the modified hopping amplitude  $\tilde{J} = -\sum_d t_d$  gives the effective coupling within the mean-field scheme. The phase diagram can now be found by diagonalizing the mean-field Hamiltonian (2.32). The diagonalization can be done either exactly by means of perturbation theory or numerically, setting an upper bound for the maximal number of bosonic excitations in the system.

The ground state energy is then given by  $\min_\Psi E[\Psi]$ . The Mott Insulator is distinguished from the Superfluid by the value of  $\Psi$  for the minimal energy. For  $\Psi = 0$ , the system is in a Mott-insulating state and for  $\Psi > 0$ , the ground state is a superfluid. This is the condition that sets the point of the transition from Mott-insulator to the Superfluid state. The important point to note here is that this method gives inadequate results in one-dimension but is exact when the dimension goes to infinity. Also it should be mentioned here that the effective hopping  $\tilde{J}$  must be larger than zero to yield useful results.

## Chapter 3

# Approximative Determination of the Phase Boundaries

In the present chapter, we introduce two different approximation schemes. In the first scheme, namely, effective strong-coupling model, the effective Hamiltonian in the limit of a strong coupling between the photonic and atomic modes is calculated. Then the chemical potentials in the upper and lower boundaries of the  $n$ th Mott lobe is calculated. In the second scheme, namely, the fermionic approximation, the spin operators are re-written in terms of the fermionic operators, which in turn, smoothens the Fourier transformation of the Hamiltonian and lead to the easy calculation of the phase boundaries.

### 3.1 Effective Strong-Coupling Model:

In the present section, the aim is to derive the effective Hamiltonian in the strong-coupling limit and thereby the chemical potentials in the upper and lower boundaries of the  $n$ th Mott lobe can be calculated. With this, the particle-hole gap can be calculated upto first order of the hopping amplitudes  $t_d$ . To do so we employ a procedure equivalent to the polariton mapping discussed below. The procedure is called degenerate perturbation theory and uses Kato's expansion up to first order with  $H_{eff} = \mathcal{PVP}$ . This procedure is equivalent to the polariton mapping considered in [5]. First of all, it is useful to note that the state  $|+, n\rangle$  is separated from the ground state by a large energy gap  $|-, n\rangle$ . Hence,  $|+, n\rangle$  can be completely ignored in the present section. Now we look at the energy of the ground state with  $N = nL$ , from the perturbation theory, no first-order contributions are present. So the Hilbert space per site is one dimensional, consisting of the single state  $|-, n\rangle$ . Thus, up to first order, the energy is given by  $E(nL) = LE_n^-$ . When adding an excitation, the local Hilbert space increases; now (locally), the two states  $|-, n\rangle$  and  $|-, n+1\rangle$  need to be taken into account. So, in this limit, the system for an additional particle can be understood as one consisting of effective spin-half particles. For simplicity, we identify the state

$|-, n\rangle$  with the state  $|\Downarrow\rangle$  and the state  $|-, n+1\rangle$  with the state  $|\Uparrow\rangle$ . In order to derive the effective spin-half model, we have to investigate the action of the hopping operator  $\hat{a}_{j+1}^\dagger \hat{a}_j$  on the states in the Hilbert space.

Using equations (2.6) to (2.9) and neglecting the contributions from the states  $|+, n\rangle$  and  $|+, n+1\rangle$ , the action of the hopping operator  $\hat{a}_{j+1}^\dagger \hat{a}_j$  can be found as follows:

$$\begin{aligned}
\hat{a}_{j+1}^\dagger \hat{a}_j |\Downarrow\rangle_{j+1} |\Uparrow\rangle_j &= \hat{a}_{j+1}^\dagger |\Downarrow\rangle_{j+1} \hat{a}_j |\Uparrow\rangle_j, \\
&= \hat{a}_{j+1}^\dagger |-, n\rangle_{j+1} \hat{a}_j |-, n+1\rangle_j, \\
&= \left[ A_n^- |+, n+1\rangle_{j+1} + B_n^- |-, n+1\rangle_{j+1} \right] \\
&\quad \left[ C_{n+1}^- |+, n\rangle_j + D_{n+1}^- |-, n\rangle_j \right], \\
&= B_n^- |-, n+1\rangle_{j+1} D_{n+1}^- |-, n\rangle_j, \\
&= B_n^- D_{n+1}^- |-, n+1\rangle_{j+1} |-, n\rangle_j.
\end{aligned}$$

Hence we get

$$\hat{a}_{j+1}^\dagger \hat{a}_j |\Downarrow\rangle_{j+1} |\Uparrow\rangle_j = B_n^- D_{n+1}^- |\Uparrow\rangle_{j+1} |\Downarrow\rangle_j \quad (3.1)$$

within the considered subspace. This expression can be developed by defining a new general operator, called the polariton operator:

$$P_{j, [\pm, n]}^\dagger = |\pm, n\rangle_j \langle -, 0|_j,$$

from which we get the expression:

$$P_{\pm n}^\dagger P_{\pm n} = |\pm, n\rangle_j \langle \pm, n|_j.$$

We can see that for our case:

$$\hat{\sigma}_j^+ = P_{j, [-, (n+1)]}^\dagger P_{j, [-, n]} = |-, (n+1)\rangle_j \langle -, n|_j = |\Uparrow\rangle_j \langle \Downarrow|_j,$$

and

$$\hat{\sigma}_j^- = P_{j, [-, n]}^\dagger P_{j, [-, (n+1)]} = |-, n\rangle_j \langle -, (n+1)|_j = |\Downarrow\rangle_j \langle \Uparrow|_j.$$

Using the above equations, we can readily write:  $\hat{\sigma}_j^+ |\Downarrow\rangle_j = |\Uparrow\rangle_j$  and  $\hat{\sigma}_j^- |\Uparrow\rangle_j = |\Downarrow\rangle_j$ . Then;

$$B_n^- D_{n+1}^- |\Uparrow\rangle_{j+1} |\Downarrow\rangle_j = B_n^- D_{n+1}^- \hat{\sigma}_{j+1}^+ |\Downarrow\rangle_{j+1} \hat{\sigma}_j^- |\Uparrow\rangle_j = B_n^- D_{n+1}^- \hat{\sigma}_{j+1}^+ \hat{\sigma}_j^- |\Downarrow\rangle_{j+1} |\Uparrow\rangle_j.$$

Therefore, by introducing the spin operators  $\hat{\sigma}_j^\pm$ , we got the hopping term which is equivalent to a nearest neighbor spin-spin interaction with;

$$\hat{a}_{j+1}^\dagger \hat{a}_j = B_n^- D_{n+1}^- \hat{\sigma}_{j+1}^+ \hat{\sigma}_j^-. \quad (3.2)$$



Using the Expression ,

$$\hat{H}^{JC} - \mu\hat{N} = (\omega - \mu)\sum_j \hat{a}_j^\dagger \hat{a}_j + (\Delta - \mu)\sum_j \hat{\sigma}_j^\dagger \hat{\sigma}_j^- + g\sum_j (\hat{\sigma}_j^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{\sigma}_j^-), \quad (3.3)$$

and substituting for  $\hat{\sigma}_j^+ \hat{\sigma}_j^-$  and  $\hat{\sigma}_j^- \hat{\sigma}_j^+$  the Hamiltonian (3.3) could be written as follows:

$$\begin{aligned} (\hat{H}^{JC} - \mu\hat{N})|-, n\rangle_j &= \sum_j E_{-,n}^\mu |-, n\rangle_j, \\ &= \sum_j E_{-,n}^\mu |-, n\rangle_j \langle -, n|_j |-, n\rangle_j, \\ &= \sum_j E_{-,n}^\mu P_{j,[-,n]}^\dagger P_{j,[-,n]} |-, n\rangle_j, \\ (\hat{H}^{JC} - \mu\hat{N})|-, n\rangle_j &= \sum_j E_{-,n}^\mu P_{j,[-,n]}^\dagger P_{j,[-,n]} |-, n\rangle_j. \end{aligned}$$

Proceeding in a similar manner, it could be shown that:

$$(\hat{H}^{JC} - \mu\hat{N})|-, (n+1)\rangle_j = \sum_j E_{-, (n+1)}^\mu P_{j,[-, (n+1)]}^\dagger P_{j,[-, (n+1)]} |-, (n+1)\rangle_j.$$

Thus the effective Hamiltonian in the strong coupling limit reads:

$$\tilde{H} = \hat{H}^{JC} - \mu\hat{N} + H^{hop},$$

$$\begin{aligned} \tilde{H} &= \sum_j E_n^- P_{j,[-,n]}^\dagger P_{j,[-,n]} + \sum_j E_{n+1}^- P_{j,[-, (n+1)]}^\dagger P_{j,[-, (n+1)]} \\ &\quad + \sum_d t_d \sum_j (\hat{a}_j^\dagger \hat{a}_{j+d} + \hat{a}_{j+d}^\dagger \hat{a}_j). \end{aligned} \quad (3.4)$$

Rewriting the above equation (3.4) in terms of the effective spin operators the Hamiltonian is

$$\tilde{H} = E_n^- \sum_j \tilde{\sigma}_j^- \tilde{\sigma}_j^+ + E_{n+1}^- \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- + B_n^- D_{n+1}^- \sum_d t_d \sum_j (\tilde{\sigma}_{j+d}^+ \tilde{\sigma}_j^- + \tilde{\sigma}_j^+ \tilde{\sigma}_{j+d}^-). \quad (3.5)$$

The first two terms of the RHS of the above equation (3.5) can be rewritten by making use of the relations;

$$\hat{\sigma}_j^+ \hat{\sigma}_j^- + \hat{\sigma}_j^- \hat{\sigma}_j^+ = \hat{1}, \quad \sum_j (\hat{\sigma}_j^+ \hat{\sigma}_j^- + \hat{\sigma}_j^- \hat{\sigma}_j^+) = L\hat{1} \text{ as;}$$

$$\begin{aligned}
E_n^- \sum_j \tilde{\sigma}_j^- \tilde{\sigma}_j^+ + E_{n+1}^- \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- &= E_n^- \left( L\hat{1} - \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- \right) + E_{n+1}^- \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^-, \\
&= (E_{n+1}^- - E_n^-) \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- + E_n^- L,
\end{aligned}$$

from which, we can readily write

$$\left[ E_n^- \sum_j \tilde{\sigma}_j^- \tilde{\sigma}_j^+ + E_{n+1}^- \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- \right] \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- = [(L-1)E_n^- + E_{n+1}^-] \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^-,$$

which give us the expression

$$E_n^- \sum_j \tilde{\sigma}_j^- \tilde{\sigma}_j^+ + E_{n+1}^- \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- = (L-1)E_n^- + E_{n+1}^-,$$

since

$$\sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- \tilde{\sigma}_j^+ \tilde{\sigma}_j^- = \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^-.$$

Thus we get,

$$\tilde{H} = (L-1)E_n^- + E_{n+1}^- + B_n^- D_{n+1}^- \sum_d t_d \sum_j \left( \tilde{\sigma}_{j+d}^+ \tilde{\sigma}_j^- + \tilde{\sigma}_j^+ \tilde{\sigma}_{j+d}^- \right) \quad (3.6)$$

since we are at fixed magnetization with only one spin pointing upward. This Hamiltonian can be further simplified, by using a Jordan-Wigner transformation defined by

$$\prod_{k=1}^{j-1} (-\tilde{\sigma}_k^z) \tilde{\sigma}_j^+ = \hat{c}_j^\dagger \quad \text{and} \quad \prod_{k=1}^{j-1} (-\tilde{\sigma}_k^z) \tilde{\sigma}_j^- = \hat{c}_j,$$

where,

$$\sigma_k^z = 2\sigma_k^+ \sigma_k^- - \hat{1}.$$

A few words about the Jordan-Wigner transformation is relevant in this discussion because of its relation to quantum computation. Jordan-Wigner transformation is a beautiful application of the fermionic canonical commutation relations. This powerful tool helps us to map a system of interacting qubits onto an equivalent system of interacting fermions, or, vice versa, to map a system of fermions onto a system of qubits. This mapping is interesting because it means that anything we understand about one type of system (e.g., Fermions) can be immediately applied to learn something about the other type of system (e.g., qubits). Also, this transformation can be applied in quantum simulation of

a system of fermions. In particular, this transformation allows us to map a system of interacting fermions onto an equivalent model of interacting spins, which can then, in principle, be simulated using standard techniques on a quantum computer. This enables us to use quantum computers to efficiently simulate systems of interacting fermions. Here it is interesting to note that a non-interacting gas of fermions is still highly correlated since the exclusion principle introduces a hard-core interaction between fermions in the same quantum state, and this is the feature exploited in the Jordan-Wigner representation of spins.

Now using the Jordan-Wigner transformation and the relation connecting  $\sigma_j^z$  and  $\sigma_j^\pm$ , we can see that:

$$\hat{c}_{j+d}^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_{j+d} = \prod_{k=1}^{j+d-1} \tilde{\sigma}_k^z \tilde{\sigma}_{j+d}^+ \prod_{k=1}^{j-1} \tilde{\sigma}_k^z \tilde{\sigma}_j^- + \prod_{k=1}^{j-1} \tilde{\sigma}_k^z \tilde{\sigma}_j^+ \prod_{k=1}^{j+d-1} \tilde{\sigma}_k^z \tilde{\sigma}_{j+d}^-.$$

But, since  $\sigma_j^z = 2\sigma_j^+ \sigma_j^- - \hat{1}$ , we can write;

$$\begin{aligned} \prod_{k=1}^{j-1} (\tilde{\sigma}_k^z) \tilde{\sigma}_{j+d}^+ &= \prod_{k=1}^{j-1} (2\tilde{\sigma}_k^+ \tilde{\sigma}_k^- - \hat{1}) \tilde{\sigma}_{j+d}^+, \\ &= \prod_{k=1}^{j-1} 2\tilde{\sigma}_k^+ \tilde{\sigma}_k^- \tilde{\sigma}_{j+d}^+ - \tilde{\sigma}_{j+d}^+, \\ &= 2 \prod_{k=1}^{j+d-1} |-, n+1\rangle_k \langle -, n+1|_k |-, n+1\rangle_{j+d} \langle -, n|_{j+d} - \sigma_{j+d}^+. \end{aligned}$$

Here, the first term goes to zero as  $k$  is always less than  $j+d$ . Hence,

$$\prod_{k=1}^{j+d-1} (\tilde{\sigma}_k^z) \tilde{\sigma}_j^+ = -\sigma_{j+d}^+.$$

Similarly we get,

$$\prod_{k=1}^{j-1} (\tilde{\sigma}_k^z) \tilde{\sigma}_j^+ = -\sigma_j^+,$$

$$\prod_{k=1}^{j-1} (\tilde{\sigma}_k^z) \tilde{\sigma}_j^- = \sigma_j^-,$$

and

$$\prod_{k=1}^{j+d-1} (\tilde{\sigma}_k^z) \tilde{\sigma}_j^- = \sigma_{j+d}^-.$$

Then we obtain,  $\hat{c}_{j+d}^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_{j+d} = \sigma_{j+d}^+ \sigma_j^- + \sigma_j^- \sigma_{j+d}^-$ , so that the effective Hamiltonian  $\tilde{H}$  becomes

$$\tilde{H} = (L-1)E_n^- + E_{n+1}^- + B_n^- D_{n+1}^- \sum_d t_d \sum_j \left( \hat{c}_{j+d}^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_{j+d} \right).$$

Performing a Fourier transformation on the above equation:

$$\hat{c}_j = \frac{1}{\sqrt{L}} \sum_k e^{-2\pi i k j / L} \hat{c}_k, \quad (3.7)$$

we see that the ground-state wave function factorizes since the Hamiltonian decouples in momentum space.

$$\tilde{H} = (L-1)E_n^- + E_{n+1}^- + 2B_n^- D_{n+1}^- \sum_d t_d \sum_k \cos\left(2\pi \frac{kd}{L}\right) \hat{c}_k^\dagger \hat{c}_k. \quad (3.8)$$

This model is equivalent to free fermionic particles with hopping amplitude given by  $t_d$ . In momentum space, a single fermion will occupy the mode with the lowest energy. Thus the total energy of the single particle and therefore the total energy of an additional excitation on top of the  $n$ th Mott insulator in the JCH model is given by:

$$E(nL+1) = (L-1)E_n^- + E_{n+1}^- + F_n(k'), \quad (3.9)$$

where,

$$F_n(k) = 2B_n^- D_{n+1}^- \sum_d t_d \cos\left(2\pi \frac{kd}{L}\right). \quad (3.10)$$

Here, the momentum mode  $k'$  is chosen such that the value of  $F_n(k)$  at  $k'$  is minimal. It should be mentioned here that the product  $B_n^- D_{n+1}^-$  is positive for any  $(\Delta, \omega, n)$ , so the momentum mode is purely determined by the minimum of  $\sum_d t_d \cos\left(2\pi \frac{kd}{L}\right)$ .

To calculate the energy for a hole in the  $n$ th Mott insulator, we follow exactly the same route. In this case, the state  $|\downarrow\rangle$  is associated with  $|-, n-1\rangle$  and  $|\uparrow\rangle$  with  $|-, n\rangle$ . The hopping operator act as:

$$\hat{a}_{j+1}^\dagger \hat{a}_j |\downarrow\rangle_{j+1} |\uparrow\rangle_j = B_{n-1}^- D_n^- |\uparrow\rangle_{j+1} |\downarrow\rangle_j, \quad (3.11)$$

and the effective Hamiltonian is given by:

$$\tilde{H} = E_{n-1}^- \sum_j \tilde{\sigma}_j^- \tilde{\sigma}_j^+ + E_n^- \sum_j \tilde{\sigma}_j^+ \tilde{\sigma}_j^- + B_{n-1}^- D_n^- \sum_d t_d \sum_j \left( \tilde{\sigma}_{j+d}^+ \tilde{\sigma}_j^- + \tilde{\sigma}_j^+ \tilde{\sigma}_{j+d}^- \right). \quad (3.12)$$

Here, the magnetization consists of one spin pointing downward. Again, after making use of a Jordan-Wigner transformation, and subsequently, a Fourier transformation, the energy of a single hole is given by:

$$E(nL - 1) = (L - 1)E_n^- + E_{n-1}^- + F_{n-1}(k''), \quad (3.13)$$

where the same condition holds for  $k''$ . Now putting the calculated energies (3.9) and (3.13) together, the chemical potentials and therefore the boundaries of the  $n$ th Mott-insulating lobe can be easily derived.. They are given by:

$$\mu_n^+ = E_{n+1}^- - E_n^- + 2B_n^- D_{n+1}^- \sum_d t_d \cos\left(2\pi \frac{k'd}{L}\right), \quad (3.14)$$

$$\mu_n^- = E_n^- - E_{n-1}^- - 2B_{n-1}^- D_n^- \sum_d t_d \cos\left(2\pi \frac{k''d}{L}\right), \quad (3.15)$$

where  $k'$  is chosen such that  $\mu_n^+(k')$  is minimal and  $k''$  is chosen such that  $\mu_n^-(k'')$  is maximal.

## 3.2 Fermion Approximation:

This section is devoted for the application of an even simpler approximation. It is clear to see that all the terms in the equation (1.3) are quadratic. These kinds of models are in general suited for an exact solution by means of a Fourier transform. The problem at this point is, however, that the commutation relations of spin operator  $\sigma_j^\pm$  are not as simple as that of bosons or fermions. This limits the applicability of a fourier transform since the operators in momentum space will not obey the same commutation relation as in real space. The usual step of a prior Jordan-Wigner transformation, transforming the spin operators to proper fermionic operators, is not applicable in this case since the interaction part is linear in the spin operators, so the Jordan-Wigner factors do not cancel out. Thus both transformations cannot be carried out exactly without increasing the descriptonal complexity of the problem. Nevertheless, the Hamiltonian can be diagonalized by a Fourier transform in an approximate way.

As said earlier, all modes decouple at  $t_d = 0$ . For this reason, the spin operators are in this limit equivalent to fermionic operators. If we assume that this replacement also holds for small values of  $t_d$ , the JCH model (1.3) can be rewritten in the fermionic approximation:

$$\hat{H} = \omega \sum_j \hat{a}_j^\dagger \hat{a}_j + \Delta \sum_j \hat{c}_j^\dagger \hat{c}_j + g \sum_j (\hat{c}_j^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{c}_j) + \sum_d t_d \sum_j \left( \hat{a}_j^\dagger \hat{a}_{j+d} + \hat{a}_{j+d}^\dagger \hat{a}_j \right). \quad (3.16)$$

Here, the spin operators are replaced by fermionic operators as discussed in the earlier section. Within this approximation, a Fourier transform of both the bosonic and fermionic degrees of freedom can be easily accomplished as:

$$\hat{a}_j = \frac{1}{\sqrt{L}} \sum_k e^{-2\pi i k j / L} \hat{a}_k, \quad (3.17)$$

$$\hat{c}_j = \frac{1}{\sqrt{L}} \sum_k e^{-2\pi i k j / L} \hat{c}_k. \quad (3.18)$$

Here the operators  $\hat{a}_k$  and  $\hat{c}_k$  are operators in the momentum space. Doing so, the JCH Hamiltonian transforms to that of uncoupled Jaynes-Cummings systems,

$$\hat{H} = \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + \Delta \sum_k \hat{c}_k^\dagger \hat{c}_k + g \sum_k (\hat{c}_k^\dagger \hat{a}_k + \hat{a}_k^\dagger \hat{c}_k), \quad (3.19)$$

with,

$$\omega_k = \omega + 2 \sum_d t_d \cos\left(2\pi \frac{k d}{L}\right). \quad (3.20)$$

The ground state in any mode is given by the Jaynes-Cummings ground state (2.3) with frequency  $\omega_k$ . The energy of mode  $k$  with  $n$  excitations is given by:

$$E_k^n = (1 - \delta_{n,0}) \left[ n\omega_k + \frac{\Delta - \omega_k}{2} - \frac{1}{2} \sqrt{(\Delta - \omega_k)^2 + 4ng^2} \right]. \quad (3.21)$$

Since the total number of excitations,

$$\hat{N} = \sum_j (\hat{a}_j^\dagger \hat{a}_j + \hat{\sigma}_j^+ \hat{\sigma}_j^-) \mapsto \sum_k (\hat{a}_k^\dagger \hat{a}_k + \hat{c}_k^\dagger \hat{c}_k), \quad (3.22)$$

commutes with the Hamiltonian (3.19), a common basis can be chosen. Thus the full solution of equation (3.19) for a fixed total number of excitations  $N = nL$  is given by the distribution  $\vec{n} = \{n_{k_1}, n_{k_2}, n_{k_3}, \dots\}$  of  $N$  excitations on  $L$  momentum modes with minimal energy  $E_N[\vec{n}] = \sum_k E_k^{n_k}$  together with the constraint  $\sum_k n_k \equiv N$ . Note that the total number of momentum modes  $L$  is equal to the number of sites.

When constructing the phase diagram, the energy of  $N = nL - 1$ ,  $N = nL$ , and  $N = nL + 1$  excitations needs to be calculated. In the limit of vanishing hopping ( $t = 0$ ) and for commensurate filling, i.e.,  $N = nL$ , the distribution of occupation numbers, which has the lowest energy, is again  $\vec{n} = \{n, n, \dots, n\}$ . This corresponds to a Mott-insulating state with an integer number of excitations on every lattice sites. The phase is gapped with a particle-hole gap, as described in the previous chapter. When  $t$  is increased, the ground state remains the same, but the gap closes and a quantum phase transition occurs from the Mott-insulating to the Superfluid phase at some critical value of  $t$ . The

only remaining thing in order to calculate the chemical potentials is to find the momentum mode, where the addition of an excitation gives the maximum reduction in the total energy and the removal of an excitation gives the minimum increase in the total energy. This yields:

$$\mu_n^+ = E_{k'}^{n+1} - E_{k'}^n, \quad (3.23)$$

$$\mu_n^- = E_k^n - E_k^{n-1}, \quad (3.24)$$

where  $k'$  is chosen such that  $\mu_n^+(k')$  is minimal and  $k$  is chosen such that  $\mu_n^-(k)$  is maximal. The actual values of  $k$  and  $k'$  depend mainly on the sign of the hopping amplitudes  $t_d$ .

## Chapter 4

# Application of to Specific Realizations of the JCH Model

In this chapter we use the two approximation schemes explained in Chapter 3 to two systems namely a JCH model with positive effective mass with nearest neighbor hopping and to another modified model describing the physics of a linear ion chain. The first case the simple JCH where the hopping is restricted to nearest neighbors, essentially serves as a testing ground for our approximation schemes, including a comparison of the analytical results to numerical data from density-matrix renormalization group (DMRG) and mean-field calculations. Later on, the generalized JCH where the hopping term is not restricted will be treated by both approximations giving analytic results for the phase diagram in a wide range of parameters.

### 4.1 JCH with Positive Effective-mass and Nearest Neighbor Hopping:

In this section, we apply both the approximation schemes to a system namely, JCH with positive effective-mass and nearest neighbor hopping [4]. For each approximation, the chemical potentials  $\mu_n^+$  and  $\mu_n^-$  are calculated. The results are plotted in the figure (4.1).

In the current subsection, the discussion is based on the case where  $d = 1$ ,  $\omega = \Delta$ ,  $t_d = -t\delta_{n,1} \Rightarrow \sum_d t_d = -t$ , and hence  $\chi_n = 2g\sqrt{n}$ . The Hamiltonian (1.3) becomes:



$$\hat{H} = \omega \sum_j \hat{a}_j^\dagger \hat{a}_j + \Delta \sum_j \hat{\sigma}_j^+ \hat{\sigma}_j^- + g \sum_j (\hat{\sigma}_j^+ \hat{a}_j + \hat{a}_j^\dagger \hat{\sigma}_j^-) - t \sum_j (\hat{a}_j^\dagger \hat{a}_{j+1} + \hat{a}_{j+1}^\dagger \hat{a}_j). \quad (4.1)$$

Again, for calculating the phase boundaries of the Mott lobes, we need to find the chemical potentials. For this, we first have to determine the momentum modes  $k'$  and  $k''$ , which contribute to the energy. For  $\omega = \Delta$ , the coefficients in the equation (2.3) are;

$$\alpha_n^\pm = \frac{1}{\sqrt{2}} = \beta_n^\pm,$$

and therefore,

$$B_n^- = D_{n+1}^- = \begin{cases} \frac{\sqrt{n} + \sqrt{n+1}}{2}, & n > 0 \\ -\frac{1}{\sqrt{2}}, & n = 0. \end{cases} \quad (4.2)$$

With this, the function  $F_n(k)$  is given by

$$F_n(k) = -t \frac{(\sqrt{n} + \sqrt{n+1})^2}{2 - \delta_{n,0}} \cos\left(2\pi \frac{k}{L}\right). \quad (4.3)$$

A good observation tells us that the chemical potential have its minimum at  $k = 0$ , since at this point,

$$\mu_n^+ = E_{n+1}^- - E_n^- - t \frac{(\sqrt{n} + \sqrt{n+1})^2}{2 - \delta_{n,0}},$$

and also using,  $E_{n+1}^- - E_n^- = \omega - \frac{\chi_{n+1}}{2} + (1 - \delta_{n,0}) \frac{\chi_n}{2} + \delta_{n,0} \frac{\Delta - \omega}{2}$  from the equation (2.26), it can be immediately written that

$$\mu_n^+ = \omega - \frac{1}{2} \chi_{n+1} + \frac{1 - \delta_{n,0}}{2} \chi_n - t \frac{(\sqrt{n} + \sqrt{n+1})^2}{2 - \delta_{n,0}}, \quad (4.4)$$

for any  $n$ . In an exactly similar way, we see that the chemical potential has its maximum at  $k = \frac{L}{2}$ , since at this point,

$$\mu_n^- = E_n^- - E_{n-1}^- + t \frac{(\sqrt{n} + \sqrt{n+1})^2}{2 - \delta_{n,0}}.$$

Now using,  $E_n^- - E_{n-1}^- = \omega - \frac{\chi_n}{2} + (1 - \delta_{n,1}) \frac{\chi_{n-1}}{2} + \delta_{n,1} \frac{\Delta - \omega}{2}$  from the equation (2.29), it can be seen that;

$$\mu_n^- = \omega - \frac{1}{2} \chi_n + \frac{1 - \delta_{n,1}}{2} \chi_{n-1} + t \frac{(\sqrt{n} + \sqrt{n-1})^2}{2 - \delta_{n,1}}, \quad (4.5)$$

for any  $n > 0$ .

Remember here the conditions imposed initially in this section :  $d = 1$ ,  $\omega = \Delta$ , and  $t_d = -t\delta_{n,1} \Rightarrow \sum_d t_d = -t$ . This allows us to determine the critical amplitude  $t_{crit}$ , where  $\mu_n^+ = \mu_n^-$ . Substituting for  $\mu_n^+, \mu_n^-$ ; and simplifying by taking into account the fact that  $\chi_{n+1} \Rightarrow 2g\sqrt{n+1}$ ,  $\chi_n \Rightarrow 2g\sqrt{n}$  and  $\chi_{n-1} \Rightarrow 2g\sqrt{n-1}$ ; we obtain:

$$\frac{t_{crit}}{g} = 2 \frac{2\sqrt{n} - \sqrt{n+1} - \sqrt{n-1}}{(\sqrt{n} + \sqrt{n+1})^2 + (\sqrt{n} + \delta_{n,1} + \sqrt{n-1})^2}. \quad (4.6)$$

Now we apply the second approximation to the same model. With the given system parameters, the momentum-dependent phonon energies from equation (3.20) are given by;

$$\omega_k = \omega - 2t \cos\left(2\pi \frac{k}{L}\right), \quad (4.7)$$

and the energy in the  $k$ th momentum mode, [see equation (3.21) for a given filling  $n$  read as:

$$E_k^n = (1 - \delta_{n,0}) \left[ n\omega - 2nt \cos\left(2\pi \frac{k}{L}\right) + t \cos\left(2\pi \frac{k}{L}\right) - \sqrt{t^2 \cos^2\left(2\pi \frac{k}{L}\right) + ng^2} \right]. \quad (4.8)$$

Finally, following equations (3.23) and (3.24), the momentum mode  $k'$  which minimizes the chemical potential and the momentum mode  $k''$  which maximizes the chemical potential need to be found out. In the present case, these are  $k' = 0$  and  $k = \frac{L}{2}$  respectively. Thus the resulting chemical potentials are

$$\mu_n^+ - \omega = -2t + t\delta_{n,0} - \sqrt{t^2 + (n+1)g^2} + (1 - \delta_{n,0}) \sqrt{t^2 + ng^2}, \quad (4.9)$$

for any  $n$ , and

$$\mu_n^- - \omega = 2t - t\delta_{n,1} - \sqrt{t^2 + ng^2} + (1 - \delta_{n,1}) \sqrt{t^2 + (n-1)g^2}, \quad (4.10)$$

for any  $n > 0$ . For this approximation too, a closed form for the critical amplitude can be found which is omitted here due to its length.

Now, we may compare the analytical results with various numerical calculations. The following figure shows both analytic approximations along with numerical data from Density-matrix renormalization group (*DMRG*) and mean-field calculations, where the modified hopping amplitude in the mean-field Hamiltonian (2.32) evaluates as  $\tilde{J} = t$ . The DMRG is a numerical variational technique devised to obtain the low energy physics of quantum many-body systems with high accuracy. It is nowadays the most efficient method for 1-dimensional systems.

From the figure (4.1), it can be seen that the effective model gives a much better agreement with the numerical DMRG [6, 7] data, especially, the slopes

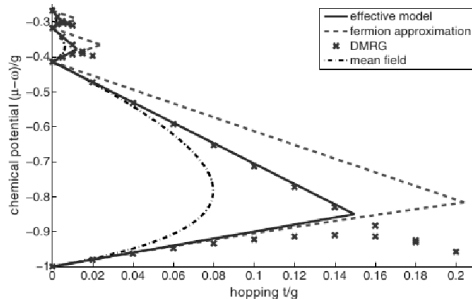


Figure 4.1: Comparison of ground state phase diagram of the 1D JCH Model (4.1) obtained by DMRG as well as mean-field results (dot-dashed line) with the prediction from the present approach (solid line: strong coupling effective Hamiltonian; dashed line: fermion approximation) for  $\Delta = \omega = g = 1$ . Taking into account the simplicity of both the approaches, the agreement with the DMRG data is rather good while the mean-field predictions are rather poor, as expected for 1D systems. The critical hopping amplitudes estimated from the DMRG data agree surprisingly well with those predicted within the fermion approximation, although the shape of the Mott lobe is different.

of the lobes agree perfectly at small hopping. The fermion approximation overestimates the size of the Mott lobe. In particular, while the lower boundaries are rather well reproduced, the upper boundaries have the wrong slope. Surprisingly though the critical hopping amplitudes seem to agree better with the DMRG data than the results obtained from the effective strong-coupling Hamiltonians. Although the fermion approximation is quantitatively worse than the effective strong-coupling Hamiltonians, it provides a simple approximative solution to the JCH beyond the mean-field level, which has the advantage of giving a closed form of the ground state.

## 4.2 Linear Ion Chain:

Now, let us consider a linear string of ions in a trap [8], where the ions are coupled to an external laser field and interact with each other due to the coulomb repulsion via phonon exchange [4]. This system is well described by a modified JCH model with a specific short range hopping with negative effective-mass and site-dependent parameters. First, we will introduce the model and give a derivation of the corresponding homogenous limit. Afterwards, we will apply both the approximations and discuss the phase boundaries within these approximations, giving explicit analytic results for them.

The Hamiltonian of a linear string of  $L$  ions simultaneously irradiated by a laser, which is tuned close to the red radial motional sideband and in the Lamb-Dicke regime, as shown in [9] is given by

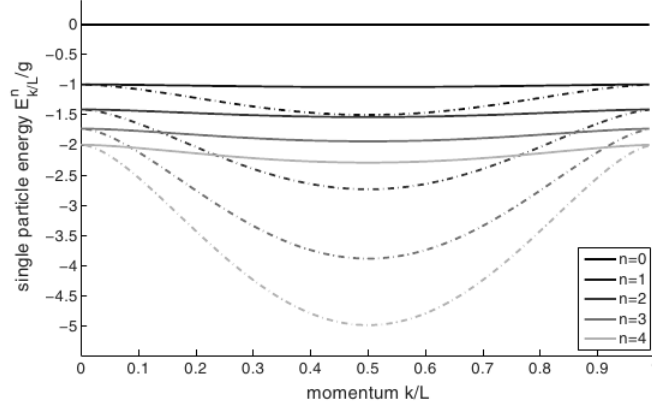


Figure 4.2: Energies of the JCH Hamiltonian for fixed filling  $n$  as function of momentum  $k$ . Shown are the energies from equation 2.4 for the five lowest fillings  $0, \dots, 4$  (from top to bottom) for  $\Delta = 0$  and  $g = 1$ . Solid lines:  $t/g = 0.02$ ; dashed lines:  $t/g = 0.2$ . One clearly recognizes the minimum at  $k = L/2$  and the flat dispersion for  $t/g \rightarrow 0$ .

$$\begin{aligned}
\hat{H} = & \sum_j^{L-1} \omega_j \hat{a}_j^\dagger \hat{a}_j + \Delta \sum_j \hat{\sigma}_j^+ \hat{\sigma}_j^- + g \sum_j (\hat{\sigma}_j^+ \hat{a}_j + \hat{a}_j^\dagger \hat{\sigma}_j^-) \\
& + t \sum_{j=0}^{L-2} \sum_{d=0}^{L-j-1} t_{j,j+d} \left( \hat{a}_{j+d}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+d} \right).
\end{aligned} \tag{4.11}$$

Here,  $\hat{a}_j^\dagger$  and  $\hat{a}_j$  describe the creation and annihilation of a local phonon at the  $j$ th site (ion),  $\hat{\sigma}_j^+$  and  $\hat{\sigma}_j^-$  are the raising and lowering operators between the internal states of the ion, and  $\Delta$  is the detuning of the external laser field from the red motional sideband.  $g$  describes the phonon-ion coupling in the Lamb-Dicke limit.

The local oscillation frequencies  $\omega_j$  and the hopping amplitudes  $t_{j,j+d}$  are determined by the longitudinal and transversal trap frequencies  $\omega_z$  and  $\omega_x$  via

$$\omega_j = -\frac{\omega_z^2}{2\omega_x} \sum_{\substack{l=0 \\ l \neq j}}^{L-1} \frac{1}{|u_j - u_l|^3}, \quad t_{j,j+d} = \frac{\omega_z^2}{2\omega_x} \frac{1}{|u_j - u_d|^3}, \tag{4.12}$$

where  $u_j$  are the equilibrium positions of the ions. For sufficiently large  $L$ , the equilibrium positions of the ions at the centre are approximately equidistant, giving  $u_j = j\tilde{u}$ , with  $\tilde{u}$  being the distance of two adjacent ions.

Let us now discuss the limit of a homogenous chain neglecting any boundary effect. In this limit, equation (4.12) can be rewritten for  $L \rightarrow \infty$ , yielding position-independent phonon energies  $\omega_j \equiv -\omega$  and hopping amplitudes  $t_{j,j+d} \equiv t_d$ ,

$$t_d = \frac{\omega_z^2}{2\omega_x \tilde{u}^3} \frac{1}{d^3} = t \frac{1}{d^3}, \quad (4.13)$$

$$\omega = 2 \frac{\omega_z^2}{2\omega_x \tilde{u}^3} \zeta(3) = 2t\zeta(3), \quad (4.14)$$

where  $t = \frac{\omega_z^2}{2\omega_x \tilde{u}^3}$  acts as a small parameter and  $\omega > 0$ .  $\zeta(x)$  is the Riemann zeta function defined by:

$$\zeta(p) = \sum_{n=1}^{\infty} \frac{1}{n^p},$$

for  $p > 1$ .

One notices a negative oscillator energy  $-\omega$  and a negative effective-mass, which is a result of the positive hopping strength  $t$ . This negative mass is the reason why the application of the mean-field theory is not that straight forward. When simply calculating the modified hopping amplitude  $\tilde{J} = -t \sum_d \frac{1}{d^3} = -t\zeta(3)$ , the hopping becomes negative and, therefore, the mean-field theory is inapplicable. This problem can be overcome by first applying a canonical transformation to all used operators. The transformation:

$$\hat{a}_j \mapsto (-1)^j \hat{a}_j, \quad (4.15)$$

for the annihilation operator and accordingly to all the other operators  $\hat{a}_j^\dagger, \hat{\sigma}_j^\pm$ , maps the JCH model(1.3) back onto itself, but with  $t_d \mapsto (-1)^d t_d$ . After this transformation, the modified hopping evaluates to  $\tilde{J} = -t \sum_d \frac{(-1)^d}{d^3} = 3t\zeta(3)/4$  being positive. Now the application of the mean-field theory is stright forward.

After having introduced the homogenous limit of the model, both the approximations introduced in the previous chapter will be applied. Starting with the effective strong-coupling theory; the first approximation, the chemical potentials for the upper and the lower boundaries of the lobes are given by equations (3.14) and (3.15). The proper momentum modes  $k'$ , which minimizes the chemical potential and the modes  $k''$ , which maximizes the chemical potential are, as already found,  $k = L/2$ . This results from the negative mass. Due to the complexity of the problem, especially the analytic form of  $B_n^-$  and  $D_n^-$ , analytic representation of the chemical potentials are left out here. They can be found straight forwardly just as in the case of the simple JCH model.

When following the second approximative method, i.e., the fermionic approximation scheme, the Hamiltonian for the uncoupled JC models is given by equation (3.19), with the phonon energies being

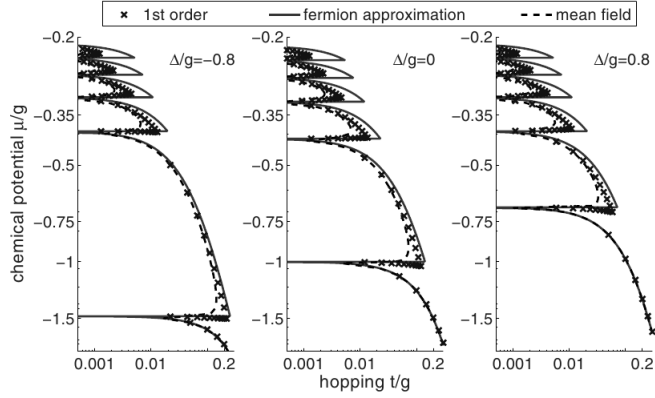


Figure 4.3: Phase diagram of the JCH model for a linear ion chain for three depicted values  $\Delta/g = -0.8, 0, +0.8$ . Shown are the upper boundary of the zero filling lobe (always lowest line) and the boundaries of the lobes with filling from 1 to 5 on a double-logarithmic scale. Beside the used approximations (solid line: fermion approximation; crosses: first order effective theory), the results from the mean-field theory (dot-dashed line) after the canonical transformation are shown. It can be seen that the fermionic approximation again over-estimates the phase boundary (compared to the more reliable effective strong-coupling theory) but gives a better agreement compared to the mean-field theory (mind the logarithm scale).

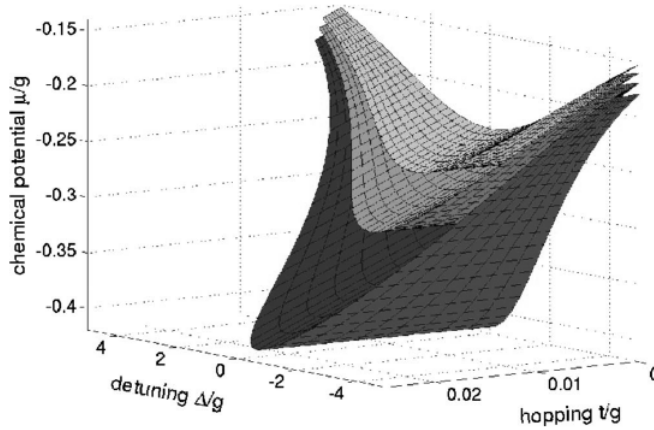


Figure 4.4: Phase diagram of the JCH model for a linear ion chain from the fermion approximation. Boundaries of the Mott-insulating lobes (from bottom to top) for  $n = 2, 3, 4$ . The lobes  $n = 0$  and  $n = 1$  are not displayed since they are unbound for  $\Delta \rightarrow -\infty$ .

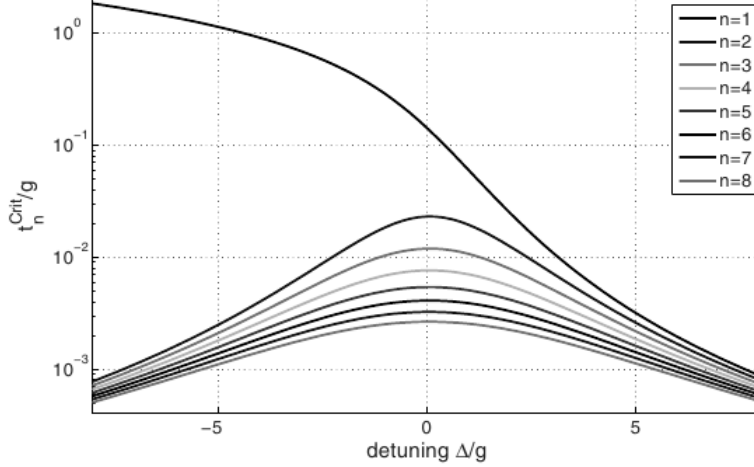


Figure 4.5: Critical hopping amplitude  $t_n^{crit}(\Delta)$ , giving the point where the Mott-insulator to superfluid transition takes place. From top to bottom:  $n = 1, \dots, 8$ , all for  $g = 0.05$ .

$$\omega_k = -\omega + 2t \sum_d \frac{\cos\left(2\pi \frac{kd}{L}\right)}{d^3}, \quad (4.16)$$

according to equation (3.20). Note that, since  $\omega = 2t\zeta(3)$ , all  $\omega_k$ 's are negative. Using the poly logarithm  $Li_n(x) = \sum_{d=1}^{\infty} \frac{x^d}{d^n}$ , one can write them in the explicit form

$$\omega_k = t \left[ Li_3\left(e^{2\pi ik/L}\right) + Li_3\left(e^{-2\pi ik/L}\right) - 2t\zeta(3) \right]. \quad (4.17)$$

The minimum value of  $\omega_k = -7t\zeta(3)/2$  is attained for  $k = \frac{L}{2}$ , as expected from the positive sign of the hopping term. The energies for each momentum mode are given by the solution (3.21) of the JC model and the corresponding spectrum is shown in the figure (4.2).

From the knowledge of the dispersion relation for different fillings, it is now easy to construct the phase diagram. As discussed in the fermionic approximation scheme, the flat dispersion for  $t = 0$  leads to the ground state having an equal number of excitations in every momentum mode  $k$ . The chemical potentials for  $t > 0$  are then determined by the  $k'$  and  $k$  values, minimizing or maximizing equations (3.23) and (3.24). When looking at the dispersion in figure (4.2), one recognizes that this is given for  $k' = L/2$  and  $k = 0$ . So, the chemical potentials are given by:

$$\mu_n^+ = E_{L/2}^{n+1} - E_{L/2}^n, \quad (4.18)$$

$$\mu_n^- = E_0^n - E_0^{n-1}, \quad (4.19)$$

and when using the analytic form, that is, equations (3.21) and (4.17), the phase boundaries of the  $n$ th Mott lobe read as

$$\begin{aligned} \mu_n^+ = \frac{1}{2} \left\{ -\sqrt{4(n+1)g^2 + \left[\frac{7}{2}\zeta(3)t + \Delta\right]^2} - \frac{7}{1+\delta_{n,0}}\zeta(3)t + \delta_{n,0}\Delta \right. \\ \left. + (1 - \delta_{n,0})\sqrt{4ng^2 + \left[\frac{7}{2}\zeta(3)t + \Delta\right]^2} \right\}, \end{aligned} \quad (4.20)$$

and

$$\mu_n^- = \frac{1 - \delta_{n,1}}{2}\sqrt{4(n-1)g^2 + \Delta^2} - \frac{1}{2}\sqrt{4ng^2 + \Delta^2} + \frac{\delta_{n,1}}{2}\Delta. \quad (4.21)$$

Figure (4.3) shows the resulting phase diagram for three values of  $\Delta$  comparing the different approaches. One recognizes the typical lobe structure of the Mott-insulating phases with a closing of the lobes at some value  $t_n^{crit}(\Delta)$ . While the mean-field results underestimate the extent of the Mott-insulator regions, our fermionic approach overestimates them but with a better agreement with the first order effective strong-coupling model compared to the mean-field solution. The main advantage of the fermionic approximation is the easy closed form for the chemical potentials as well as for the ground state and more reasonable agreement of the critical hopping amplitude  $t_n^{crit}(\Delta)$ , as can be seen from the figure. Figure (4.4) shows the full phase diagram of the model as a function of the detuning  $\Delta$  obtained from the fermionic approximation only.

The critical hopping amplitude  $t_n^{crit}(\Delta)$  can easily be calculated from the analytic expressions for the chemical potential given above. Figure (4.5) shows the dependence of the critical hopping amplitude from the detuning  $\Delta$  for the different Mott lobes. One recognizes the unboundness of the first lobe, i.e.,  $t_n^{crit}(\Delta) \rightarrow \infty$ , as  $\Delta \rightarrow -\infty$ .



## Chapter 5

# Summary of the Work

Phase transitions always attracted the attention of researchers. Quantum phase transition, characterized by a non-thermal control parameter have been of recent interest. The aim of this thesis is to study the quantum phase transition in the Jaynes-Cummings-Hubbard model, which corresponds to a fundamental configuration exhibiting the quantum phase transition of light. First, we introduced the JCH model and discussed some of its features. Then we introduced the way of calculation of the chemical potential which is crucial in the determination of the phase boundaries between the Mott-insulator phase and the Superfluid phase. Then we used a transformation to decouple the hopping term in the JCH Hamiltonian and derived the corresponding mean-field Hamiltonian.

Next, we presented two simple analytic approximation schemes for the determination of the phase boundaries of the Jaynes-Cummings-Hubbard model. The first approximation described the particle-hole excitations in the vicinity of the Mott-insulator to superfluid transition for a specific filling by a simple effective spin model, which generalizes the known results to arbitrary short-range hopping. The second approximation treats the spins as fermions, which allows for a simple solution of the model by means of a Fourier transformation. A comparison of both the methods to the results of density-matrix renormalization group (DMRG) and mean-field data shows reasonable agreement to the numerics. As a testing ground, we selected two systems and applied both the approximation schemes to them. The first one is a JCH model with positive effective-mass and nearest-neighbor hopping and the second, a linear ion chain.

The approximative description by effective strong-coupling Hamiltonians makes very good quantitative predictions for the phase boundaries of the Mott-insulating lobes for small hopping and can be straightforwardly written down upto second order. The fermion approximation also performs very well for the lower boundaries but is less accurate for the upper ones. It does make, however, rather good predictions for the critical hopping at commensurate fillings and has the advantage of giving a closed form for the ground state in the whole parameter regime. Altogether, both methods provide quite reasonable results for the phase boundaries compared to numerical results from DMRG simulations.

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