Phase Transition in 1 – D Holstein – Hubbard Model

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in

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By

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DECLARATION

I, **Mohammed Zahid Malik**, hereby declare that this thesis entitled **" Phase transition in 1 – D Holstein – Hubbard Model "** submitted by me in the School of Physics, University of Hyderabad, India, under the supervision and guidance of **Prof. Ashok Chatterjee** is a bonafide research work which is also free of plagiarism. I also declare that it has not been submitted previously in part or in full to this University or any other University or Institution for the award of any degree or diploma. I hereby agree that my thesis can be deposited.

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CERTIFICATE

This is to certify that the research work described in this thesis entitled **" Phase transition in 1 – D Holstein – Hubbard Model "** has been carried out by **Mohammed Zahid Malik** (Reg. No. 15PHPH16) under my direct guidance and supervision and this has not been submitted for any degree of diploma at this or any other University.

Further, the student has the following publications (1, 2 & 3) in international peer reviewed journals and conference proceedings (4 – 5) before the submission of the thesis for adjudication.

1. **M. Z. Malik**, S. Mukhopadhyay & A. Chatterjee, *Ground state phase diagram of 1D Holstein – Hubbard model, Phys. Lett. A*, 383, *1516 – 1519* (2019).

2. **M. Z. Malik** & A. Chatterjee, *An intervening metallic phase at the CDW – SDW transition region in the one – dimensional Holstein – Hubbard model at half filling: a semi – exact solution.* J. Phys. Commun. 4 (2020) 105005.

3. **M. Z. Malik** & A. Chatterjee, *Quantum entanglement entropy and Double occupancy in a one – dimensional Holstein – Hubbard model at half filling.* Physica E 133 (2021) 114784.

4. **Mr. Zahid Malik**, Soma Mukhopadhyay and Ashok Chatterjee, Existence of *a metallic phase in the charge – density – wave – spin – density – wave crossover region in the 1 – D Hubbard – Holstein model at half filling.* AIP Conf. Proc. 2115 (2018) 030375.

5. **M. Zahid Malik**, Soma Mukhopadhyay & Ashok Chatterjee, Existence of *an intervening metallic phase at the transition region of the charge – density – wave and spin – density – wave in the 1 – D Hubbard – Holstein model.* AIP Conf. Proc. 2142 (2019) 110014.

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PY804	Advanced Electromagnetic Theory	04	Pass
PY821	Research Methodology	04	Pass

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PREFACE

It is well – known that the pairing mechanism for the high – temperature superconductivity (HTCS) in cuprates is still not clear. A number of researchers have advocated the electronic mechanism as the cause of superconductivity in the cuprates. However, quite a few researchers have also suggested the phonon mechanism. Since high – T_c materials like cuprates are strongly correlated narrow – band systems, the Holstein – Hubbard (HH) model should be the suitable model to investigate the HTSC in cuprates. Unfortunately, however, the explanation of superconductivity using the HH model runs into a serious difficulty. To understand this, one has to look into the nature of the ground states provided by the HH model. The HH system can have different quantum phases. When the electron (el) – phonon (ph) interaction is small, the ground state of the HH system is a spin – density – wave (SDW) state and when the el – ph interaction is strong, the ground state of the system is a charge – density – wave (CDW) state. This is not an encouraging scenario from the point of view of superconductivity because to achieve high transition temperature one needs to have strong el – ph interaction, while the strong el – ph interaction leads the system into a CDW insulator. Thus, superconductivity looks impossible in the HH model. Of course, one may be curious to study the transition region. In fact, Hirsch and Fradkin performed a Monte – Carlo study of the HH model and showed that the transition from SDW phase to CDW phase is direct so that there is no metallic phase in the HH model at all.

Takada and Chatterjee (TC) in 2003 took up the 1D half – filled HH model for a more critical analytical investigation and studied the SDW –

CDW transition in this system using a variational method coupled with the Bethe – ansatz technique. Their analysis shows that there exists an intervening metallic phase at the crossover of the SDW – CDW transition.

This theoretical observation is important because the existence of such a metallic state would be just ideal for High – *Tc* superconductivity. The work of TC has been supported by many researchers [*Phys. Rev. Lett. 95, 096401 (2005), Phys. Rev. B. 75, 245103 (2007), Phys. Rev. B 83 033104 (2011)*], but there also exist a few investigations [*Phys. Rev. Lett. 95 226401 (2005), Phys. Rev. B 76 155114 (2007), Phys. Rev. B 75 161103 (R) (2007)*] which refute the existence of the metallic phase predicted by TC. Chatterjee and collaborators [*Physica C. 457, 55 – 59 (2007), Adv. Con. Matt. Phys. 2010, 350787 (2010), Physica B 489, 17 – 22 (2016)*] have therefore studied this problem analytically with more improved variational wave functions. Interestingly, they have shown that each improvement in the variational wave function leads to a broadening of the intermediate metallic phase. This result is important because if an improved variational calculation predicts a narrower metallic phase, the very existence of the intermediate metallic phase will be doubtful. Since the variational calculations performed by Chatterjee and collaborators are still approximate, they can be further modified and improved. In the present work, we make attempts in this direction. We propose more improved variational functions as compared to [*Physica C. 457, 55 – 59 (2007)*] by incorporating the phonon coherence and correlation in a more accurate way and then deal with the effective electronic problem by the exact Bethe – ansatz method [*Phys. Rev. Lett. 20, 1445 – 1448 (1968)*] to accomplish a lower ground state energy. These works are expected to unravel the nature of the phase transition in the HH model more accurately and we will be in a position to make a make more authentic prediction on the width of the metallic phase.

The organization of the thesis is as follows. In Chapter 1, we introduce the subject of the thesis in general and discuss the motivation for carrying out this work. We first describe the Tight – Binding model and then introduce electron correlation and the Hubbard Model. Thereafter we touch upon the concept of phonons and present the Holstein model. In this context we discuss polarons and bipolarons. Next, we present a brief introduction to the Holstein – Hubbard model and discuss the SDW and CDW phases.

In chapter 2, we present our recent work on the HH model in one – dimension (1D) at half filling by where we have used an improved variational calculation. We have employed a series of unitary transformations [*Physica C. 457, 55 – 59 (2007)*] to take into account the coherence and correlation of phonons. To treat the phonon subsystem more accurately a new squeezing transformation is introduced to incorporate the electron – density – dependent phonon correlations to lower the ground energy further. The effective electronic Hamiltonian is next obtained by averaging the transformed Hamiltonian with respect to the zero – phonon state and the resulting effective electronic Hamiltonian is then solved exactly using the method of Bethe – ansatz. Finally, the ground state is obtained by minimizing the energy with respect to all the variational parameters. The method gives better results as compared to the earlier works [*Physica C. 457, 55 – 59 (2007), Adv. Con. Matt. Phys. 2010, 350787 (2010), Physica B 489, 17 – 22 (2016)*], for the ground state energy and also suggests the existence of a wider intermediate metallic phase at the SDW – CDW. The present results lend credence to the initial observation of TC. It may be noted here that it is not important by how much amount the metallic phase widens in an improved approach, rather what is important is that the metallic phase does widen and does not shrink.

In Chapter 3, we study the 1D half – filled HH model with a more improved variational wave function for the phonons than the one used in Chapter 2. In fact, here we consider a Generalized many – phonon state to obtain an effective Hubbard model which we then solve exactly by using Bethe – ansatz technique to obtain the ground state energy. The present variational state leads to a lower ground state energy as compared to those obtained from all the previous variational calculations. Furthermore, we show that the width of the metallic phase also increases with the present improved method.

In Chapter 4, for the same system as in Chapter 3, we study two new parameters namely, the Double Occupancy and the Entanglement Entropy at the boundary of the SDW – CDW phases of the 1D HH system at half filling. The results reconfirm that an intermediate metallic phase exists at the cross – over region of the SDW – CDW phases.

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3.1 Ground state energy (ε_0) per site as a function of onsite Coulomb energy (U) for el – ph interaction strength $\alpha = 1$ and for $t = 0.5\ \omega_0$.

LIST OF ABBREVIATIONS

HTSC	High Temperature Superconductivity
BCS	Bardeen, Cooper, and Schrieffer
GS	Ground State
SDW	Spin Density Wave
0 – D	Zero Dimension
1 – D	One Dimension
2 – D	Two Dimension
3 – D	Three Dimension
CDW	Charge Density Wave
BCS	Bardeen, Cooper and Schrieffer
el – ph	Electron – Phonon
el – el	Electron – Electron
ph – ph	Phonon – Phonon
HH	Holstein Hubbard
TC	Takada Chatterjee
KC	Krishna Chatterjee
HHH	Holstein Hubbard Hamiltonian

VDLF	Variable – Displacement Lang – Firsov
CS	Coherent State
SC	Shankar Chatterjee
MMC	Malik, Mukhopadhyay, and Chatterjee
NN	Nearest Neighbor
NNN	Next Nearest Neighbour
QE	Quantum Entanglement
LO	Longitudinal Optical
AF	Anti – Ferromagnetic
EE	Entanglement Entropy
MC	Malik Chatterjee
QC	Quantum Correlations
DO	Double Occupancy

LIST OF SYMBOLS

T_{BCS}	Transition Temperature for the Superconductivity of Polarons
T_{BP}	Temperature at which two polarons will frame a stable local bi – polaron
T_{BEC}	Bose – Einstein Condensation Temperature for the bi – polarons
H_e	Hamiltonian for Electrons
H_p	Hamiltonian for Phonons
H_{ep}	Hamiltonian for Electron – Phonon Interactions
$c_{i\sigma}^{\dagger}$	Creation Operator for an Electron with spin σ
$c_{j\sigma}$	Annihilation Operator for an Electron with spin σ
$n_{i\sigma}$	Electron Number Operator
t_{ij}	Hopping Integral
U	Coulomb Interaction Energy
$b_i^{\dagger}$	Creation Operator for a Phonon

b_i	Annihilation Operator for a Phonon
ω_0	Frequency of a Phonon
α	Electron – Phonon Coupling Constant
J	Polaron Self – Energy
U_{eff}	Modified Effective Onsite Coulomb Correlation Energy
t_{eff}	Renormalized Hopping Integral
$J_0(x)$	Bessel Function of Zero – th Order
$J_1(x)$	Bessel Function of First Order
S_{av}	Average Local Spin Moment
E_v	Entanglement Entropy
ω	Polaron Self – Energy
D_R	Reduced Density Matrix

Dedicated to my ‘ *Sweet Family* ‘

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***Nephew*: Zohaan Malik**

***Bhabhi*: Mehreen Malik**

***Brother – in – Laws*: Ifqar Mirza & Atif Mirza**

CONTENTS

Chapter 1

Introduction

1.1 Introduction and Motivation

The theory of high – temperature superconductivity in cuprates [1 – 3] has remained a topic of debate in the field of Condensed matter physics for the past few decades. These superconductors are found different from the old superconductors in many ways. For instance, the transition temperature in these new superconductors is much higher compared to the old superconductors in which the superconductivity is caused by Cooper pairing induced by phonon mechanism which can be explained by the BCS (Bardeen, Cooper, and Schrieffer) theory [4]. Furthermore, in high T_c superconductors (HTSC) the coherence length is much smaller than that in the usual superconductors in which the coherence length is of the order of 10^{-4}cm. Though different kinds of mechanisms [5] were recommended in the past, a general agreement has been lacking. In fact, so far no single theory could explain all the properties of HTSC successfully.

One of the prospective mechanisms proposed for causing superconductivity in HTSC is electron (el) – phonon (ph) interaction [6 – 11] which is responsible for creating polarons and bound – pair of polarons called bipolarons. According to some of these models, the normal phase of

these materials ought to contain polarons or bipolarons as quasiparicles. Since these systems are correlated structures, the Holstein model can be considered more suitable than the standard Frohlich model for the description of the corresponding polarons or bipolarons in these systems. Several temperature scales exist in this problem. First is T_{BCS}, the critical temperature corresponding to BCS superconductivity induced by Cooper – pairing of polarons [4]. T_{BP} is another temperature scale. At this temperature, two individual polarons will interact to make a bound state in the real space, which is a static local bipolaron. If T_{BP} is greater than T_{BCS}, the system's normal phase will be characterized by bosonic quasiparticles namely the bipolarons. In this scenario, one can think of another temperature scale namely, T_{BEC} at which bipolarons may undergo the Bose condensation. So, in this case, the Bose condensate of bipolarons can be claimed to be the superconducting phase. A number of properties of cuprates can be explained by the polaronic or bipolaronic mechanism [12 – 17], but some analysts have been critical of this mechanism. The reason is the following. The formation of polarons and bipolarons requires a strong el – ph interaction, which according to these analysts is, however, the biggest stumbling – block of the polaronic theories. If the el – ph coupling is small in strength, a system will be inclined to stay in a spin – density – wave (SDW) ground state (GS) that may be characterized as an antiferromagnetic polaronic state. This is also referred to as the Mott insulating phase. If the el – ph interaction is made strong enough to dominate over the el – el Coulomb repulsion, the net onsite interaction may become attractive and in that case, the GS may be a charge – density – wave (CDW) state. This would be, of course, a bipolaronic state. In this phase, the system behaves as an insulator and may be referred to as the peierls insulator. Thus, on increasing the el – ph interaction from a low value to a high value, one may transform the system from a Mott insulator

to the Peierls insulator. Based on this argument, the system should be in an insulating phase irrespective of the strength of the el – ph interaction. From this point of view, the el – ph mechanism was discounted in the beginning. But one would still like to know the detailed transition behaviour at the CDW – SDW cross – over region. In fact, the SDW – CDW cross – over behaviour of the Holstein – Hubbard model [19 – 23] was explicitly investigated by Hirsch and Fradkin (HF) [18] by using a Monte – Carlo calculation. This study has revealed that as the strength of the el – ph coupling is enhanced, at some el – ph interaction coefficient, the HH system undergoes a direct SDW – CDW transition. In 2003, Takada and Chatterjee (TC) [24] considered the HH Hamiltonian again and looked into SDW – CDW cross – over region more carefully. This study has been on the speculation that the competition between the el – ph interaction and the Coulomb correlation may cause some sort of compromise or frustration leading to an intermediate phase which may not be insulating. TC employed an analytical method and performed a variational calculation coupled with the exact Bethe – ansatz technique [25 – 26] to show the existence of an intervening phase at the SDW – CDW cross – over region in the one – dimensional (1D) HH system and interestingly this intermediate phase has a metallic character. Chatterjee and Takada [27] have subsequently shown that the anharmonicity increases the extent of the conducting region.

The results of TC threw a challenge among the researchers in the area and motivated further investigations on this issue [28 – 35] which supported the prediction of TC. However, there have also been a few investigations [36 – 38] which predicted results that are not in agreement with the results of TC. Since the approach of TC is variational, it would be interesting to make improvements in the calculation of TC and analyze the modified results. An improved variational calculation will of course lower

the GS energy but the important point is to find how the width of the metallic phase changes. It may so happen that in the improved calculation the metallic phase disappears or the extent of the metallic region shrinks. In that case one can have a serious doubt about the presence of the metallic phase. However, if the metallic phase broadens, then one can have more confidence in the prediction of TC. With this goal in mind, Chatterjee and collaborators [39 – 43] have modified the variational calculation of TC and the results of these investigations have supported the result of TC. Since these calculations are approximate, it is important to make more and more accurate calculations and examine the veracity of the results of TC. The main purpose of this thesis is to make attempt in this direction.

1.2 Model

High T_C cuprate superconductors are narrow band materials and electrons in these materials would mostly be localized at the lattice sites and will move from one site to other site only by hoping. To deal with such electrons, one would normally use the Tight – Binding model [44 – 45].

1.2.1 Tight – Binding Model

It is well known that the Tight Binding model [44] is a suitable approach for the calculations of electronic band structures for localized electrons. The method uses a superposition of atomic orbitals. The tight – binding Hamiltonian (H_{TB}) in second quantization notation can be written as:

$$H_{TB} = -\sum_{<ij>} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \ , \qquad (1)$$

where $c_{i\sigma}^{\dagger}(c_{j\sigma})$ is the creation (annihilation) operators of an electron with spin σ, where the notation $\langle i,\ j\rangle$ implies that the summation is over nearest neighbours i and j only and t_{ij} is the hopping integral given by

$$t_{ij} = \int d\boldsymbol{r}\ \varphi_i^*(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U(\boldsymbol{r})\right]\varphi_j(\boldsymbol{r}),$$

where $U(\boldsymbol{r})$ refers to the lattice potential at $\boldsymbol{r}$, $\varphi_{i(j)}(r) = \varphi(r - r_{i(j)})$ are the atomic orbitals, $\boldsymbol{r}_{i(j)}$ being the coordinate of $i(j)$ – th site. The hopping integral finally assumes the following expression:

$$t_{ij} \cong \frac{1}{N}\sum_k \varepsilon_k e^{ik(r_i - r_j)} \qquad (2)$$

where ε_k is the energy of an electron in state $\boldsymbol{k}$.

We calculate the energy of the system using the Bloch function $\psi_k(\boldsymbol{r}_i) = e^{i\boldsymbol{k}.\boldsymbol{r}_i}u_{\boldsymbol{k}}(\boldsymbol{r}_i)$, which is a periodic function and where u has the same periodicity as the lattice. In many systems, t_{ij} would be equal for all nearest neighbours, therefore we choose $t_{ij} = t$. The tight – binding energy for a three – dimensional (3D) system can be written as:

$$\varepsilon_k = -t\sum_\alpha cos(\boldsymbol{k}.\boldsymbol{\alpha})\ . \qquad (3)$$

For a one – dimensional system, there are two nearest neighbours and we have: $\alpha = \pm a$, where a is the lattice constant and the energy of an electron in state k will be given as:

$$\varepsilon_k = -2tcos(ka). \qquad (4)$$

The energy dispersion relation is plotted schematically in Fig. 1.1. If the band contains N (number of unit cells in the system) k states and since each k state can have two electrons, the band can contain $2N$ electrons.

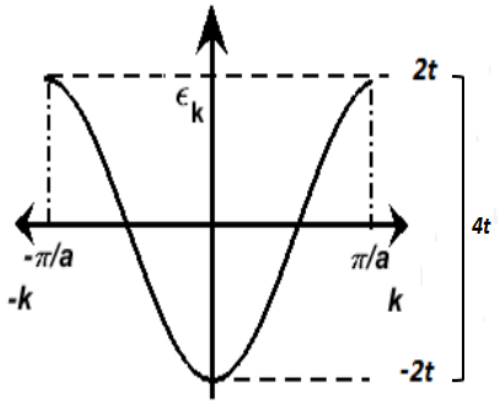

Fig. 1.1 Energy dispersion relation of a Tight – binding model for a $1D$ lattice chain of lattice spacing a.

Fig. 1.1 shows that the Brillouin zone spreads from $-\pi/a$ to π/a and the width of the band is 4t. The Tight – Binding model is a useful model to categorize the materials into metals and insulators, based upon the overlap of the wave functions, band filling factor and the lattice constant. As mentioned above, in narrow band materials, electrons would mostly stay localized at lattice sites and would move from one site to another only by hopping as shown in Fig. 1.2. We consider a one – dimensional (1D) chain of electrons with the assumption that the chain is half filled i.e. we have just one electron per site.

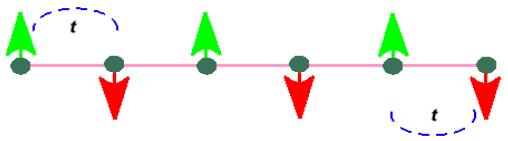

Fig. 1.2 Hopping of an electron from one site to another in a 1D chain of electrons. The parameter t denotes the strength of hopping.

An electron can hop from a certain site to its nearest site by hopping, only if that site is unoccupied or occupied by an electron of opposite spin. The tight – binding model suggests that if we consider one electron per site (which can contain in general two electrons of opposite spins), the band will be half filled and the system should behave as a metal. According to this model, substances like V_2O_3, Fe_3O_4, VnO_2 etc. should be metals but experimentally they turned out to be insulators. So, the simple Band theory cannot justify the non – metallic properties of the systems mentioned above. Mott and Hubbard later elucidated the insulating properties of these materials. They suggested that the insulating behaviour of the aforementioned materials could be attributed to the el – el Coulomb correlation, and these materials are known as Mott insulators. Hubbard proposed a model that provides the necessary framework for dealing with correlated systems and this model is known as the Hubbard model.

1.2.2 Hubbard Model

As mentioned above, Hubbard demonstrated the insulating properties of certain materials introducing the phenomenon of el – el coulomb correlation. The el – el interaction term proposed by Hubbard is given by [20]

$$H_{corr} = U \sum_{i} n_{i\uparrow} n_{i\downarrow} ,$$

where U is the on – site el – el interaction strength (Coulomb correlation strength) and $n_{i\sigma}$ denotes the number operation for spin – σ electrons at the i – th site. $\sigma = \uparrow$ refers to the up – spin state and $\sigma = \downarrow$ refers to the down – spin state of the electron. When the above el – el interaction term is combined with the tight binding Hamiltonian, we get the celebrated Hubbard model which is given by

$$H_{Hubbard} = -t \sum_{ij\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (5)$$

This model permits electrons to hop between neighbouring sites while also allowing them to be localized at the lattice sites. As a result, both the scenarios of localization and delocalization are addressed in this model. The Hubbard model has proved useful in explaining several phenomena in condensed matter physics.

1.3 Polarons and Bipolarons

The concept of polaron was introduced in 1933 by Landau [46]. If we have an impurity electron in an ionic crystal, as shown in the Fig. 1.3, the electron will repel the negative ions and attract the positive ions in its vicinity because of the Coulomb interaction. This will lead to the distortion of the lattice around the electron and consequently a polarization potential for the electron. The electron can then get trapped in this potential, if the potential becomes sufficiently deep. This bound electron will have its own energy levels and was later referred to as a strong – coupling polaron. The name

"polaron" was coined by Pekar. Later, Landau and Peker [47] determined the energy of the polaron and its effective mass.

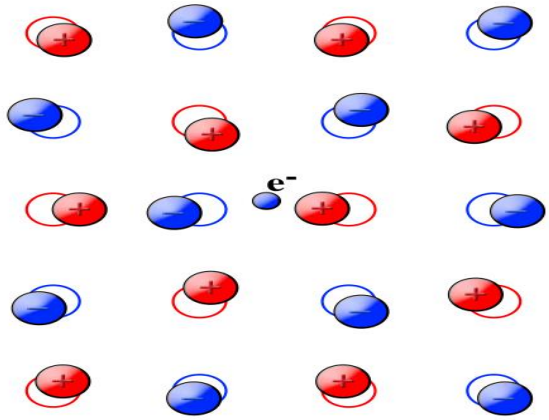

Fig. 1.3 A conduction electron in an ionic crystal.

To characterize a polaron, Frohlich [48] devised a quantum mechanical Hamiltonian. In this picture, an electron distorts the lattice in its neighbourhood and carries the lattice distortion together with it as it moves through the lattice (Fig. 1.4). This complex i.e. the electron together with the lattice distortion constitutes a quasi – particle which is called a polaron [49 – 50].

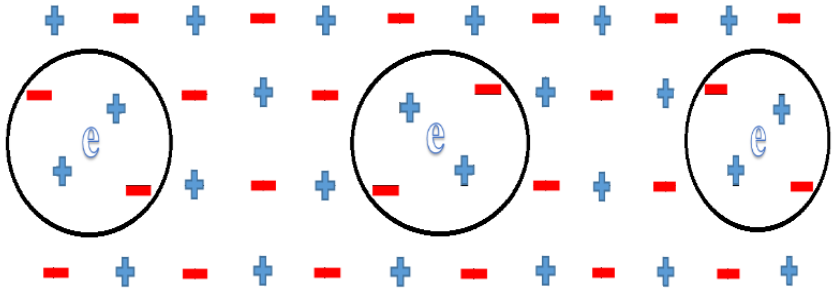

Fig. 1.4 An impurity electron distorting the lattice in its neighborhood as it moves.

If the deformation of the lattice is restricted over a single lattice distance, the corresponding polaron is called a small polaron (Fig. 1.5). This happens when the el – ph interaction is strong. Because in this case, the lattice distortion will be more and the corresponding polarization potential will be deep and as a result, the electron will be trapped in the potential and the polaron will be small. On the other hand, if the lattice distortion is not restricted to one lattice spacing, but extends over a few lattice points in the crystal, then we call it a large polaron, as shown in Fig. 1.5. In this case, the interaction of the electron with the phonons is weak and so the potential created by the electron will be shallow and the corresponding polaron will be large in size. The Fröhlich model is based on the continuum model and therefore it is more suitable for a large polaron.

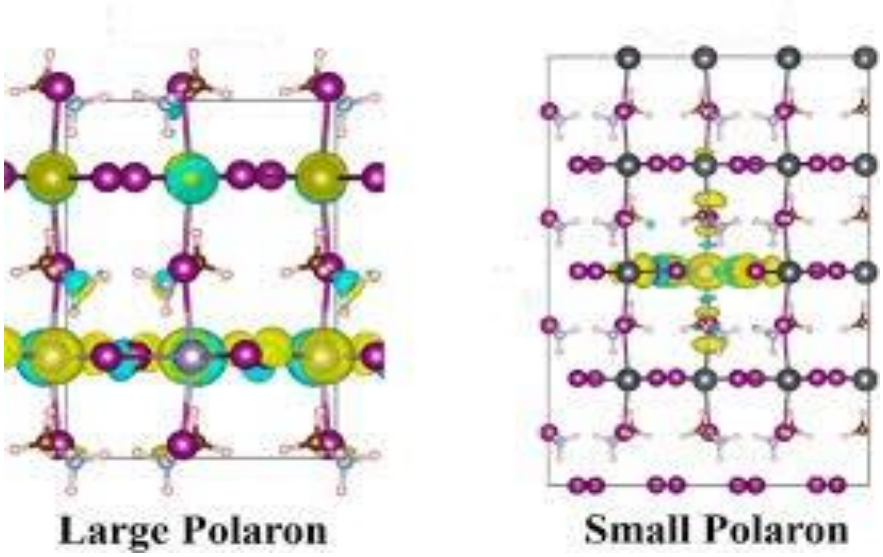

Fig. 1.5 Small and Large polarons

1.4 Holstein Polaron/Polaron in Tight binding model

Based on the Tight – Binding model, Holstein [19] proposed a new formulation for the polaron problem which is more suitable for a small polaron. The Holstein Hamiltonian is given by

$$H = -t\sum_{ij\sigma}\left(c_{i\sigma}^{\dagger}c_{j\sigma}\right) + \hbar\omega_0\sum_{i} b_i^{\dagger}b_i + \; g\sum_{i\sigma} n_{i\sigma}\left(b_i^{\dagger} + b_i\right). \qquad (6)$$

In Eq. (6), the first term is the hopping term where the operator $c_{i\sigma}^{\dagger}(c_{j\sigma})$ creates (annihilates) an electron of spin σ at site i and the parameter t gives the strength of hopping. The second term denotes the phonon Hamiltonian, where the operator $b_i^{\dagger}(b_i)$ creates (annihilates) a phonon of dispersionless frequency ω_0 at site i. The third term gives the el – ph interaction, where g is the el – ph interaction strength.

In a certain situation, the phonon – induced attraction between two electrons may dominate over the repulsive el – el interaction. In such a scenario, two electrons can form a bound pair, which is referred to as a bipolaron [49].

1.5 Holstein – Hubbard Model

When we include lattice dynamics (phonons) in the Hubbard model, then one can also have el – ph interaction in the system (Fig. 1.6).

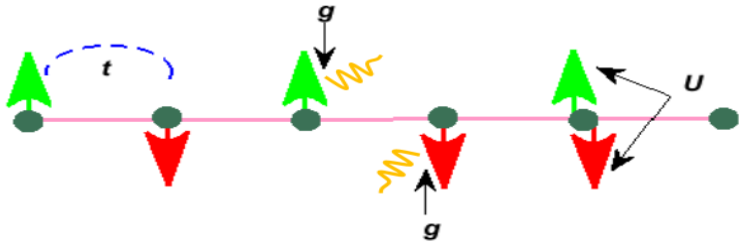

Fig. 1.6 The parameter t gives the strength of hopping, g denotes the strength of the onsite el – ph interaction and U refers to the onsite el – el interaction strength in a 1D chain.

The Holstein – Hubbard (HH) Hamiltonian [21, 22] is given by

$$H = -t\sum_{ij\sigma}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + \hbar\omega_0\sum_{i} b_i^{\dagger}b_i + g\sum_{i\sigma} n_{i\sigma}\left(b_i^{\dagger} + b_i\right) \qquad (7)$$

The el – ph interaction coefficient g is often written as: $g = \sqrt{\alpha}\omega_0$, where α is called the el – ph coupling constant.

Now we have three parameters in the problem, the hopping parameter t, the onsite el – el Coulomb correlation strength U and the onsite el – ph interaction coefficient g. In order to see the competition between the el – el interaction and el – ph interaction, one has to keep the value of t at a certain finite value. The parameter that dominates over the others will decide the ground state of the system.

1.5.1 Spin Density Wave

The antiferromagnetic GS of metals is the spin – density – wave (SDW) state, in which the density of conducting electrons' spins at Fermi level is spatially modulated (Fig. 1.7). Mostly SDW state can be observed in metals and alloys having high density of states at Fermi level. The most leading element where SDW can be observed is Chromium and its alloys. Albert Overhauser [51] was the first to show the existence of SDW for the first time.

If $U \gg g$, all the electrons will stay localized on their respective sites and hence there will not be any movement of electrons from one site to the other. Thus, this is an insulating state and is called a Mott insulating state. In this state, GS of the system will be an SDW state (Fig. 1.7). This is obviously an antiferromagnetic state and this can also be referred to as a polaronic state because in this state the quasi – particles are polarons which form because of the interaction of electrons with the local phonons.

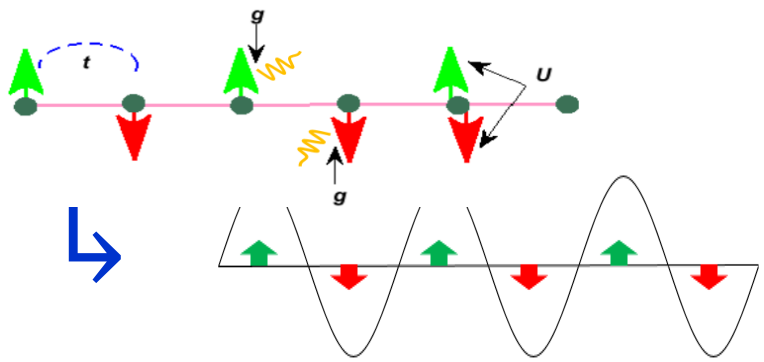

Fig. 1.7 Spin density wave, when on – site el – el interaction strength (U) is greater than the el – ph interaction strength (g) at some finite value of hopping parameter (t).

1.5.2 Charge Density Wave

An orderly placement of electrons in a layered crystal or linear chain compound is the charge density wave (CDW) state (Fig. 1.8). Like SDW, this state also occurs in low dimensional materials at low temperature or in metals and alloys having high density of states at Fermi level. Scanning tunneling microscopy or electron diffraction techniques can be used to observe the periodicity associated with CDWs. Peierls [52] was one of the first to put forward the theory of CDWs, while trying to explain the concept of superconductivity.

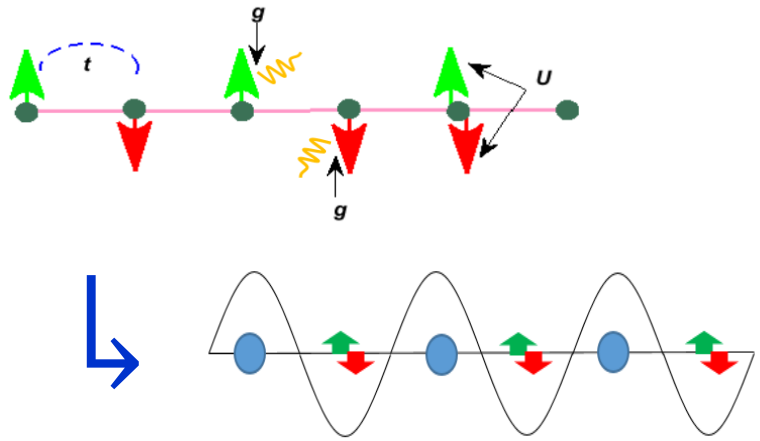

Fig. 1.8. Charge density wave when el – ph interaction strength (g) is greater than the on – site el – el interaction strength (U) at some finite value of hopping parameter (t).

If $g \gg U$, the phonon induced el – el interaction can overcome the repulsive Coulomb correlation giving rise to an effective attractive el – el attraction. An electron can then hop from one site to another and form a bound pair of two electrons. Thus, we will have two bound electrons or a

bipolaron localized on every site and there will not be any movement of electrons after the formation of these bound pairs. This state is called a CDW state in which a gap appears due to Peierls distortion. Such an insulator can therefore be called a Peierls insulator.

1.5.3 Phase Transition in Holstein – Hubbard model

As mentioned above, GS of the HH model can be a SDW state or a CDW state depending on the relative strengths of the el – ph and el – el interactions. However, both are insulating phases and therefore as the el – ph interaction is increased, one would expect the system to undergo an SDW – CDW transition, which is an insulator – to – insulator transition. Thus, the possibility of superconductivity in the HH model looked rather bleak. However, one can still like to find out what happens at the transition region. Hirsch and Fradkin [18] have indeed investigated the behaviour of the SDW – CDW transition in a 1D Holstein – Hubbard system numerically by using a Monte – Carlo simulation technique. It has been shown that the SDW – CDW transition is direct. This suggested that superconductivity in the HH model was impossible.

TC [24] gave a critical re – look at the nature of the SDW – CDW phase transition in a 1D HH model and obtained an analytical solution for the GS energy of the system using a variational calculation coupled with the exact Bethe – Ansatz formalism. TC have claimed the possible existence of an intervening metallic phase at the crossover region of CDW – SDW phases. This finding is naturally important because if such a phase really exists, then it may become superconductive at low temperature. In a subsequent paper, Chatterjee and Takada [24] have demonstrated that the

existence of phonon anharmonicity may increase the extent of the intervening metallic region even further. This work is important because the apex oxygen in the cuprate superconductors does have a substantial anharmonic motion and this anharmonicity has a sizable effect on the properties of these materials **[53 – 57].**

The work of TC has drawn a lot of attention and motivated a good number of investigations because it brought the role of el – ph interaction in high T_c materials again in the forefront of research. Clay and Hardikar [28 – 29] have examined the assertion of TC by studying the same HH model using a numerical approach based on density – matrix renormalization group (DMRG). Their results support the prediction of TC. They have also suggested by calculating the Luttinger liquid correlation exponent that the existing metallic phase can become superconductive. Another study has been carried out by Fehske et al [30] by using density – matrix – renormalization – group technique. They have shown that there exists an intermediate metallic phase particularly for large – phonon frequencies. Payeur and Senechal [31] have employed an exact diagonalization technique and a cluster perturbation theory and have revealed that the possibility of existence of an intermediate – metallic state at the CDW phase boundary cannot be rejected. A determinant quantum Monte – Carlo analysis has been carried out by Nowadnick et al. [32] in two – dimensions (2D). This investigation also reveals the presence of an intervening metallic region. Assaad and Hohenadler [33] have also verified the presence of such an intermediate metallic phase. Bourbonnais and Bakrim [34] have shown that the renormalization group technique and the quantum Monte – Carlo technique yield similar results and both the techniques support the existence of the intermediate metallic phase. Wang. et al. [35] have studied the GS features of the 2D HH Hamiltonian using an exact diagonalization

technique and provided an evidence for the presence of an intermediate phase flanked by the SDW and CDW states.

However, a few investigations have also disagreed with the assertion of TC [36 – 38]. Tezuku et al. [36] have used DMRG to investigate the HH Hamiltonian for large values of el – el and el – ph coupling strengths. The study of the region flanked by the adiabatic and anti – adiabatic regimes has shown that pairing and CDW correlations are degenerate when the el – el and el – ph interactions are of equivalent strength. It has also been discovered that when the phonons have much larger energy compared to the el – ph interaction energy and also the electron – hole symmetry is absent, the CDW and the on – site superconducting phases overlap, requiring no intermediate phase in the SDW – CDW transition. Tezuka et al. [37] have generated correlation functions using real – space dynamics in a modified study and discovered a metallic gap between the SDW and CDW phases in the pure (un – doped) HH model, but the pairing correlation has been found more significant in the doped HH model in the absence of electron – hole symmetry. Tam et al. [38] have used the renormalization group (RG) method to investigate the 1D HH model at half – filling treating the el – ph and el – el interactions on an equal footing. They have also considered the probable retardation effects of the phonon dynamics. Their results show a direct transition from the CDW state to the SDW state.

According to the findings of the above studies it is therefore important to examine the authenticity of the result of TC through more accurate analytical calculations. The aim is to find out the extent of the intervening metallic phase by using more accurate phonon wave functions. As has been mentioned earlier, if a more accurate wave function leads to the shrinking of the width of the intermediate metallic phase or its disappearance

altogether, then the prediction of TC is certainly questionable. On the other hand, if the width of metallic phase increases, then the results of TC will have more credibility. With this motivation, Chatterjee and collaborators [39 – 43] have modified the variational calculation of TC and the results of these investigations have supported the result of TC. However, these calculations are variational in nature and thus approximate and therefore systematic attempts to improve the variational phonon state are called for to bring out the accurate picture of the nature of the SDW – CDW transition. Recently we have made attempts in this direction [58 – 61] The purpose of this thesis is to present these works.

1.6 Organization of the thesis

In the chapter following the present one i. e. in Chapter 2, we analyze the 1D HH model at half – filling using a sequence of unitary transformations that incorporate coherence and correlations of the phonons followed by a zero – phonon averaging. The phonon wave function chosen here is more accurate than the one used in [24]. We have introduced a new squeezing transformation that depends on the electron concentration to treat the phonon sub – system. This new transformation treats the phonon correlation in a more realistic way. The effective Hamiltonian obtained after phonon averaging is exactly solved by the technique of Bethe – ansatz and finally the GS energy and the intermediate metallic phase are obtained.

In the Chapter 2, we performed a series of canonical transformed and used a zero – phonon state to obtain the effective electron Hamiltonian which has been solved by the Bethe – ansatz technique. In Chapter 3, we extend the work of Chapter 2 by introducing a generalized many – phonon state to eliminate the phonon degrees of freedom. We show that this

modified variational method broadens the width of the intermediate metallic phase.

In Chapter 4, we take up the same 1D HH model and present our calculation of two parameters namely, the Quantum Entanglement Entropy and Double Occupancy. We show that in a plane of Coulomb correlation strength and el – ph coupling constant, a phase exists which is flanked by the CDW and SDW phases and this phase is proven to be a metallic phase.

In the final chapter i. e., Chapter 5, we briefly present a summary of our results and prove some concluding remarks.

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Chapter 2

Ground – state phase diagram of the one dimensional Holstein – Hubbard model

2.1 Introduction

We have already explained in Chapter 1 that it is important to examine the nature of the spin – density – wave (SDW) [1] charge – density – wave (CDW) [2] transition in a Holstein – Hubbard (HH) system analytically in the context of high T_c superconductivity. In this context, Takada and Chatterjee (TC) [3] made an interesting study in 2003 on the one – dimensional (1D) half – filled HH model [4 – 8] to show that there exists an intermediate metallic phase at the SDW – CDW transition region. Several investigations [9 – 16] supported this result, though a few [17 – 19] also discounted it. Later, Chatterjee and collaborators [20 – 24] modified the analytical calculation of TC using more improved phonon states and supported the claim of TC. Since these calculations are variational and hence approximate, calculations with more accurate phonon states are called for to confirm the veracity of the assertion of TC. In this chapter, we improve the variational phonon state used by (KC) [20] and show that this modification leads to a wider metallic phase at the crossover region of SDW – CDW phases.

2.2 The Hubbard – Holstein (HH) Hamiltonian

The HH Hamiltonian to be studied has been introduced in Chapter 1. It is given by:

$$H = H_e + H_p + H_{ep}\,, \tag{1}$$

where H_e is the electronic Hamiltonian given by

$$H_e = -t \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

H_p is the free phonon Hamiltonian given by:

$$H_p = \omega_0 \sum_{i} b_i^{\dagger} b_i, \tag{3}$$

and H_{ep} is the el – ph interaction given by

$$H_{ep} = g \sum_{i\sigma} n_{i\sigma}\,(b_i^{\dagger} + b_i), \tag{4}$$

Though all the symbols in the above equations have already been defined in Chapter 1, we define them again here for the sake of completeness. In Eq. (2), t denotes the bare hopping integral, $c_{i\sigma}^{\dagger}(c_{j\sigma})$ refers to the creation (annihilation) operator for an electron of spin σ at the i^{th} site and $< \cdots >$ denotes that the summation is to be carried out over nearest neighbours only. In Eq. (2), U denotes the onsite correlation energy and $n_{i\sigma}\left(\equiv c_{i\sigma}^{\dagger} c_{i\sigma}\right)$ stands for the "number operator" for electrons of spin σ at the i^{th} site. In Eq. (3), $b_i^{\dagger}(b_i)$ represents the creation (annihilation) operator for an optical phonon with dispersion – less frequency ω_0 at the i^{th} site and g is called

the el – ph interaction coefficient. We write: $g = \sqrt{\alpha}\omega_0$, where α is called the el – ph coupling constant and is dimensionless.

2.3 Formulation

The Hamiltonian (1) is not exactly soluble. So we carry out a set of unitary transformations to solve it approximately. We first perform a variable – displacement Lang – Firsov transformation (VDLFT) [25]:

$$S_1 = e^{R_1} , \tag{5}$$

with the generator R_1 given by

$$R_1 = \frac{g'}{\omega_0} \sum_{i\sigma} n_{i\sigma} \left(b_i^{\dagger} - b_i \right) , \tag{6}$$

where g' has to be obtained variationally. We make the following choice of g':

$$g' = \sqrt{\alpha}\eta \, \omega_0 , \tag{7}$$

where η is to be treated as a new variational parameter. The Hamiltonian H now transforms to

$$H_1 = e^{R_1} H e^{-R_1} . \tag{8}$$

Using the following variant of the Baker – Cambell – Haudroff formula

$$\tilde{A} = e^{S} H e^{-S}$$

$$= A + [S, A] + \frac{1}{2\,!} \left[S, [\, S, A\,] \right] +$$

$$+ \frac{1}{3!} \left[S, \left[S, [\, S, A\,] \right] \right] + .. , \tag{9}$$

we have

$$H_1 = H + [R_1, H] + \frac{1}{2!}[R_1, [R_1, H]] + \ldots\ldots \qquad (10)$$

where $H = H_e + H_p + H_{ep}$, as given in Eq. (1). Now we need to calculate the commutators appearing in Eq. (9). Let us first consider $[R_1, H]$ which can be written as

$$[R_1, H] = [R_1, H_e] + [R_1, H_p] + [R_1, H_{ep}]\,. \qquad (11)$$

We obtain the following results.

$$[R_1, H_e] = -\,t\eta\sqrt{\alpha} \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \left(\left(b_i^{\dagger} - b_i \right) - \left(b_j^{\dagger} - b_j \right) \right), \qquad (12)$$

$$\left[R_1, [R_1, H_e]\right] = -t\alpha\eta^2 \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \left(\left(b_i^{\dagger} - b_i \right) - \left(b_j^{\dagger} - b_j \right) \right)^2, \qquad (13)$$

$$\left[R_1, H_p\right] = -\sqrt{\alpha}\eta\, \omega_0 \sum_{i\sigma} n_{i\sigma} \left(b_i^{\dagger} + b_i \right), \qquad (14)$$

$$\left[R_1, \left[R_1, H_p\right]\right] = \left(\sqrt{\alpha}\eta\right)^2 \omega_0 \sum_{i\sigma\sigma'} n_{i\sigma}\, n_{i\sigma'}, \qquad (15)$$

$$\left[R_1, H_{ep}\right] = -2g\sqrt{\alpha}\eta \sum_{i\sigma\sigma'} n_{i\sigma}\, n_{i\sigma'}, \qquad (16)$$

$$\left[R_1, \left[R_1, H_{ep}\right]\right] = 0\,. \qquad (17)$$

In order to calculate the above commutators, we use the following result

$$[\,A\,B\,,C\,D\,] = A\,\{\,B\,,C\,\}\,D - A\,C\,\{\,B\,,D\,\}$$

$$+\,\{\,A\,,C\,\}\,D\,B - C\,\{\,A\,,D\,\}\,B \qquad (18)$$

and the relation

$$\sum_{i\,\sigma} n_{i\,\sigma}^{\,2} = \sum_{i\,\sigma\,\sigma'} n_{i\sigma}\,n_{i\sigma'} = \sum_{i} [(n_{i\uparrow} + n_{i\downarrow})(n_{i\uparrow} + n_{i\downarrow})]$$

$$= \sum_{i\,\sigma} n_{i\sigma} + \sum_{i} 2n_{i\uparrow}n_{i\downarrow} \quad . \qquad (19)$$

Thus, the transformed Hamiltonian after the first transformation becomes

$$H_1 = -\,t \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}\, e^{x_i - x_j} + U_{eff} \sum_{i} n_{i\uparrow}n_{i\downarrow}$$

$$+\,\omega_0 \sum_{i} b_i^{\dagger} b_i + P \sum_{i\sigma} n_{i\sigma}\,(b_i^{\dagger} + b_i) + Q \sum_{i\,\sigma} n_{i\,\sigma}^{\,2}, \quad (20)$$

where the operator x_i is given by:

$$x_i = \sqrt{\alpha}\eta\,\left(b_i^{\dagger} - b_i\right) \qquad (21)$$

and the parameters P, Q and the effective onsite Coulomb correlation energy U_{eff} are given by

$$U_{eff} = U - 2\alpha\omega_0\eta(2-\eta)\,, \qquad (22)$$

$$P = \omega_0\sqrt{\alpha}(1-\eta)\ , \qquad (23)$$

$$Q = \alpha\omega_0\eta(\eta-2)\ \ . \qquad (24)$$

In the usual LF method [25], η is chosen to be equal to 1, which implies: $g' = g$. One then calculates the effective electronic Hamiltonian of the system by zero – phonon averaging. This would be a fairly good assumption for strong el – ph coupling in the anti – adiabatic regime. By varying η, however, a more accurate GS may be obtained in the weak and intermediate – coupling region. In VDLFT, the phonon coherence is assumed to be proportional to the electron density, n_i and the parameter η provides an information about the extent of lattice distortion. In the large – α regime, $\eta \to 1$, but in the intermediate – coupling region, it decreases, resulting in a better total energy by balancing the tendency for an electron to localize due to el – ph coupling and the tendency to delocalize due to the hopping term.

We next perform the transformation by the operator

$$S_2 = e^{R_2} , \tag{25}$$

where

$$R_2 = h \sum_{k\sigma} \left(b_k^{\dagger} - b_k \right) , \tag{26}$$

where h is considered as a variational parameter. The transformed Hamiltonian H_2 obtained after the transformation by S_2 can be written as

$$H_2 = H_1 + [R_2, H_1] + \frac{1}{2!} [R_2, [R_2, H_1]] + \cdots . \tag{27}$$

To obtain H_2, we use calculate the following commutators.

$$[\,R_2, e^{x_{i-j}}] = e^{x_{i-j}} \tag{28}$$

$$\left[\,R_2, b_i^\dagger b_i\right] = -h\left(b_i^\dagger + b_i\right)\ , \tag{29}$$

$$\left[R_2, \left[R_2, b_i^\dagger b_i\right]\right] = h^2\ , \tag{30}$$

$$\left[\,R_2, \left(b_i^\dagger + b_i\right)\right] = -2h\ . \tag{31}$$

where we use the relation

$$[AB, CD] = AC[B, D] + A[B, C]D + C[A, D]B + [A, C]DB\ . \tag{32}$$

The transformed Hamiltonian after second transformation is given by

$$H_2 = -t \sum_{<i,j>\sigma} c_{i\sigma}^\dagger c_{j\sigma}\, e^{x_{i-j}} + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_i b_i^\dagger b_i + h^2\omega_0$$

$$-h\omega_0 \sum_i \left(b_i^\dagger + b_i\right) + P \sum_{i\sigma} n_{i\sigma}\left(b_i^\dagger + b_i - 2h\right) + Q \sum_{i\sigma} n_{i\sigma}^2\ , \tag{33}$$

where the parameters x_{i-j}, U_{eff}, P and Q have already been defined. A solution with non – zero h yields a significantly lesser energy, particularly when U is positive and large. The two transformations S_1 and S_2 together can be generated by the generator

$$R_{12} = \sum_{k\sigma} \left[h + \eta\sqrt{\alpha}\left(n_{k\sigma} - \frac{h}{\sqrt{\alpha}}\right)\right]\left(b_k^\dagger - b_k\right). \tag{34}$$

The first transformation with generator R_1 takes cares of the anti – adiabatic regime $(\eta = 1)$, whereas the second transformation takes care of the adiabatic regime $(\eta = 0)$. So, by optimizing η between 0 and 1, we make our calculation valid over the entire adiabatic and antiadiabatic regions.

Next, we perform a two – phonon coherence state transformation, also known as a squeezing transformation [26] by S_3 :

$$S_3 = e^{R_3} \tag{35}$$

where

$$R_3 = \alpha_s \sum_i \left(b_k b_k - b_k^\dagger b_k^\dagger\right) \tag{36}$$

where α_s is a variational parameter. This transformation, also called a Bogolubov transformation, addresses the phonon correlation at the same site. It also incorporates the phonon anharmonicity partly.

The transformed Hamiltonian H_3 after carrying out the transformation by S_3, can be written as:

$$H_3 = H_2 + [R_3, H_2] + \frac{1}{2!}[R_3, [R_3, H_2]] + \ldots\ldots . \tag{37}$$

To obtain the expression for H_3, we calculate the following commutators.

$$\left[R_3, b_i^\dagger\right] = 2\alpha_s b_i \ , \tag{38}$$

$$\left[R_3, \left[R_3, b_i^\dagger\right]\right] = (2\alpha_s)^2 b_i^\dagger \ , \tag{39}$$

$$[R_3, b_i] = 2\alpha_s b_i^\dagger \ , \tag{40}$$

$$\left[R_3,[R_3,b_i]\right]=(2\alpha_s)^2 b_i \quad . \tag{41}$$

$$[\,R_3,e^{x_{i-j}}]=e^{x_{i-j}e^{-2\alpha_s}} \tag{42}$$

$$\left[\,R_3,\left(b_i^\dagger+b_i\right)\right]=\left(b_i^\dagger+b_i\right)e^{2\alpha_s} \tag{43}$$

$$\left[R_3,b_i^\dagger b_i\right]=\left(b_i^\dagger cosh(2\alpha_s)+b_i sinh(2\alpha_s)\right)$$

$$\times\left(b_i cosh(2\alpha_s)+b_i^\dagger sinh(2\alpha_s)\right) \tag{44}$$

The transformed Hamiltonian H_3 obtained after third canonical transformation reads

$$H_3=-\,t\sum_{<i,j>\sigma}c_{i\sigma}^\dagger c_{j\sigma}\exp(x_{i-j}e^{-2\alpha_s})+U_{eff}\sum_i n_{i\uparrow}n_{i\downarrow}+Q\sum_{i\sigma}n_{i\sigma}^2$$

$$+\omega_0\left(h^2-h\sum_i\left(b_i^\dagger+b_i\right)e^{2\alpha_s}\right)+P\sum_{i\sigma}n_{i\sigma}((b_i^\dagger+b_i)e^{2\alpha_s}-2h)$$

$$+\omega_0\sum_i\left\{\left(b_i^\dagger+b_i\right)^2\frac{e^{4\alpha_s}}{4}-\left(b_i^\dagger-b_i\right)^2\frac{e^{-4\alpha_s}}{4}-\frac{1}{2}\right\}. \tag{45}$$

Here we have used the relation

$$\left(\,b_i^\dagger\,cosh\,(\,2\,\alpha_s\,)\,+\,b_i\,sinh\,(\,2\,\alpha_s\,)\,\right)$$

$$\times\left(\,b_i\,cosh\,(\,2\,\alpha_s\,)+\,b_i^\dagger\,sinh\,\,(\,2\,\alpha_s\,)\,\right)$$

$$=\left\{\left(\,b_i^\dagger\,+\,b_i\,\right)^2\,\frac{e^{\,4\,\alpha_s}}{4}\,-\,\left(\,b_i^\dagger\,-\,b_i\,\right)^2\,\frac{e^{\,-\,4\,\alpha_s}}{4}\,-\,\frac{1}{2}\right\}. \tag{46}$$

The parameter α_s has always been treated as a constant in the context of HH model. This implies that the phonon correlation is unaffected by electron density. However, in reality, this is not true, particularly if the electron density is high. We therefore propose a new squeezing transformation that takes into account the electron density – dependent phonon correlation. We assume that the phonon correlation is proportional to the electron density at a given particular site. Thus our new canonical transformation is given by

$$S_4 = e^{R_4} \quad , \tag{47}$$

where

$$R_4 = \alpha_d \sum_{k\sigma} n_{k\sigma}(b_k b_k - b_k^\dagger b_k^\dagger) \ , \tag{48}$$

α_d being a variational parameter. As before, H_4 can be written as

$$H_4 = H_3 + [R_4, H_3] + \frac{1}{2!}[R_4, [R_4, H_3]] + \ldots . \tag{49}$$

The commutators now become very messy. So we do not give all the commutators here expect for two general results.

$$e^{R_4}\left(b_i^\dagger \pm b_i\right)e^{-R_4} = \left(b_i^\dagger \pm b_i\right)e^{\pm 2\alpha_d \sum_\sigma n_{i\sigma}} \ , \tag{50}$$

$$\boldsymbol{e^{R_4}\left(b_i^\dagger \pm b_i\right)^2 e^{-R_4}} = \boldsymbol{\left(b_i^\dagger \pm b_i\right)^2 e^{\pm 4\alpha_d \sum_\sigma n_{i\sigma}}} . \tag{51}$$

The transformed Hamiltonian after this new canonical transformation reads

$$H_4 = -t' \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + P \sum_{i\sigma} n_{i\sigma} \left[\{ (b_i^{\dagger} + b_i) e^{\pm 2\alpha_d \sum_{\sigma'} n_{i\sigma'}} \} e^{2\alpha_s} - 2h \right]$$

$$+Q \sum_{i\sigma} n_{i\sigma}^2 + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \left[h^2 - h \sum_i (b_i^{\dagger} + b_i) e^{(2\alpha_s + 2\alpha_d \sum_{\sigma} n_{i\sigma})} \right]$$

$$+\omega_0 \sum_{ii'} \left[-\frac{1}{2} + \frac{1}{4} (b_i^{\dagger} + b_i)^2 e^{(4\alpha_s + 4\alpha_d \sum_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'})} \right.$$

$$\left. -\frac{1}{4} (b_i^{\dagger} - b_i)^2 e^{(-4\alpha_s - 4\alpha_d \sum_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'})} \right], \qquad (52)$$

where we have used the relations

$$\sum_{i\sigma} n_{i\sigma}^3 = \sum_{i\sigma} n_{i\sigma} + \sum_i 6\, n_{i\uparrow} n_{i\downarrow} \qquad (53)$$

and

$$n_{i\uparrow}^2 = n_{i\uparrow} n_{i\downarrow}^2 = n_{i\downarrow}. \qquad (54)$$

The modified parameters in Eq. (52) are given by

$$t' = t \exp(x'_{i-j}) \exp(x_{i-j} e^{-2\alpha_s - 2\alpha_d \sum_{\sigma'} n_{i\sigma'}}), \qquad (55)$$

$$x'_{i-j} = \alpha_d \left[(b_i b_i - b_i^{\dagger} b_i^{\dagger}) - (b_j b_j - b_j^{\dagger} b_j^{\dagger}) \right]. \qquad (56)$$

We have ignored all inter–site phonon correlations so far. A unitary transformation can be used to implement correlation between phonons at different sites. Following [27] we perform the transformation

$$S_5 = e^{R_5}, \qquad (57)$$

where

$$R_5 = \frac{1}{2}\sum_{k\neq k'} \beta_{kk'}\left(b_k b_{k'} - b_k^{\dagger} b_{k'}^{\dagger}\right) \ , \tag{58}$$

$\beta_{kk'}'s$ being variational parameters. For the sake of convenience, we stipulate that $\beta_{kk'} = \beta$, when k and k' refer to nearest neighbors and $\beta_{kk'} = 0$, otherwise. The Hamiltonian $H_5 = e^{R_5} H_4 e^{-R_5}$ is now given by

$$H_5 = H_4 + [R_5, H_4] + \frac{1}{2!}[R_5, [R_5, H_4]] + \ldots\ldots \ , \tag{59}$$

The relevant commutators are calculated as

$$\left[R_5, b_i^{\dagger}\right] = \sum_{k\neq i} \beta_{ki}\, b_k \ \ , \tag{60}$$

$$\left[R_5, \left[R_5, b_i^{\dagger}\right]\right] = \sum_{kj} \beta_{ik}\, \beta_{kj} b_j^{\dagger} \ , \tag{61}$$

$$\left[R_5, \left[R_5, \left[b_i^{\dagger}\right]\right]\right] = \sum_{kjl} \beta_{ik}\, \beta_{kj} \beta_{jl} b_l \ \ , \tag{62}$$

$$[R_5, b_i] = \sum_{k\neq i} \beta_{ki}\, b_k^{\dagger} \ , \tag{63}$$

$$\left[R_5, [R_5, b_i]\right] = \sum_{kj} \beta_{ik}\, \beta_{kj} b_j \ \ , \tag{64}$$

$$\left[R_5, \left[R_5, [b_i]\right]\right] = \sum_{kjl} \beta_{ik}\, \beta_{kj} \beta_{jl} b_l^{\dagger} \ \ . \tag{65}$$

We also obtain

$$e^{R_5}\left(b_i^{\dagger} \pm b_i\right)e^{-R_5} = \sum_j \left(\mu_{ij} \pm \vartheta_{ij}\right)\left(b_j^{\dagger} \pm b_j\right), \qquad (66)$$

where μ_{ij} and ϑ_{ij} are given by

$$\mu_{ij} = \delta_{ij} + \frac{1}{2!}\sum_k \beta_{ik}\beta_{kj} + \frac{1}{4!}\sum_{klm} \beta_{ik}\beta_{kl}\beta_{lm}\beta_{mj} + \ldots. \quad (67)$$

$$\vartheta_{ij} = \beta_{ij} + \frac{1}{3!}\sum_{kl} \beta_{ik}\beta_{kl}\beta_{lj} + \frac{1}{5!}\sum_{klmn} \beta_{ik}\beta_{kl}\beta_{lm}\beta_{mn}\beta_{nj} + \ldots.. \quad (68)$$

so that we can write

$$\mu_{ij} \pm \vartheta_{ij} = e^{\pm \boldsymbol{\beta}}\ . \qquad (69)$$

where $\boldsymbol{\beta}$ (having periodic boundary conditions) is an $N \times N$ matrix. Using the above equations (69) and the formula

$$e^{A+B} = e^{A} + e^{B} + e^{-\frac{1}{2}[A,B]}\ , \qquad (70)$$

we obtain

$$H_5 = -t' \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}\, U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow} + Q \sum_{i\sigma} n_{i\sigma}^2$$

$$+ P \sum_{i\sigma} n_{i\sigma} \left[\sum_j (\mu_{ij} + \vartheta_{ij})\,(b_j^{\dagger} + b_j) e^{2\alpha_d \Sigma_{\sigma'} n_{i\sigma'}} e^{2\alpha_s} - 2h\right]$$

$$+\omega_0\left(h^2-h\sum_{ij}(\mu_{ij}+\vartheta_{ij})(b_i^\dagger+b_i)e^{(2\alpha_s+2\alpha_d\sum_\sigma n_{i\sigma})}\right)$$

$$+\frac{1}{4}\,\omega_0\sum_{ijj'}\{(\mu_{ij}+\vartheta_{ij})(\mu_{ij'}+\vartheta_{ij'})(b_j^\dagger+b_j)^2 e^{(4\alpha_s+4\alpha_d\sum_{\sigma\sigma'}n_{i\sigma}n_{i\sigma'})}$$

$$-(\mu_{ij}-\vartheta_{ij})(\mu_{ij'}-\vartheta_{ij'})(b_j^\dagger-b_j)^2$$

$$\times e^{(-4\alpha_s-4\alpha_d\sum_{\sigma\sigma'}n_{i\sigma}n_{i\sigma'})}-\frac{1}{2}\}, \qquad (71)$$

where

$$t'=Tt\,e^{(-\frac{1}{2}e^{-4\alpha_s-4\alpha_d\sum_\sigma n_{i\sigma}})}\sum_k A_k^2\ , \qquad (72)$$

$$A_k^2=\left(\sqrt{\alpha}\eta(\mu_{ik}-\vartheta_{ik})-(\mu_{jk}-\vartheta_{jk})\right)^2\ , \qquad (73)$$

$$T=e^{\alpha_d\sum_{jki'}\{B_{jk}(b_jb_k-b_j^\dagger b_k^\dagger)+C_{jk}(b_jb_k^\dagger-b_j^\dagger b_k)\}}\ , \qquad (74)$$

with

$$B_{jk}=\left((\mu_{ij}\mu_{ik}-\vartheta_{ij}\vartheta_{ik})-(\mu_{i'j}\mu_{i'k}-\vartheta_{i'j}\vartheta_{i'k})\right)\ , \qquad (75)$$

$$C_{jk}=\left((\mu_{ij}\vartheta_{ik}-\vartheta_{ij}\mu_{ik})-(\mu_{i'j}\vartheta_{i'k}-\vartheta_{i'j}\mu_{i'k})\right)\ . \qquad (76)$$

Ultimately, we restore the coherence in the phonon subsystem by performing the final transformation with the operator

$$S_6=e^{R_6}\ , \qquad (77)$$

where

$$R_6 = \Delta \sum_k (b_k^\dagger - b_k) \ , \tag{78}$$

Δ being a variational parameter. We obtain the following results.

$$e^{R_6}\left(b_i^\dagger + b_i\right)e^{-R_6} \ = \ \left(b_i^\dagger + b_i\right) - 2\Delta \tag{79}$$

$$e^{R_6}\left(b_i^\dagger + b_i\right)^2 e^{-R_6} \ = \ \left(b_i^\dagger + b_i\right)^2 + 4\Delta^2 \tag{80}$$

$$e^{R_6}\left(b_i^\dagger - b_i\right)e^{-R_6} \ = \ \left(b_i^\dagger - b_i\right) \tag{81}$$

$$e^{R_6}\left(b_i^\dagger - b_i\right)^2 e^{-R_6} \ = \ \left(b_i^\dagger - b_i\right)^2 \tag{82}$$

The final transformed Hamiltonian $H_6 = e^{R_6} H_5 e^{-R_6}$ can again be written as:

$$H_6 = e^{R_6} H_5 e^{-R_6}$$

$$= H_5 + [R_6, H_5] + \frac{1}{2!}[R_6, [R_6, H_5]] + \ldots\ldots \tag{83}$$

We obtain

$$H_6 = -t' \sum_{<i,j>\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow} + Q \sum_{i\sigma} n_{i\sigma}^2$$

$$+ P \sum_{i\sigma} n_{i\sigma} \{\sum_j (\mu_{ij} + \vartheta_{ij}) ((b_j^\dagger + b_j) - 2\Delta) e^{2\alpha_d \Sigma_{\sigma'} n_{i\sigma'}} e^{2\alpha_s} - 2h\}$$

$$+\frac{\omega_0}{4}\sum_{ijj'}\{-(\mu_{ij}-\vartheta_{ij})(\mu_{ij'}-\vartheta_{ij'})(b_j^\dagger-b_j)^2 e^{(-4\alpha_s-4\alpha_d\sum_{\sigma\sigma'}n_{i\sigma}n_{i\sigma'})}$$

$$+(\mu_{ij}+\vartheta_{ij})(\mu_{ij'}+\vartheta_{ij'})\left((b_j^\dagger+b_j)^2+4\Delta^2\right)e^{(4\alpha_s+4\alpha_d\sum_{\sigma\sigma'}n_{i\sigma}n_{i\sigma'})}-\frac{1}{2}\}$$

$$+\omega_0\left(h^2-h\sum_{ij}((\mu_{ij}+\vartheta_{ij})((b_i^\dagger+b_i)-2\Delta))\exp(2\alpha_s\right.$$

$$\left.+2\alpha_d\sum_{\sigma}n_{i\sigma})\right)\ , \tag{84}$$

where

$$t'=Tt\exp\left(-\frac{1}{2}e^{-4\alpha_s-4\alpha_d\sum_\sigma n_{i\sigma}}\right)\sum_k A_k^2\ \ , \tag{85}$$

$$T=\exp(\alpha_d\sum_{jki'}\{B_{jk}(b_jb_k-b_j^\dagger b_k^\dagger)+C_{jk}(b_jb_k^\dagger-b_j^\dagger b_k)\})\ , \tag{86}$$

$$A_k^2=\left(\sqrt{\alpha}\eta(\mu_{ik}-\vartheta_{ik})-(\mu_{jk}-\vartheta_{jk})\right)^2\ \ , \tag{87}$$

with

$$B_{jk}=\left((\mu_{ij}\mu_{ik}-\vartheta_{ij}\vartheta_{ik})-(\mu_{i'j}\mu_{i'k}-\vartheta_{i'j}\vartheta_{i'k})\right)\ , \tag{88}$$

$$C_{jk}=\left((\mu_{ij}\vartheta_{ik}-\vartheta_{ij}\mu_{ik})-(\mu_{i'j}\vartheta_{i'k}-\vartheta_{i'j}\mu_{i'k})\right). \tag{89}$$

2.2.2 Averaging Phonon state

Now we calculate the expectation value of H_6 in the zero – phonon state

$$|0> = \prod_i |0_i> , \tag{90}$$

where $i = 1,2,3, \ldots, N$. The final effective electronic Hamiltonian is given by

$$H_{eff} = <0|H_6|0>$$

$$= -J \sum_{i\sigma} n_{i\sigma} + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow} - t_{eff} \sum_{ij\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \omega_0 h^2$$

$$+ \Delta\, e^{\boldsymbol{\beta}}\, e^{2\alpha_s + 2\alpha_d \sum_\sigma n_{i\sigma}} \left(2h + \Delta e^{2\alpha_s + 2\alpha_d \sum_\sigma n_{i\sigma}}\right) + K$$

$$+ \frac{\omega_0}{2} \left[(e^{2\boldsymbol{\beta}})_{00} \cosh\left(4\alpha_s + 4\alpha_d \sum_\sigma n_{i\sigma}\right) - 1 \right], \tag{91}$$

where

$$P = \omega_0 \sqrt{\alpha}(1-\eta) \tag{92}$$

$$J = \omega_0 \alpha \eta (2-\eta) + 2\sqrt{\alpha}\omega_0 (1-\eta)(h + M\Delta e^{2\alpha_s}) \tag{93}$$

$$U_{eff} = U - 2\alpha\omega_0 \eta (2-\eta) \tag{94}$$

$$M = \left(e^{\beta}\right)_{00} + 2\left[\left(e^{\beta}\right)_{01} + \left(e^{\beta}\right)_{02} + \left(e^{\beta}\right)_{03} + \ldots\right] \tag{95}$$

$$t_{eff} = t e^{-\alpha\eta^2 e^{-4\alpha_s}\left(1 - 4\alpha_d + 12{\alpha_d}^2\right)\left\{\left(e^{-2\beta}\right)_{00} - \left(e^{-2\beta}\right)_{01}\right\}} \tag{96}$$

$$K = M\Delta e^{2\alpha_s}(4h\alpha_d + 6h\alpha_d^2 + 4\alpha_d\Delta e^{2\alpha_s} + 12\alpha_d^2\Delta e^{2\alpha_s})$$

$$+\left(e^{2\beta}\right)_{00}(\alpha_d e^{4\alpha_s} + 12\alpha_d^2 e^{4\alpha_s} + 12\alpha_d^2 e^{-4\alpha_s} - \alpha_d e^{-4\alpha_s})$$

$$- 2\Delta MPe^{2\alpha_s}(3\alpha_d^2 + 2\alpha_d). \qquad (97)$$

2.2.3 The GS Energy

It is worth noting that the Hamiltonian H_{eff} given by Eq. (91), which describes an effective Hubbard model in one dimension, can be used to obtain the exact GS energy at half – filling with the help of the Bethe – ansatz approach following Lieb and Wu [28 – 29].

However, only positive U_{eff} values were considered in [28]. The exact Bethe – ansatz solution for the Hubbard model has been extended to the negative – U_{eff} – problem by TC [3]. In this case, the GS energy per site for (91) is obtained as

$$\varepsilon_0 = -J + \frac{\omega_0}{2}\left[2h^2 + (e^{2\beta})_{00}\cosh(4\alpha_s) - 2\right]$$

$$+ \frac{1}{4}\left[U_{eff} - \left|U_{eff}\right|\right] + \omega_0 M\Delta e^{2\alpha_s}(2h + \Delta e^{2\alpha_s})$$

$$+ K - 4t_{eff}\int_0^\infty \frac{J_0(x)\,J_1(x)\,dx}{x\left[1 + \exp\left\{\frac{x\left|U_{eff}\right|}{2t_{eff}}\right\}\right]}\,, \qquad (98)$$

where $J_0(x)$ and $J_1(x)$ are the Bessel functions of zero – th and first – order respectively.

2.3 Numerical Results and Discussions

To find the minimum energy, the expression (98) is varied with respect to six variational parameters $\eta, h, \alpha_s, \alpha_d, \beta$ and Δ. The results are shown in Fig. 2.1. The results obtained by TC [3] and KC [20] are also shown together with the present results for comparison.

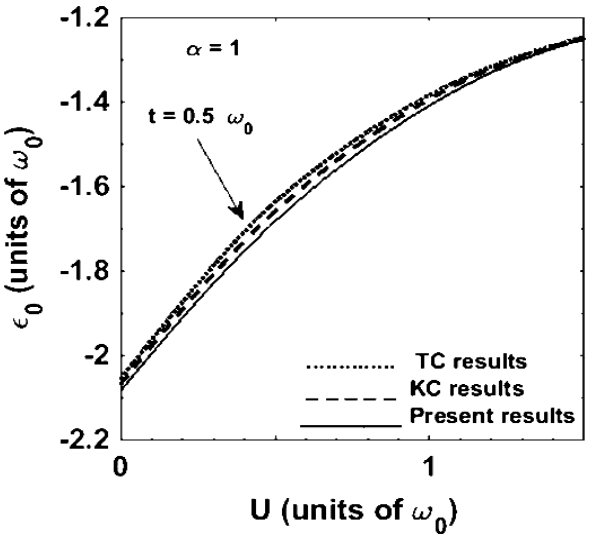

Fig. 2.1 Ground state energy (ε_0) per site as a function of onsite Coulomb energy (U) for el – ph interaction strength $\alpha = 1$ and for $t = 0.5\ \omega_0$.

The present results for the GS energy are slightly improved compared to those of [20], especially for small values of U. We can demonstrate, however, that even a small increase in energy can have a large impact on the phase diagram. This is common with variational calculations, as a small order δ error in the wave function causes an error of order δ^2 in the energy. The effective hopping parameter is a critical quantity in this problem.

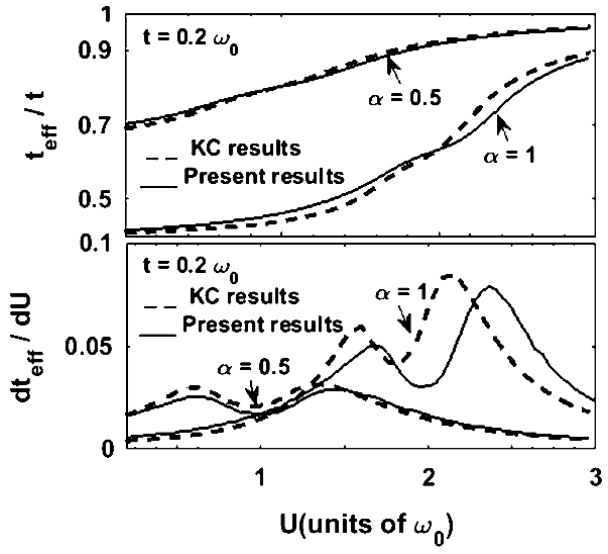

Fig. 2.2 t_{eff} and dt_{eff}/dU as a function of onsite el – el inetraction U for two values of el – ph interaction strength α and for $t = 0.2\ \omega_0$.

In Fig. 2.2, we show t_{eff} and its derivative as a function of U with respect to U. We have also plotted the results of KC for comparison. The figure shows that when U is small, U_{eff} becomes negative and t_{eff} becomes very small due to the el – ph interaction effect. This leads to the formation of bipolarons and consequently narrowing of the band. In this case, the ground state is an insulating state known as the CDW state of Peierls form. In the opposite extreme, i.e., when U becomes substantially larger than the el – ph interaction, U_{eff} becomes positive and $t_{eff} \to t$, and then one obtains the standard Hubbard – Hamiltonian and thus the ground state, in this situation, is represented by an insulating antiferromagnetic state. This is the so called SDW state of Mott type. One can observe that in – between the two phases, the t_{eff} – curves are accompanied by some fascinating attributes. To solve

this problem, we look at how dt_{eff}/dU behaves with respect to U. In the lower part of Fig. 2.2, these results are shown. Interesting dt_{eff}/dU has a double – peak structure. dt_{eff}/dU has two peaks for two different values of U for a given α. Let us say that the first peak happens at $U = U_1$ and the second peak happens at $U = U_2$. A closer look shows that $U_{eff} = 0$ in the middle of U_1 and U_2. It is also worth noting that the peak structure is asymmetric in nature. It is well understood that the band – width $2zt$, where z is the coordination number and t is the hopping parameter, must be larger/equal than/to the Hubbard gap U (which is the onsite Coulomb correlation energy) for a metallic state. As a result, the criterion for a metallic condition for a one – dimensional system is: $4t/U \geq 1$. We discover that between U_1 and U_2, t_{eff} and U_{eff} are related by the inequality: $4t_{eff}/U_{eff} \geq 1$ which, as previously said, is the characteristic of a metallic state. We also note that, in comparison to KC's results [20], the current approach predicts a wider gap between the two peaks.

The primary goal of our analysis is to find a two – dimensional $(U - \alpha)$ phase portrait. As previously mentioned, we obtain a set of U_1 and U_2 values for each value of α from the peak positions of dt_{eff}/dU. Thus U_1 and U_2 as a function of α, define the phase boundaries. Fig. 2.3 shows the corresponding phase diagram. The metallic phase is identified between the U_1 and U_2 lines, while the SDW phase is located above the U_2 line and the CDW phase is located below the U_1 line. We already know that the metallic region obtained by KC is wider than that obtained by TC and Fig. 3.3 shows that the current analysis predicts an even wider metallic region than obtained by KC. We have not plotted the phase diagram below a certain value of α because the results were unreliable due to computational error for values of α close to $\alpha = 0$.

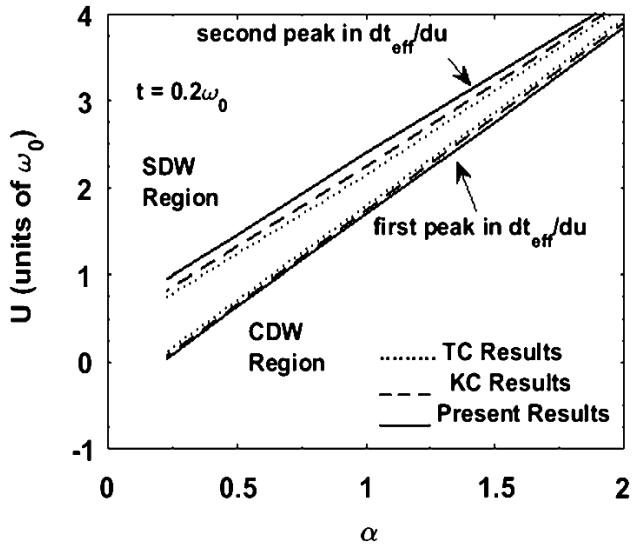

Fig. 2.3 Phase diagram in the $(\alpha - U)$ plane obtained from the peaks in dt_{eff}/dU for $t = 0.2\ \omega_0$.

The local moment may also provide details about the existence of different phases. We study this by calculating the average local spin moment per site (S_{av}) and plotting it on a contour plot in $(U - \alpha)$ – space. S_{av} can be expressed as

$$S_{av} = \frac{1}{N} \sum_i \langle S_i^2 \rangle \tag{99}$$

where S_i can be written as:

$$S_i^2 = S_{ix}^2 + S_{iy}^2 + S_{iz}^2.$$

Using

$$S_i^{\pm} = S_{ix} \pm iS_{iy}\ ; \quad S_i^{+} = c_{i\uparrow}^{\dagger} c_{i\downarrow}\ ; \quad S_i^{-} = c_{i\downarrow}^{\dagger} c_{i\uparrow}$$

$$S_i^{+} \cdot S_i^{-} = -\, n_{i\uparrow} n_{i\downarrow}\ ; \quad {n_{i\uparrow}}^2 = n_{i\uparrow}\ , \quad {n_{i\downarrow}}^2 = n_{i\downarrow}$$

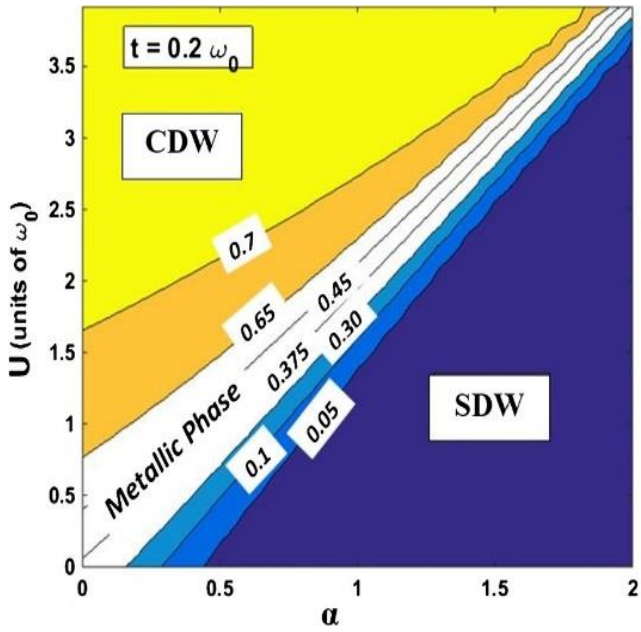

Fig. 4. Contour plots of the local spin moment S_{av} in $(\alpha - U)$ −plane.

we obtain,

$$S_{av} = \frac{1}{N}\sum_i \langle S_i^2 \rangle = \frac{3}{4} - \frac{3}{2N}\sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle \ . \tag{100}$$

From Eq. (98) we obtain

$$\frac{d\,\varepsilon_0}{d\,U} = n_{i\uparrow}\, n_{i\downarrow} \tag{101}$$

Therefore, we can write

$$S_{av} = \frac{3}{4} - \frac{3}{2}\frac{d\,\varepsilon_0}{d\,U} \quad . \tag{102}$$

For a given S_{av}, Eq. (101) returns a set of (U, α) – values. The results of S_{av} are shown in Fig. 2.4 as a contour plot in the (α, U) – plane. Eq. 98 can be used to calculate $[d\varepsilon_0/dU]$ for a system of totally uncorrelated electrons in a metallic state. Then, using Eq. (102), we get $S_{av} = 0.375$, which is the value we see in the middle of the intermediate phase. This supports TC's prediction of the occurrence of a metallic zone.

2.4 Conclusion

In this chapter, the one – dimensional HH model has been utilized to examine the interplay of el – ph interaction and Coulomb correlation at the cross – over area of the SDW and CDW phases. We have considered a correlated squeezed coherent state for the phonon sub – system. Introducing a new canonical/unitary transformation that introduces the electron – density – dependent phonon correlation, the phonon state [20] has been improved. Finally, the Bethe ansatz method is used to solve the resulting electronic Hamiltonian exactly. We show that, when compared to TC's and KC's calculations, the improved variational calculation provides a wider metallic phase at the CDW and SDW phase boundary cross – over area. The broadening of the intermediate metallic phase by an improved variational calculation strengthens the conjecture made by TC regarding the existence of such a phase.

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Chapter 3

An Intervening metallic phase at the CDW – SDW transition region in the one – dimensional Holstein – Hubbard model at half filling: A Semi – Exact solution

3.1 Introduction

In this chapter, we extend the work presented in the previous chapter by modifying the phonon state. We have mentioned in the previous chapter that the spin – density – wave (SDW) charge – density – wave (CDW) – transition problem is important for high temperature supercoonductivity (HTSC) in cuprates [1 – 3] and has been studied through several methods [4]. We have also briefly discussed in Chapter 2 that Chatterjee and collaborators [5 – 11] have studied the one – dimensional (1D) half – filled Holstein – Hubbard (HH) model [13 – 17] variationally to obtain an analytical solution. Recently, Malik, Mukhopadhyay, and Chatterjee (MMC) [11] have modified the variational method of Krishna and Chatterjee (KC) [7] by proposing a new squeezing transformation in addition to the ones considered by KC. This work has been the subject matter of Chapter 2. In this work, we have shown that a better variation calculation widens the metallic phase further.

It should be noted that the variational method of MMC [11] is still approximate as far as the averaging phonon state is concerned and therefore there are opportunities to modify this calculation. One would like to see what happens to the width of the metallic region, if the phonon wave function in the MMC – calculation is replaced by a more accurate state. More recently, Malik and Chatterjee (MC) [12] have used a modified calculation using a very accurate many – phonon state and in this sense, their calculation can be considered as semi – exact. The basic aim is again the same. If a more refined variational approach produces a broader metallic phase, then the possibility of existence of the intervening metallic phase is reinforced while, on the other hand, if a better variational approach results in the shrinkage of the metallic phase, then the presence of the metallic phase is questionable.

In the present chapter, we present the work of MC [12].

3.2 Formulation of the Model

The 1D HH Hamiltonian is given by

$$H = -t \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_{i} b_i^{\dagger} b_i + g \sum_{i\sigma} n_{i\sigma} \left(b_i^{\dagger} + b_i\right) , \quad (1)$$

where all the symbols have the same meaning as discussed in chapter 2.

To deal with the above Hamiltonian, we use a variational method with the following modified phonon state:

$$|\Phi\rangle = e^{R_1}\, e^{R_2}\, e^{R_3}\, e^{R_4}\, e^{R_5}\, e^{R_6}\, |\chi\rangle, \tag{2}$$

where $R_1,\ R_2,\ R_3,\ R_4\ , R_5$ and R_6 are the same as introduced in Chapter 2 and are given by

$$R_1 = \sqrt{\alpha}\,\eta \sum_{i\sigma} n_{i\sigma}\left(b_i^{\dagger} - b_i\right)\ , \tag{3}$$

$$R_2\ = \sum_{i} h_i\left(b_i^{\dagger} - b_i\right)\ , \tag{4}$$

$$R_3\ =\ \alpha_s \sum_{i}\left(b_i b_i - b_i^{\dagger} b_i^{\dagger}\right)\ , \tag{5}$$

$$R_4 =\ \alpha_d \sum_{i\sigma} n_{i\sigma}\left(b_i b_i - b_i^{\dagger} b_i^{\dagger}\right)\ , \tag{6}$$

$$R_5 = \frac{1}{2}\sum_{i\neq j} \beta_{ij}\left(b_i b_j - b_i^{\dagger} b_j^{\dagger}\right)\ , \tag{7}$$

$$R_6 = \Delta \sum_{i} (b_i^{\dagger} - b_i)\ , \tag{8}$$

and $|\chi\rangle$ is the phonon state which we choose as:

$$|\chi\rangle\ = \prod_i |\phi_i\rangle\ = \prod_i \left(\sum_{n=0,1,2,..m} A_n \frac{{b_i^{\dagger}}^n}{\sqrt{n!}} |0_i\rangle \right). \tag{9}$$

The transformed Hamiltonian H_6 has been obtained in the previous chapter and is given by

$$H_6 = e^{-R_6}\, e^{-R_5}\, e^{-R_4}\, e^{-R_3}\, e^{-R_2}\, e^{-R_1} H e^{R_1}\, e^{R_2}\, e^{R_3}\, e^{R_4}\, e^{R_5}\, e^{R_6}$$

$$= -t' \sum_{<i,j>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U_{eff} \sum_{i} n_{i\uparrow} n_{i\downarrow} + Q \sum_{i\sigma} n_{i\sigma}^2$$

$$+ P \sum_{i\sigma} n_{i\sigma} \{ \sum_{j} (\mu_{ij} + \vartheta_{ij}) ((b_j^{\dagger} + b_j) - 2\Delta) e^{2\alpha_d \Sigma_{\sigma'} n_{i\sigma'}} e^{2\alpha_s} - 2h \}$$

$$+ \frac{\omega_0}{4} \sum_{ijj'} \{ -(\mu_{ij} - \vartheta_{ij})(\mu_{ij'} - \vartheta_{ij'}) (b_j^{\dagger} - b_j)^2 e^{(-4\alpha_s - 4\alpha_d \Sigma_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'})}$$

$$+ (\mu_{ij} + \vartheta_{ij})(\mu_{ij'} + \vartheta_{ij'}) \left((b_j^{\dagger} + b_j)^2 + 4\Delta^2 \right) e^{(4\alpha_s + 4\alpha_d \Sigma_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'})} - \frac{1}{2} \}$$

$$+ \omega_0 \left(h^2 - h \sum_{ij} ((\mu_{ij} + \vartheta_{ij})((b_i^{\dagger} + b_i) - 2\Delta)) \exp(2\alpha_s + 2\alpha_d \sum_{\sigma} n_{i\sigma}) \right) , \qquad (10)$$

where all the parameters are defined in Chapter 2.

3.2.1 Averaging State and Effective Hamiltonian

The effective electronic Hamiltonian H_{eff} is now given by:

$$H_{eff} = \langle \Phi | H | \Phi \rangle = \langle \chi |\, H_6\, | \chi \rangle \ , \qquad (11)$$

The final averaging phonon state is a many – phonon state (Eq. (9)) with $A_n{}'s$ as the variational parameters. We assume $A_n{}'s$ to be site – independent, which is a plausible assumption for a uniform system.

It may be noted that $m = 0$ produces the standard zero – phonon state i.e.,

$$|\chi\rangle = \prod_i |0_i\rangle , \tag{12}$$

For $m = 1$, we have

$$|\chi\rangle = \prod_i (A_0 |0_i\rangle + A_1 |1_i\rangle) , \tag{13}$$

which is a many – phonon that can be written as a linear combination of different phonon states with the constraint that no single site can have more than one phonon. It is a restricted many – phonon state and is reminiscent of the intermediate – coupling polaron wave function of Gurari [18].

For $m = 2$, the averaging many – phonon state is

$$|\chi\rangle = \prod_i \left(A_0 |0_i\rangle + A_1 |1_i\rangle + \frac{A_2}{\sqrt{2!}} |2_i\rangle \right) , \tag{14}$$

which is a linear superposition of phonon states in which a given particular site can only be filled by at most two phonons. Thus, in general, Eq. (9) represents a generalized many – phonon state, in which m number of phonons can be present at any given site depending. In the numerical calculation, we choose the value of m in order to get self – consistent result. Now the effective electronic Hamiltonian, H_{eff} can be written as:

$$H_{eff} = \langle \Phi | H_6 | \Phi \rangle$$

$$= -J \sum_{i\sigma} n_{i\sigma} + U_{eff} \sum_{i} n_{i\uparrow} n_{i\downarrow} - t_{eff} \sum_{ij\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \omega_0 h^2$$

$$+ \Delta\, e^{\boldsymbol{\beta}}\, e^{2\alpha_s + 2\alpha_d \sum_\sigma n_{i\sigma}} \left(2h + \Delta e^{2\alpha_s + 2\alpha_d \sum_\sigma n_{i\sigma}}\right) + K$$

$$+ \frac{\omega_0}{2} \left[(e^{2\boldsymbol{\beta}})_{00} \cosh\left(4\alpha_s + 4\alpha_d \sum_{\sigma} n_{i\sigma}\right) - 1 \right], \qquad (15)$$

where

$$U_{eff} = U - 2\alpha\omega_0\eta(2-\eta) \qquad (16)$$

$$J = Q + P(e^{2\alpha_s} M\left(2A_0A_1 + 2A_1A_2\sqrt{2} + 2A_2A_3\sqrt{3} - 2\Delta\right) - 2h \qquad (17)$$

$$P = \omega_0\sqrt{\alpha}(1-\eta)$$

$$Q = \alpha\omega_0\eta^2 - 2\eta\omega_0\alpha = \alpha\omega_0\eta(\eta-2)$$

$$M = \left(e^{\beta}\right)_{00} + 2\left[\left(e^{\beta}\right)_{01} + \left(e^{\beta}\right)_{02} + \left(e^{\beta}\right)_{03} + \ldots\right]$$

$$K = .25Me^{4\alpha_s}\left(2A_0A_2\sqrt{2} + \left(2A_0A_2\sqrt{2} + 2A_1A_3\sqrt{6} + 4\Delta^2\right)\right)$$

$$+ PMe^{4\alpha_s}\left(2A_0A_1 + 2A_1A_2\sqrt{2} + 2A_2A_3\sqrt{3} - 2\Delta\right)\left(2\alpha_d + 3\alpha_d^2\right)$$

$$- 2Mh\alpha_s\left(2A_0A_1 + 2A_1A_2\sqrt{2} + 2A_2A_3\sqrt{3} - 2\Delta\right)\left(2\alpha_d + 3\alpha_d^2\right)$$

$$-2Mh\alpha_s + \left(2A_0A_1 + 2A_1A_2\sqrt{2} - 2\Delta + 2A_2A_3\sqrt{3}\right)$$

$$+0.25e^{4\alpha_s}(1+4\beta^2)\left(1 + 2A_1^2 + 4A_2^2 + 2A_0A_2\sqrt{2}\right.$$

$$+2A_1A_3\sqrt{6} + 6A_3^2 + 4\Delta^2)(4\alpha_d + 12\alpha_d^2)$$

$$- 0.25e^{-4\alpha_s}(1 + 4\beta^2)\,(-1 - 2A_1^2 - 4A_2^2 + 2A_0A_2\sqrt{2} +$$

$$2A_1A_3\sqrt{6} - 6A_3^2)\,(-4\alpha_d + 12\alpha_d^2)$$

$$-.25Me^{-4\alpha_s}(2A_0A_2\sqrt{2} + 2A_1A_3\sqrt{6}) \qquad (18)$$

$$t_{eff} = t\exp\big((1 + 4\beta^2) + (2\beta + 4\beta^3)\big)$$

$$\times \{1 + 2\alpha\eta^2A_0A_2\sqrt{2}\,e^{-4\alpha_s}(1 - 6\alpha_d + 36\alpha_d^2)$$

$$\times \big((1 + 4\beta^2) + (2\beta + 4\beta^3\,)\big)$$

$$- 2\alpha A_0A_2A_1^2\eta^2e^{-4\alpha_s}(1 - 6\alpha_d + 36\alpha_d^2)$$

$$\times \big((1 + 4\beta^2) + (2\beta + 4\beta^3)\big)$$

$$- 4\alpha A_2^2\eta^2e^{-4\alpha_s}(1 - 6\alpha_d + 36\alpha_d^2)\big((1 + 4\beta^2) + (2\beta + 4\beta^3)\big)$$

$$+0.5\alpha^2A_2^2\eta^4e^{-8\alpha_s}(1 - 36\alpha_d)((1 + 4\beta^2)^2 + (2\beta + 4\beta^3\,)^2)$$

$$+2\alpha A_1A_3\eta^2\sqrt{6}e^{-4\alpha_s}(1 - 6\alpha_d + 36\alpha_d^2)$$

$$\times \Big((1 + 4\beta^2) - \big((-1)(2\beta + 4\beta^3)\big)\Big)$$

$$-6\alpha A_3^2\eta^2e^{-4\alpha_s}(1 - 6\alpha_d + 36\alpha_d^2)\big((1 + 4\beta^2) + (2\beta + \ 4\beta^3)\big)$$

$$-1.63A_1A_3\alpha^2\eta^4e^{-8\alpha_s}(1 - 36\alpha_d)$$

$$\times ((1 + 4\beta^2)^2 + (2\beta + 4\beta^3)^2)$$

$$+3A_3^2\alpha^2\eta^4e^{-8\alpha_s}(1 - 36\alpha_d)$$

$$\times ((1 + 4\beta^2)^2 + (2\beta + 4\beta^3)(2\beta + 4\beta^3)^2)$$

$$- 0.33A_3^2\alpha^4\eta^6 e^{-12\alpha_s}(1 - 198\alpha_d)$$

$$\times \left((1 + 4\beta^2)^3 + (2\beta + 4\beta^3)^3\right)\Big\}. \qquad (19)$$

We have already noted that $\left(e^{\beta}\right)_{i0}$ can be written in a compact way as

$$\left(e^{\pm\beta}\right)_{j\,0} = \sum_{i\,=\,0,1,2,\ldots} (\pm)^i \frac{\beta^{2\,i\,+\,j}}{i\,!\,(i\,+\,j)\,!}. \qquad (20)$$

3.2.2 The GS Energy

To calculate the exact GS energy of H_{eff} per site (ε_0) for both positive and negative U_{eff} we use the Bathe – Ansatz method [19 – 20]. We obtain

$$\varepsilon_0 = -J + \frac{\omega_0}{2}\left[2h^2 + (e^{2\beta})_{00}\cosh(4\alpha_s) - 2\right]$$

$$+ \frac{1}{4}\left[U_{eff} - |U_{eff}|\right] + \omega_0 M\Delta e^{2\alpha_s}(2h + \Delta e^{2\alpha_s})$$

$$+ K - 4t_{eff}\int_0^{\infty} \frac{J_0(x)\,J_1(x)\,dx}{x\left[1 + \exp\left\{\frac{x|U_{eff}|}{2t_{eff}}\right\}\right]}, \qquad (21)$$

where $J_0(x)$ denotes zero – th order Bessel function and $J_1(x)$ denotes the first – order Bessel function.

3.3 Results and Explanations

The GS energy is obtained by minimizing ε_0 with respect to the variational parameters $\eta, h, \alpha_s, \alpha_d, \beta, \Delta,$ and $A_0, A_1, A_2, A_3,$ .... etc.. Fig. 3.1

shows the GS energy results. The dotted line represents the TC results [5], the dashed line represents the results of KC [7], the dotted – dashed line the MMC results [11] and the solid line represents the present results. As can be seen from the figure, the present GS energy results are only somewhat better than the previous variational calculation. We will show again that this small increase in energy can have a significant effect on the phase diagram.

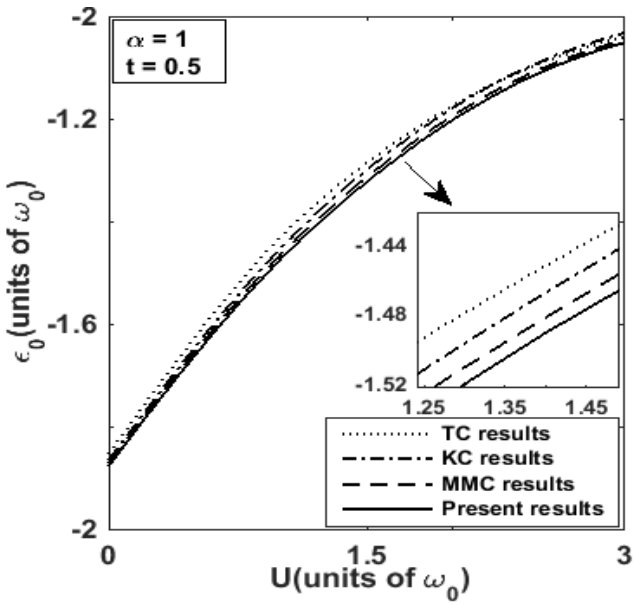

Fig. 3.1 Ground state energy (ε_0) per site as a function of onsite Coulomb energy (U) for el – ph interaction strength $\alpha = 1$ and for $t = 0.5\ \omega_0$.

As before, the effective hopping parameter (t_{eff}/t) is studied with respect to the on – site Coulomb correlation energy U. The results are shown in Fig. 3.2. Again we observe that for small U and a reasonable value of the el – ph coupling constant α, t_{eff} is small. As a result, the band is narrow in this limit, and massive bi – polarons can form. This is the insulating CDW state, in which Peierl's instability occurs and the possibility of double occupancy

increases. For large U and reasonable values of el – ph interaction, the system behaves essentially as the Hubbard model and an anti – ferromagnetic Mott insulating state becomes the GS of the system. This is the SDW state. As in [5, 7, 11], some interesting features can be seen here as well, between the SDW and CDW states.

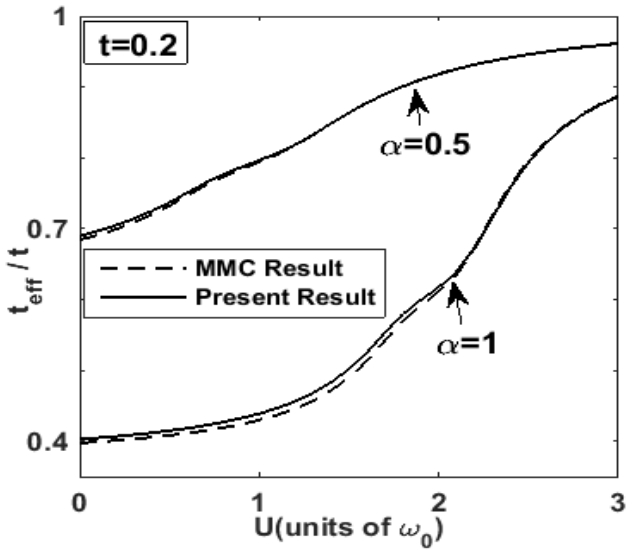

Fig. 3.2 t_{eff}/t as a function of onsite el – el inetraction U for two values of el – ph interaction strength α and for $t = 0.2\ \omega_0$.

To gain a better understanding of these interesting features, we again investigate the behaviour of the derivative of the renormalized hopping integral (dt_{eff}/dU) with respect to U, as we did previously. Fig. 3.3 depicts this behaviour. The double – peak structure is clearly visible again. As previously stated, the system is in a charge – density – wave phase at small U, and the system's GS is in a SDW phase at large U.

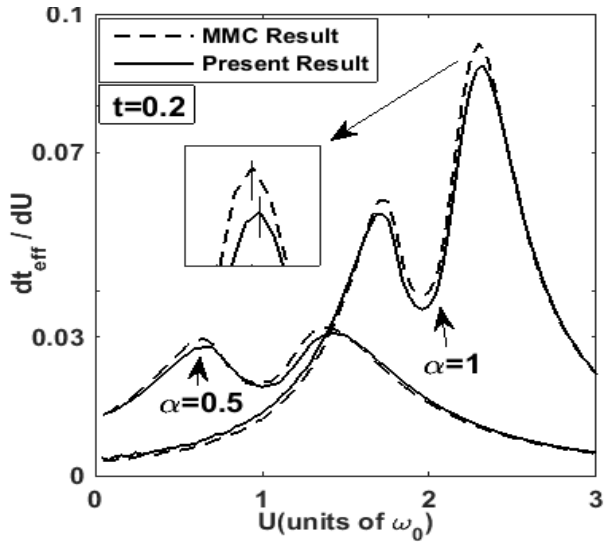

Fig. 3.3 dt_{eff}/du as a function of onsite el – el inetraction U for two values of e – p interaction strength α and for $t = 0.2\ \omega_0$.

The broad valley at the crossover between CDW and SDW phases suggests that the CDW – SDW transition is not direct rather it occurs through an intermediate phase. For $t = 0.2\ \omega_0$ and a certain value of α, let us say U_1 and U_2 are the two values of U at which (dt_{eff}/U) shows the peaks. Thus, for a range of $\alpha -$ values, we can obtain the phase diagram: (U_1, U_2) versus α as we have shown in Chapter 2. Fig. 3.4 illustrates the phase diagram. We obtain results for two cases, one with a Restricted many – phonon state (RMPS) and the other with a generalized many – phonon state (GMPS). We also compare our results with those of TC [5], KC [7], and MMC [11]. In the case of GMPS, we find that beyond $m = 3$, the results do not change any more. As has been observed earlier by TC, KC and MMC, the presents results also show that for a given value of α, the region between the $U_1 -$ line and the $U_2 -$ line, satisfies the metallicity criterion: $4t_{eff}/U_{eff} \geq 1$ (both with RMPS and GMPS). One can see that above the

$U_1 -$ line, strong correlation would win and the system would be in an SDW phase, whereas the el – ph interaction would win below the $U_2 -$ line, and the system would then be in a CDW phase. The phase boundaries are thus described by the $U_1 -$ and $U_2 -$ lines. Therefore, we can say that, the SDW and the metallic phase are separated by the $U_1 -$ line, while the metallic phase and the CDW phase are separated by the $U_2 -$ line.

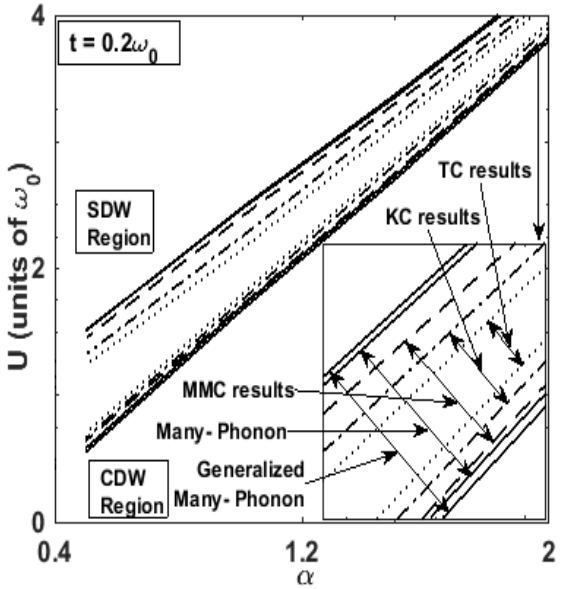

Fig. 3.4 Phase diagram in the $(\alpha - U)$ plane obtained from the peaks in dt_{eff}/dU for $t = 0.2\ \omega_0$.

It can be noticed that, compared to the variational results of TC, KC, and MMC, the present work provides a wider metallic phase, GMPS giving even broader metallic phase than RMPS. The fact that successive improvements and modifications in variational calculations widen the metallic phase lends credence to the conjecture of TC regarding the presence of an metallic region between the CDW and SDW regions. Since the most general state has been chosen for the phonons and the effective electronic problem has been dealt

with exactly by the Bethe ansatz approach, the calculation with GMPS can be considered as semi – exact. However, the method is still not exact because the total wave function is chosen as a product state.

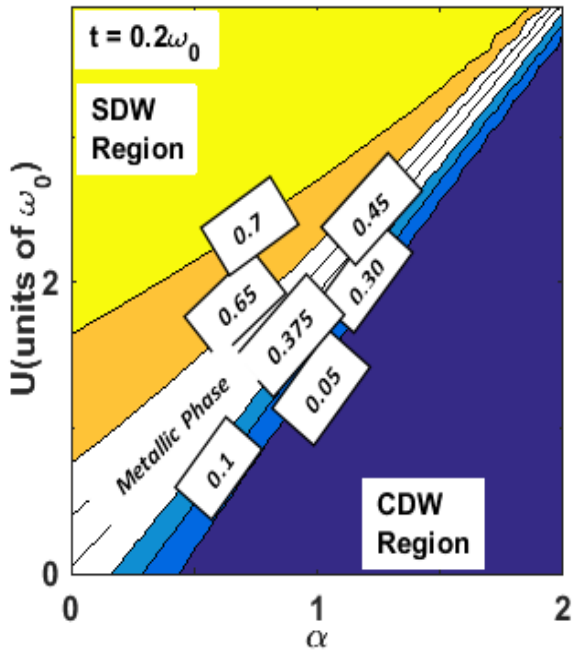

Fig. 3.5 Contour plots of the local spin moment L_0 in $(\alpha - U) -$ plane.

We also calculate the average local spin moment L_0 per site, which provides an additional proof for the existence of a metallic state at the transition region of the CDW and the SDW phases. Following Chapter 2, we have

$$L_0 = \frac{1}{N}\sum_i \langle S_i^2 \rangle = \frac{3}{4} - \frac{3}{2}\frac{d\,\varepsilon_0}{d\,U}, \qquad (22)$$

where S_i denotes to the electronic spin at the $i - th$ site.

The contour plots for L_0 are shown in the (α, U) – plane in Fig. 3.5. If the electrons' motion is completely uncorrelated, as it is in a gas of non – interacting electrons, Eq. 19 gives $L_0 = 0.375$, which is similar to the value seen in the intermediate state. Hence, this supports the evidence that an intermediate metallic phase exists at the CDW and SDW transition region.

3.4 Conclusion

The GS energy of the 1D Holstein Hubbard model has been examined variationally by employing a series of unitary canonical transformations and a generalized many – phonon state to obtain an effective electronic Hamiltonian, which is then solved exactly by using Bethe – ansatz technique to obtain the system's GS energy. Comparison of our results with the previous variational ones reveal that the present semi – exact calculation provides a broader metallic phase at the CDW – SDW crossover region lending credence to TC's original conjecture [5]. It should be noted that the amount by which the metallic phase broadens in an improved modified variational calculation is not so important; what is important is that the metallic phase widens and does not shrink when we improve our variational calculations. The existence of a metallic phase in the HH model is important not only in the context of high – temperature superconductivity, but also for fundamental physics related to the existence of different phases in strongly correlated Fermi systems.

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Chapter 4

Quantum – Entanglement Entropy and Double Occupancy in a one dimensional Holstein – Hubbard model at half – filling

4.1 Introduction

The subject of quantum phase transition has emerged in recent times as one of the most exciting and fascinating areas of research, both in experimental and theoretical fields of modern quantum condensed matter physics. A phase transformation can be called a quantum phase transition (QPT) if the change of phase occurs due to a change in the material properties such as interaction strengths, doping concentration, and so on [1 – 3]. The physics of quantum phase transition is intimately linked to the notion of quantum entanglement (QE) [4 – 7] and therefore the study of quantum entanglement for a condensed matter system is important to understand some of the interesting aspects of the quantum phase transition the system may undergo. Quantum entanglement is, of course, a fundamental property of a quantum system, and therefore studying and analyzing it, can provide fundamental information and knowledge about non – local quantum correlations, which could be important in the fields of quantum information, quantum computing, and quantum teleportation. Furthermore, the measure of

quantum entanglement can be utilized to determine the nature of a many – body ground state (GS) of a quantum system and this information can be used to investigate and identify the nature of QPTs [8 – 18]. In this work, we consider the theory of quantum entanglement to investigate [19] the possibility and nature of quantum phase transition in the Holstein – Hubbard (HH) model [20 – 24].

4.2 Model

As already introduced in the earlier chapters, the Holstein – Hubbard Hamiltonian is given by

$$H = -\sum_{<i,j>\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_{i} b_i^{\dagger} b_i + g \sum_{i\sigma} n_{i\sigma} (b_i^{\dagger} + b_i) \ , \qquad (1)$$

where all the symbols have already been explained earlier. We use the method [25 – 26] discussed in Chapter 3 to obtain the GS energy per site for (1). This is given by

$$\varepsilon_0 = -J + \frac{\omega_0}{2}\left[2h^2 + (e^{2\beta})_{00}\cosh(4\alpha_s) - 2\right] + \frac{1}{4}\left[U_{eff} - |U_{eff}|\right] + \omega_0 M \Delta e^{2\alpha_s}(2h + \Delta e^{2\alpha_s}) + K - 4t_{eff}\int_0^{\infty} \frac{J_0(x)\, J_1(x)\, dx}{x\left[1 + \exp\left\{\frac{x|U_{eff}|}{2t_{eff}}\right\}\right]} \ , \qquad (2)$$

where all symbols have been defined in Chapter 3.

4.3 Entanglement Entropy and Double Occupancy

Quantum entanglement can be used to identify interesting phases of the Hubbard model emerging from quantum correlations. Shankar and Chatterjee (SC) [27] has considered the Hamiltonian [28] and calculated the Quantum Etanglement Entropy (QEE) and Double Occupancy (DO) of the system. We have recently modified the work of SC using the method [29] discussed in Chapter 3 and calculated QEE and DO for the Hamiltonian (1).

We examine a subsystem with four possible states as: $:|0\rangle, |\uparrow\rangle, \langle\downarrow|$ and $|\uparrow\downarrow\rangle$ and calculate the single – site Entanglement entropy (EE) (E_v) and Double occupancy (ω) as follows:

$$E_v = -Tr\,(D_R \log_2 D_R)\ ; \tag{4}$$

$$\omega = \langle n_{i\uparrow} n_{i\downarrow} \rangle \tag{5}$$

where D_R stands for the reduced density matrix, which can be written as

$$D_R = \omega^0 |0\rangle\langle 0| + \omega^+ |\uparrow\rangle\langle\uparrow| + \omega^- |\downarrow\rangle\langle\downarrow| + \omega |\uparrow\downarrow\rangle\langle\uparrow\downarrow|\ , \tag{6}$$

where the occupation numbers $\omega^0, \omega^+, \omega^-$ are given by:

$$\omega^+ = \omega^- = n/2 - \omega \tag{7}$$

$$\omega^0 = 1 - \omega^+ - \omega - \omega \tag{8}$$

In order to obtained the value of D_R, we substitute the values of ω^+, ω^- and ω^0 in Eq. (6) which then reads

$$D_R = 2\left(\frac{1}{2} - \omega_{\uparrow\downarrow}\right) + 2\,\omega_{\uparrow\downarrow} \tag{9}$$

Thus, E_v can be expressed as

$$E_v = -\Big\{(2\,\omega_{\uparrow\downarrow}\log_2 2\,\omega_{\uparrow\downarrow}) + \left(2\left(\frac{1}{2} - \omega_{\uparrow\downarrow}\right)\log_2 2\left(\frac{1}{2} - \omega_{\uparrow\downarrow}\right)\right)\Big\}. \tag{10}$$

Using the Hellman – Feynman theorem, we can derive:

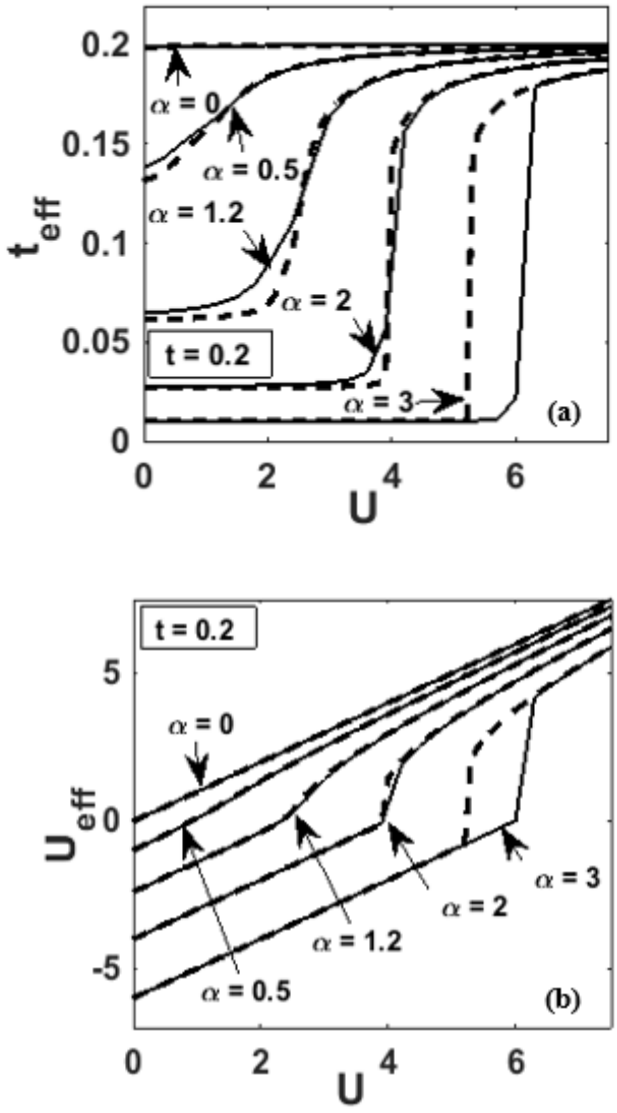
$$\frac{d\,E}{d\,U} = \langle n_{i\uparrow} n_{i\downarrow} \rangle \tag{11}$$

and consequently ω is determined.

4.4 Numerical Results and Discussions

In Fig. 4.1, we investigate the dynamics of the effective hopping integral (t_{eff}), the modified on – site Coulomb correlation strength (U_{eff}), the double occupancy parameter (ω), and the single – site EE (E_v) as a function of U for various α values. For the sake of comparison, the results of SC [27] are also included. The plot of t_{eff} vs U (Fig. 4.1(a)) shows that for small α, when U is increased, t_{eff} grows continuously to the bare hopping parameter t, which is the Hubbard value, but when α is large, t_{eff} goes to t through a finite discontinuous jump at some crucial value of U.

Fig. 4.1(b) shows that U_{eff} may become negative if α becomes sufficiently large compared to U. The reason behind this is not difficult to understand. If α is significantly large, the phonon – induced el – el attractive interaction may take precedence over the usual Coulomb repulsion between the electrons, resulting in an overall effective attractive el – el interaction.



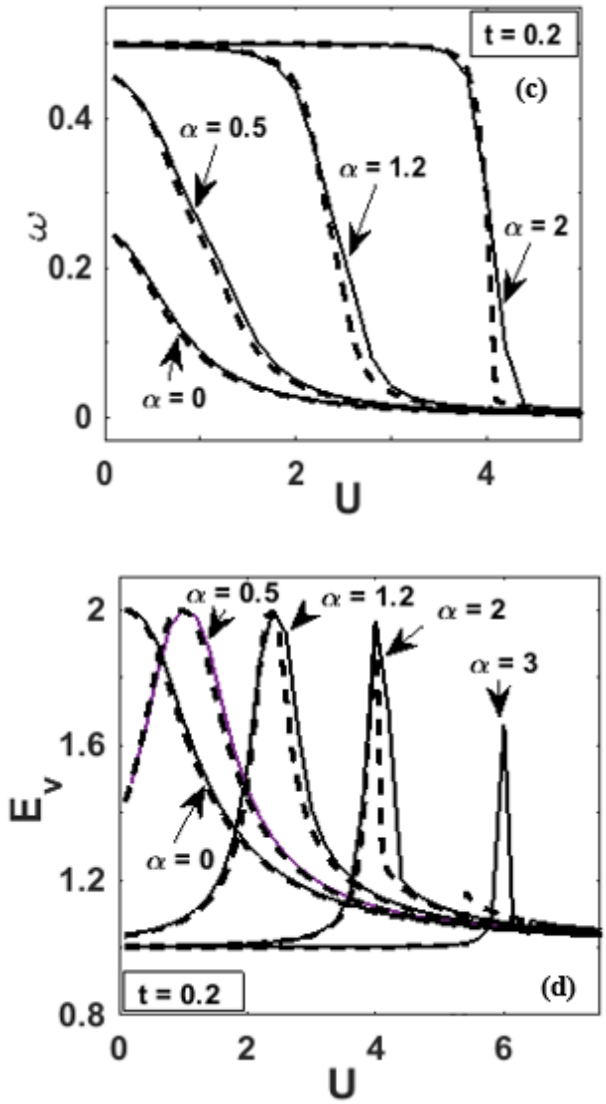
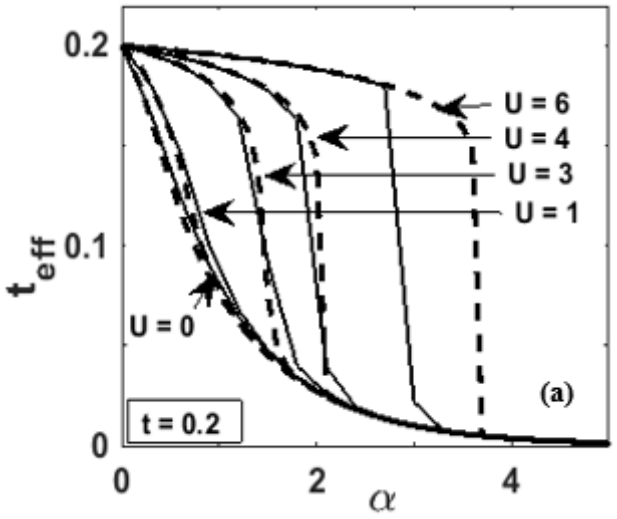


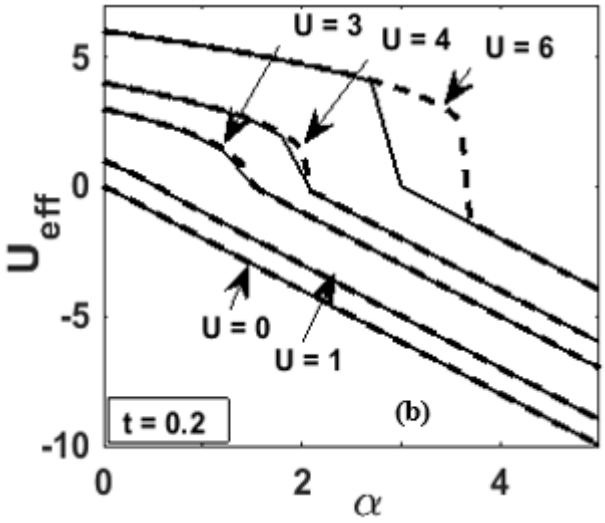
Fig. 4.1 (a) t_{eff} vs U for different values of α; (b) U_{eff} vs U for different values of α; (c) Double occupancy parameter (ω) vs. U for different values of α; (d) Entanglement entropy (E_v) vs. U for different values of α, for $t = 0.2$ at half filling. The solid lines represent the present results and the dashed lines refer to those of SC [27].

In other words, if α is large enough, U_{eff} can become negative, resulting in the formation of bi – polaronic bound states consisting of polaronic pairs.

The parameter ω can be used to quantify the presence of bipolaronic pairs at a lattice site, giving a measure of double – occupancy. The $\omega\ vs\ U$ plot in Fig. 4.1(c) shows that as U increases, ω decreases, and eventually becomes zero as U reaches a critical value (U_c), which of course is dependent on α. If U_{eff} has a positive value, one would conclude that ω will be zero. As a result, we can assume that for certain α, there exists a critical value of U (U_c) above which the system's GS is represented by a single polaronic state in which phonon – dressed electrons with opposite spins are localized at nearby neighboring sites. This is similar to a SDW state or the Mott insulating phase. As a result, when $U_{eff} > 0$, the SDW condition is expected to arise. As can be seen, ω increases as α increases, and U_c increases in general as α increases. U_{eff} is negative below U_c, implying that the system is unstable against Peirels transition. The system enters a CDW state or a bi – polaronic state. As a result, we can safely conclude that very small values of ω belong to a SDW state, while large values of ω correspond to a CDW state. The fascinating aspect is that at and near $U_{eff} = 0$, GS could be an unstable weakly correlated anti – ferromagnetic state that may not be a Mott insulating state. A real Mott insulating GS emerges at $U_{eff} \geq W_e = 2zt_{eff}$, where W_e is the band – width and z is the coordination number [51, 52]. The results for double occupancy clearly illustrate that for a small positive U_{eff}, ω can have a small finite value. This could be a SDW state for weak correlation. A ground state corresponding to a pure Mott insulator will arise for $U_{eff} \geq W_e$. This state will have a value of ω equal to zero. Similarly, $U_{eff} \lesssim 0$, on the other hand, might not belong to a pure CDW state. The system will be in a pure CDW state if U_{eff} is substantially smaller than zero. The variation of $E_v\ vs\ U$ is shown in Fig. 4.1(d). It can be seen that E_v has a peak at a given critical value of U (U_{QC}) for every value of α. As the value

of α is increased, the peak becomes shorter, sharper, and shifts towards the higher values of U. U_{QC} is the quantum critical point, and the peaks in E_v indicate a quantum phase transition. The peak found in E_v refers to a metallic phase. Before and after the peak in E_v, U is relatively much smaller.





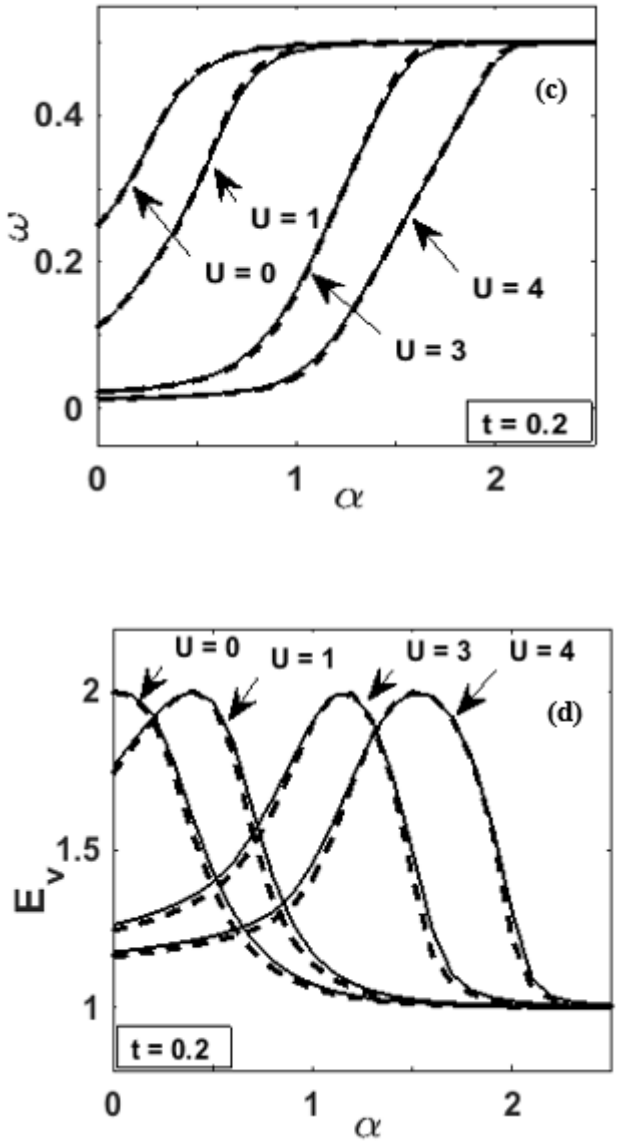


Fig. 4.2 t_{eff} vs α for different values of U; (b) U_{eff} vs. α for different values of U; (c) ω vs. α for different values of U; (d) E_v vs. α for different values of U, for $t = 0.2$ at half filling. The solid lines represent the present results and the dashed lines refer to those of SC [27].

As a result, one can conclude that, the region before U_{QC} corresponds to a CDW phase, whereas the region following U_{QC} corresponds to a SDW phase. As U is increased, the system undergoes a quantum phase transition from a CDW phase to an SDW phase via an intermediate metallic phase for a given value of α.

Next, we show the behaviour of t_{eff}, U_{eff}, and ω with respect to α for different U values in Figs. 4.2 (a, b, c, d). Again, the SC results are shown for comparison. For small α, $t_{eff} = t$, $U_{eff} > 0$ and ω is zero or small depending on the value of U and GS of the system appears to be the SDW state. For a large value of α, we find that $U_{eff} \ll 0$, $t_{eff} \cong 0$ and ω saturates to its maximum value and the system settles in a CDW GS. Fig. 4.2(d) shows that for a given value of U, E_v exhibits a maximum at some critical value of (α_{QC}) and the maxima shifts towards higher values of α as U increases. Therefore, as the value of α increases from the small and intermediate coupling zone to the strong coupling regime, ω increases until it exceeds the average value of 0.25, at which time U_{eff} switches sign and E_v goes through a maximum value. The maxima in E_v again suggest a metallic phase, and the figures show a quantum phase transition through an intermediate metallic phase from an insulating polaronic SDW phase of antiferromagnetic Mott type to an insulating CDW bipolaronic phase of Peierls type.

In Fig. 4.3, we draw a three – dimensional (3D) plot of ω versus α and U to show the combined effect of α and U on the GS phase diagram. It is evident that at small α and large U, ω is very small, which indicates that the system is in the SDW phase. On the other hand, at large α and small U, GS is a CDW state. From Figs. 4.1 and 4.2, we expect that in Fig. 4.3, there will be some region bordered by the SDW and CDW phases that will be

metallic. The Mott – Hubbard criterion: $t_{eff} \geq |U_{eff}|/4$, which is a criteria for a metallic state, is used to examine this. We find that the requirement $t_{eff} \geq |U_{eff}|/4$ is indeed satisfied in the region between the SDW and CDW phases.

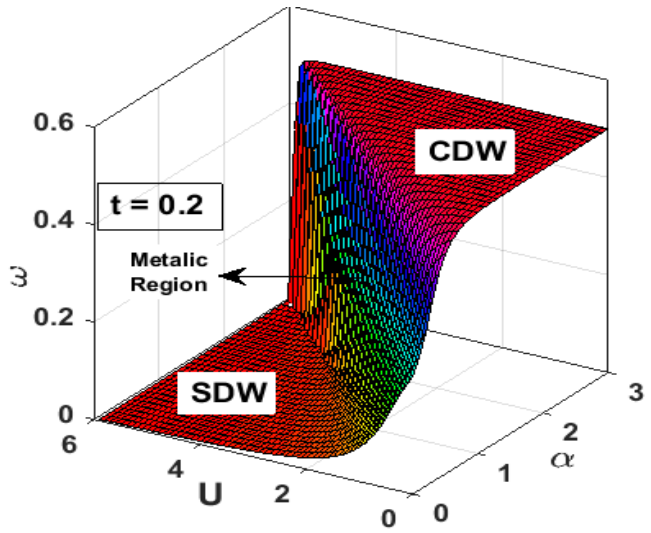


Fig. 4.3 3D plot of ω vs. α and U for $t = 0.2$ at half filling.

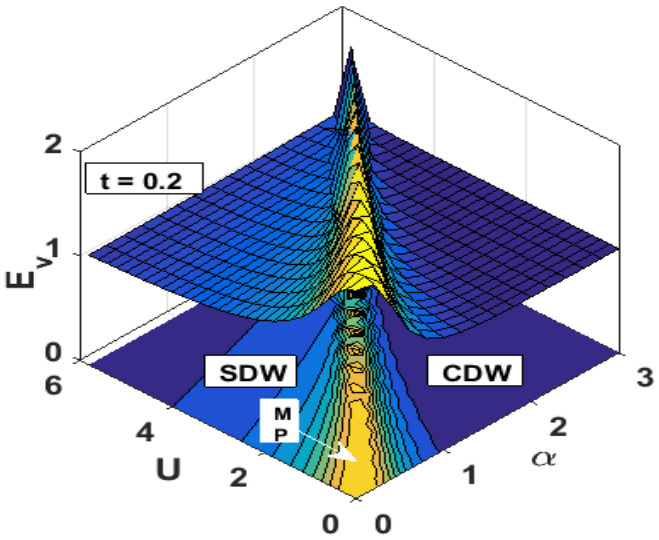


Fig. 4.4 3D plot of E_v vs. α and U for $t = 0.2$ at half filling. MP refers to the metallic phase.

The $3D$ plot of E_v with respect to α and U is shown in Fig. 4.4. One can see that there is a zone flanked by the SDW and CDW regions, where E_v is maximum, which is the signature of a metallic phase.

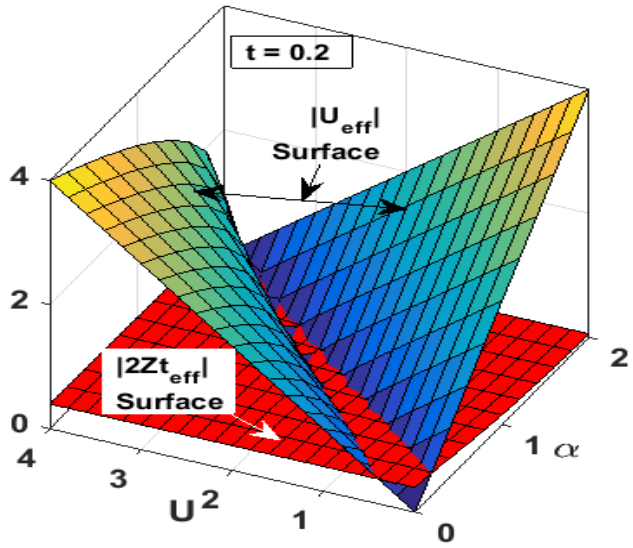


Fig. 4.5 3D plots of $2zt_{eff}$ and $|U_{eff}|$ surfaces for $t = 0.2$ with respect to α and U.

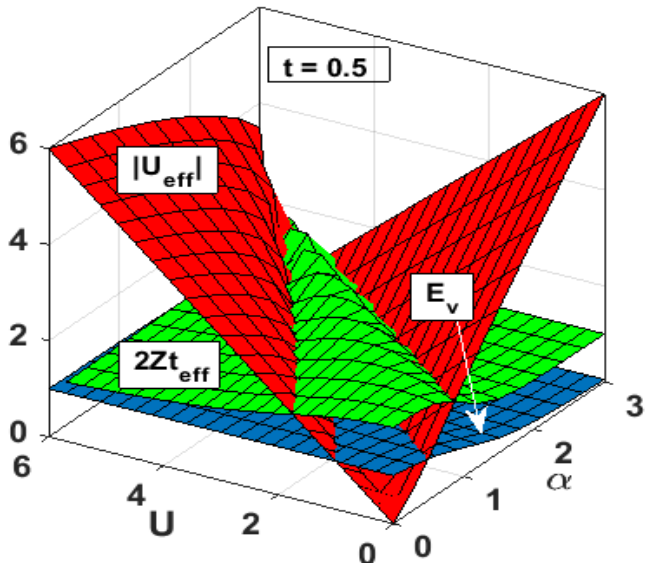


Fig. 6 3D plots of E_v, $2Zt_{eff}$ and $|U_{eff}|$ surfaces for $t = 0.5$ with respect to α and U.

In Fig. 4.5, we plot the $|U_{eff}|$ and $2Zt_{eff}$ surfaces as a function of α and U. One can see that the metallic phase satisfying the Mott – Hubbard condition corresponds to the same metallic phase seen in Fig. 4.4 through the concept of quantum entanglement. In Fig. 4.6, we illustrate the variation of $|U_{eff}|$, $2zt_{eff}$ and E_v with respect to U and α for $t = 0.5$ through a multidimensional plot. The metallic phase is manifestly clear from the EE peaks and the criterion: $4t_{eff} \geq |U_{eff}|$. In Fig. 4.7, we show the contour plots for QEEs for the SDW and CDW phases in the (U, α) plane with $t = 0.4$. The Mott – Hubbard condition is again used to obtain the metallic phase.

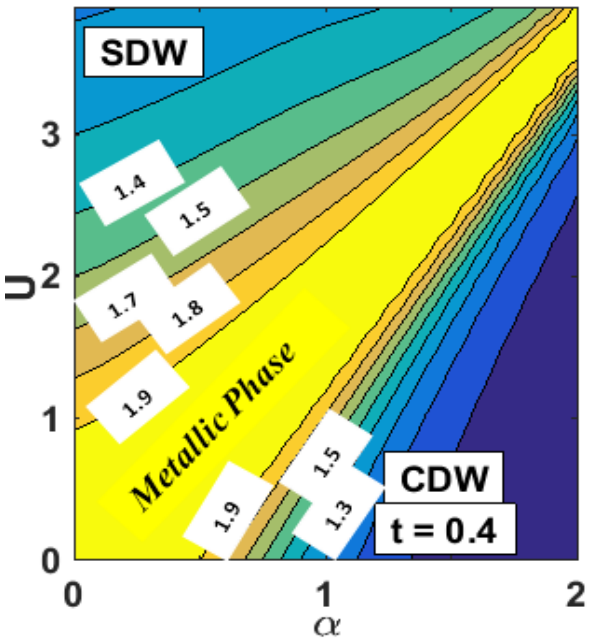


Fig. 4.7. Phase diagram for $t = 0.4$. in the $(\alpha - U) -$ plane.

In Fig. 4.8 we show the contour plots for $t = 0.8$. We can immediately see that as t increases, the metallic phase is widened. We also show the contour plots obtained from the calculation of SC [27]. It is clearly evident

that the present work that uses an improved variational calculation predicts a broader metallic phase.

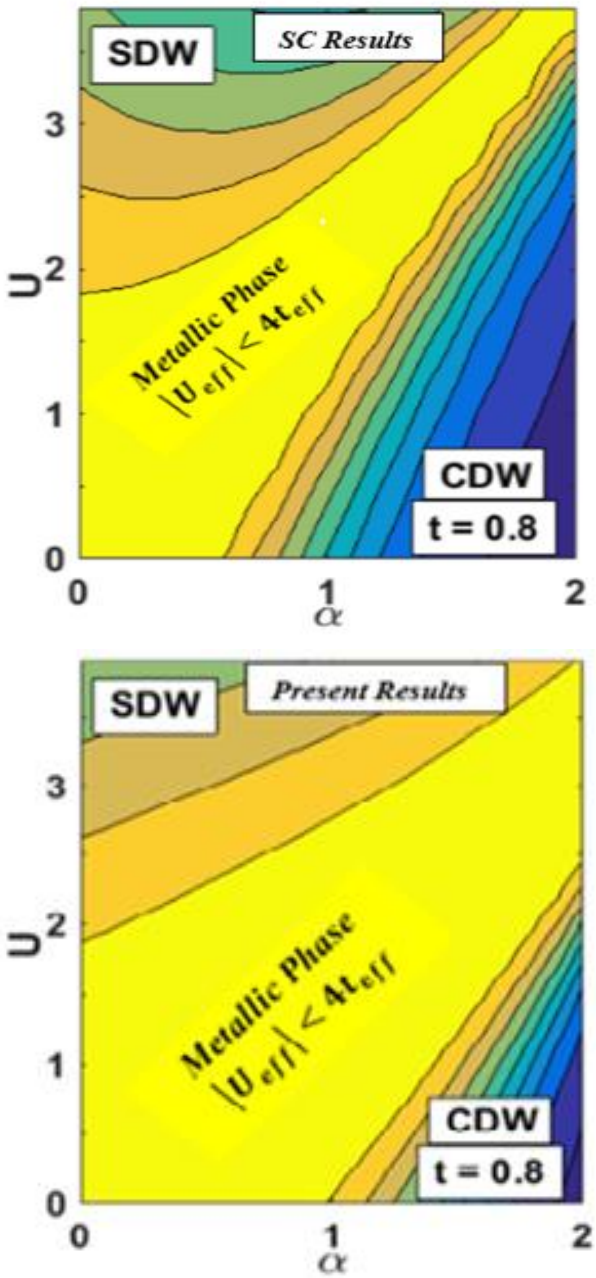


Fig. 4.8 Phase diagram for $t = 0.8$. in the $(\alpha - U) -$ plane. 'SC' refers to the phase diagram obtained by SC [27].

4.1 Conclusion

In this chapter, we have investigated and analyzed the detailed nature of the SDW – CDW transition in a 1D correlated electron – system in the presence of el – ph interaction using the half – filled 1D HH model. After performing a series of unitary transformations to the HH Hamiltonian, we averaged the modified transformed Hamiltonian with respect to a generalized many – phonon state. This has resulted in an effective Hubbard Hamiltonian. The GS energy of this Hamiltonian is finally determined by using the Bethe – ansatz approach. The quantum entanglement entropy and the double occupancy parameters are then calculated at and around the SDW – CDW transition regions to examine the existence of an intermediate phase. An intermediate phase is observed and it turns out to be metallic. When the present results are compared with those SC, it becomes clear that the present modified variational calculation predicts a larger metallic phase. This lends credence to the original prediction of TC [28].

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Chapter 5

Conclusion

The summary of the present thesis entitled, **'Phase transition in 1 – D Holstein – Hubbard model'** is presented in this final chapter. The mechanism of high T_c superconductivity has remained inconclusive. A number of reports have proposed the electron (el) – phonon (ph) mechanism. However, the problem with the el – ph mechanism is that it suggests an insulating spin – density – wave (SDW) state as the ground state if the el – ph interaction is small compared to the Coulomb correlation and an insulating charge – density – wave (CDW) as a ground state if the el – ph interaction is large compared to the Coulomb correlation. Thus, one has an insulator to insular transition in this scenario. In 2003, Takada and Chatterjee (TC) [1] took up this problem for a more rigorous analytical examination and suggested the presence of an intermediate metallic phase between the SDW – CDW regions. The calculation of TC is variational and therefore Chatterjee and collaborators [2 – 6] have made a few improvements on the calculation of TC. It is interesting to point out that every improved variational calculation has led to a wider metallic phase. As we have pointed out, the calculations performed in [1] are variational and therefore there can still be room for improvement. The aim of the present thesis has been to make an attempt in this direction.

In Chapter 1, we introduced the subject matter of the thesis and the motivation. We have also discussed the basic concepts and relevant models on which our works are based. Because we have been interested in this thesis on narrow – band systems, we have started with a brief discussion on the Tight – Binding model [7] and then presented a brief overview of the Hubbard model [8]. Since the main aim of this thesis has been to study the interplay between the el – ph and el – el interactions, we have next introduced the concept of polarons and bipolarons, the Holstein polaron [9 – 13] and finally the Holstein – Hubbard (HH) model [14 – 17], that can explain the physics of an el – ph system with Coulomb correlation [18 – 20]. Finally, we have examined the issue of possible ground states that the HH model can provide. In this context, we described the SDW and CDW phases and discussed the phase transitions that can occur in HH model as the interaction parameters are changed. At the end of the chapter, we have given an overview of the thesis.

In Chapter 2, the 1D HH model is studied at half – filling to analyze the influence of el – ph interaction and coulomb repulsion at the cross over region of the CDW and SDW phases. A series of canonical transformations have been applied to the Hamiltonian followed by an averaging with respect to a zero – phonon state to obtain an effective electronic Hamiltonian that has been finally solved by the Bethe – ansatz technique. The canonical transforations have been carried out to take care of phonon coherence and correlations. In the present work, we have introduced a new canonical transformation that takes into account electron density – dependent phonon correlations that can lead to an important effect particularly if the el – ph interaction is not small. We have used the Mott criterion and the local spin – moment to obtain the phase diagram and the contour plot. We have confirmed the existence of the intermediate metallic phase at the SDW –

CDW transition region and have also shown that the present calculation provides a broader metallic phase at the phase boundaries of CDW and SDW cross – over region than the one's predicted by the previous calculations [2]. This wider metallic phase obtained from an improved variational calculation reinforces our confidence in the prediction of TC.

In Chapter 3, we have extended our work of Chapter 2 by using a generalized many – phonon state as the averaging phonon state in place of the zero – phonon state. The effective electronic Hamiltonian is then solved exactly by the Bethe – ansatz method. So, we have referred to this method as semi – exact. We have shown that this calculation widens the intermediate metallic state even further lending credence to the conjecture of TC.

In Chapter 4, we have extended the investigation of Chapter 3 to calculate Entanglement Entropy (EE) and Double Occupancy (DO) of the same system. EE and DO have been calculated at and around the transition region of SDW and CDW phases. These calculations reconfirm the presence of intervening metallic phase and also show broader metallic phase when compared with the earlier calculation of Shankar and Chatterjee [5].

It would be quite interesting to examine the nature of the SDW – CDW transition in two dimensions.

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LIST OF PUBLICATIONS

Thesis Publications

1) **M. Z. Malik**, S. Mukhopadhyay & A. Chatterjee, *Ground state phase diagram of 1D Holstein-Hubbard model,* Phys. Lett. A, 383, 1516-1519 (2019).

2) **M. Z. Malik** & A. Chatterjee, *An intervening metallic phase at the CDW–SDW transition region in the one-dimensional Holstein-Hubbard model at half filling: a semi-exact solution.* J. Phys. Commun. 4 (2020) 105005.

3) **M. Z. Malik** & A. Chatterjee, *Quantum entanglement entropy and Double occupancy in a one-dimensional Holstein-Hubbard model at half filling.* Physica E 133 (2021) 114784.

Other Publications

1) **M. Zahid Malik**, D. Sanjeev Kumar, Soma Mukhopadhyay & Ashok. Chatterjee, *Role of spin-orbit interactions on the entropy and heat capacity of a quantum dot helium placed in an external magnetic field.* Physica.E, 121 (2020) 114097.

2) Debika Debnath, **Zahid Malik** & Ashok. Chatterjee, *A semi-exact solution for a metallic phase in a half-filled Holstein-Hubbard chain with Gaussian anharmonic phonons*. Sci Rep 11 (2021) 12305.

Publications in Conference preceedings

1) **Mr. Zahid Malik**, Soma Mukhopadhyay and Ashok Chatterjee, Existence of *a metallic phase in the charge-density-wave-spin-density-wave crossover region in the 1-D Hubbard-Holstein model at half filling.* AIP Conf. Proc. 2115 (2018) 030375.

2) **M. Zahid Malik**, Soma Mukhopadhyay & Ashok Chatterjee, Existence of *an intervening metallic phase at the transition region of the charge-density-wave and spin-density-wave in the 1-D Hubbard-Holstein model.* AIP Conf. Proc. 2142 (2019) 110014.

CONFERENCES ATTENDED

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Phase transition in 1 - D Holstein - Hubbard Model

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