PAPER

An intervening metallic phase at the CDW–SDW transition region in the one-dimensional Holstein-Hubbard model at half filling: a semi-exact solution

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Abstract

The one-dimensional Holstein–Hubbard model is analyzed at half filling at the CDW-SDW transition region by using a series of unitary transformations. The phonon degrees of freedom are eliminated by averaging the transformed Hamiltonian with respect to a generalized many-phonon state and the resulting effective electronic Hamiltonian is finally solved exactly by employing the Bethe-ansatz technique. The present variational state leads to a lower ground state energy as compared to those obtained from the previous variational calculations and yields a wider intermediate metallic phase at the SDW-CDW transition region confirming the prediction of Takada and Chatterjee.

1. Introduction

High-temperature superconductivity (HTSC) in cuprates [1] was discovered more than forty years ago, but still there is no unequivocal agreement on the basic pairing mechanism responsible for inducing superconducting condensation in these materials. There have been several mechanisms [2] in the fray but none has been able to explain convincingly all the aspects of HTSC. In this context, one of the mechanisms that have been advocated as the potential candidates is again the electron-phonon (e-p) interaction [3]. However, it appeared that the e-p mechanism suffers from a fundamental problem. For example, for the transition temperature to be high, the e-p coupling has to be sufficiently strong. But, if the e–p coupling is strong enough, then the virtual phonon-mediated attractive electron-electron (e–e) interaction at the Fermi level can prevail over the usual repulsive e–e Coulomb correlation and consequently, the overall effective onsite electron correlation ($U_e$) can become negative and the system will then be unstable under Peierls distortion giving rise to a bipolaronic charge density wave (CDW) [4] ground state. While, if the e–p interaction is weak, then the ground state is, of course, an antiferromagnetic polaronic spin-density wave (SDW). Therefore, under no circumstances, the e–p interaction appears to be a suitable mechanism for inducing pairing for HTSC. In fact, Fradkin and Hirsch [5] have shown by a monte-Carlo (MC) calculation that as the e–p interaction is increased, the ground state undergoes a direct transition from an SDW state to a CDW state, which also reinforces the opinion against the e–p interaction as the cause for high-temperature superconductivity.

The SDW–CDW transition problem has been studied analytically by Takada and Chatterjee (TC) [6] in the context of Holstein-Hubbard (HH) model. This study was motivated by the conjecture that when the effective e–e interaction is close to zero, there may be an interesting interplay between the e–p interaction and the repulsive Coulomb interaction, and as a result of this competition, there might appear a new phase at the transition region of the SDW–CDW phases, which may be metallic. Takada and Chatterjee used for the phonons, instead of the standard Lang-Firsov coherent state, a more general coherent state that has two parts, one depending on the electron concentration and the other independent of it. The variational calculation of TC is equivalent to performing two canonical transformations on the HH Hamiltonian and then taking a zero-phonon averaging of the transformed Hamiltonian. This yields an effective electronic Hamiltonian which is...
essentially a Hubbard Hamiltonian with renormalized parameters. The ground state energy solution of the effective Hubbard Hamiltonian has been finally obtained by TC by means of the Bethe ansatz method following Lieb and Wu [7]. TC have indeed found that as the e-p coupling is increased, an SDW-CDW transition does occur but it is not direct, rather it goes through an intermediate phase which has the attributes of a metallic phase. This interesting result has understandably triggered quite a few investigations. Clay and Hardikar [8] have examined the results of TC by studying the same HH model using a density-matrix-renormalization-group (RG) (DMRG)-based numerical technique. Their results support the prediction of TC. They have also demonstrated that the metallic phase can become superconductive. Fehske et al [9] have also employed a DMRG technique and predicted an intermediate metallic region particularly for large phonon frequencies. Bakrim and Bourbonnais [10] have shown that the RG approach and the quantum MC (QMC) method yield the same results and both support the presence of the intervening metallic phase. Nowadnick et al [11] have carried out a determinant QMC analysis in two dimensions and have shown the existence of the intervening metallic phase. Payeur and Senechal [12] have used a cluster perturbation theory and an exact diagonalization technique and concluded that the possibility of the existence of an intermediate metallic phase at the CDW phase boundary cannot be ruled out. Hohenadler and Assaad [13] have also confirmed the existence of such a metallic region.

However there have also been a few works [14] which were in contradiction with our results. According to these works when the e-p interaction is increased, a transition from an SDW phase to a CDW phase takes place without going into a superconducting phase through polaronic or bipolaronic mechanism. This motivated Chatterjee and collaborators to investigate SDW-CDW crossover region more critically by improving the trial phonon wave function in their variational treatment. The idea is that if a more refined variational method gives rise to a wider metallic phase, then the possibility of existence of the intervening metallic phase is strengthened.

On the other hand, if an improved variational method leads to a shrinking metallic phase, this would cast a shadow of doubt on the presence of the metallic phase. With this motivation, Karisha and Chatterjee (KC) [15] have carried out a variational study of the HH model with an improved phonon state. In the standard field theoretic jargon, the electrons are considered as the source of phonons. As a phonon is emitted by an electron, the electron undergoes a recoil motion. During this motion, if another phonon is emitted by the electron, then the two successively emitted phonons will be correlated. This phonon correlation can be taken care of by introducing a squeezing transformation [16]. In addition to taking care of the phonon correlations, the squeezing transformation also incorporates, albeit partly and also indirectly at the wave function level, the phonon anharmonicity effect which, among other things, makes the phonon life-time finite. Thus the squeezing transformation also takes into account some aspect of the phonon dynamics. The wave function of KC leads to a lower energy for the system ground state and also predicts a wider metallic phase compared to the one obtained by TC. Recently, Shankar and Chatterjee [17] have calculated the Entanglement entropy of the same system and have also shown the presence of the intermediate metallic phase through a different route.

The phonon correlation effect incorporated by KC is in tune with the squeezing transformation of Zheng [16]. According to this prescription, the squeezing parameter does not depend on the electron concentration at a particular site. More recently, Malik, Mukhopadhyay and Chatterjee (MMC) [18] have introduced a new squeezing transformation (hereafter called MMC transformation) that involves electron-density-dependent squeezing transformation. This implies incorporation of onsite phonon correlation effect that depends on the electron density on the corresponding site, which is obviously an important improvement of the phonon state. This will be referred to as the MMC transformation. Using the variational treatment of MMC is equivalent to employing a series of six canonical transformations and then performing a zero-phonon averaging. The calculation of MMC lowers the ground state energy and widens the metallic phase even further.

However as mentioned above, MMC [18] have used a zero-phonon state as the final averaging state after giving a series of six canonical transformations to obtain the effective Hubbard Hamiltonian which is then solved exactly by the Bethe ansatz technique to obtain the ground state energy. In the present work, we shall improve the calculation of MMC further by taking a many-phonon state instead of a zero-phonon state. In this sense, the present calculation can be considered as a semi-exact calculation.

### 2. Model and formulation

The one-dimensional (1D) Holstein-Hubbard chain can be modeled by the following Hamiltonian:

\[
H = - \sum_{\langle i,j \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_i b_i^\dagger b_i + g \sum_i n_{i\omega}(b_i^\dagger + b_i),
\]

where \(c_{i\sigma}^\dagger\) (\(c_{i\sigma}\)) is the creation (annihilation) operator of an electron at site \(i\) with spin \(\sigma\), \(n_{i\sigma} = (c_{i\sigma}^\dagger c_{i\sigma})\) being the corresponding electron number operator, \(t_{ij}\) is the bare hopping integral, \(i, j\) indicating that the summation is...
over nearest neighbours only, \( U \) is the on-site Coulomb interaction energy, \( b^\dagger_i (b_i) \) is the creation (annihilation) operator for a dispersion-less optical phonon of frequency \( \omega_0 \) at the site \( i \). \( g \) characterizes the strength of the e-p interaction we write as \( g = \sqrt{\alpha} \omega_0 \), where \( \alpha \) is the e-p coupling constant which is dimensionless. Since we consider a uniform chain, we can consider: \( t_{ij} = t \).

In order to solve the above Hamiltonian, we have to first decouple the electrons and phonons and obtain an effective electronic Hamiltonian. To accomplish this task, we use, as mentioned in the introduction, a variational method with a modified phonon state which is given by

\[
|\Phi\rangle = e^{R_{01}} e^{R_{21}} e^{R_3} e^{R_4} |\chi\rangle,
\]

where

\[
R_0 = \sqrt{\alpha} \eta \sum_{i} n_{i\omega} (b_i^\dagger - b_i),
\]

\[
R_2 = \sum_{i} h_i (b_i^\dagger - b_i),
\]

\[
R_3 = \alpha_i \sum_{i} (b_i b_i^\dagger - b_i^\dagger b_i),
\]

\[
R_4 = \alpha_d \sum_{i=0}^n (b_i b_i^\dagger - b_i^\dagger b_i),
\]

\[
R_5 = \frac{1}{2} \sum_{i<j} \beta_{ij} (b_i b_j - b_j^\dagger b_i^\dagger),
\]

\[
R_6 = \Delta \sum_{i} (b_i^\dagger - b_i),
\]

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

\[
|X\rangle = \prod_i |\phi_i\rangle = \prod_i \left( \sum_{n=0,1,2 \ldots \infty} A_{n} \frac{b_i^{n\dagger}}{\sqrt{n!}} |0_i\rangle \right).
\]

Thus the effective electronic Hamiltonian \( H_{\text{eff}} \) is given by:

\[
H_{\text{eff}} = \langle \Phi | H | \Phi \rangle = \langle \chi | H_{\text{d}} | \chi \rangle,
\]

where

\[
H_0 = e^{-R_0} H_5 e^{R_0}, \quad H_5 = e^{-R_5} H_4 e^{R_5}, \quad H_4 = e^{-R_4} H_3 e^{R_4},
\]

\[
H_3 = e^{-R_3} H_2 e^{R_3}, \quad H_2 = e^{-R_2} H_1 e^{R_2}, \quad H_1 = e^{-R_1} H e^{R_1}.
\]

Thus our variational treatment is equivalent to performing six unitary transformation followed by an averaging with a many-phonon state \( |\chi\rangle \). Here \( R_0 \) generates the well-known variable-displacement Lang–Firsov transformation VDLFT [19], where \( \eta \) is a variational parameter. This takes in account the coherence of the phonon state that depends on the electron density \( n_i \). \( R_2 \) generates an additional coherence in the phonon state that is independent of the electron density. Since we consider a uniform chain of atoms, we choose the variational parameter \( h_i \) to be same for all sites i.e., \( h_i = h \quad \forall \quad i \). The electron density-independent phonon correlation is taken care of by the generator \( R_3 \) with a variational parameter \( \alpha_i \). \( R_4 \) generates the MMC transformation which involves a variational parameter \( \alpha_d \) and assumes the squeezing to be linear in the electron density at a particular site. \( R_5 \) and \( R_6 \), however, neglect all the inter-site phonon correlations. Following Lo and Sollic [20], we introduce the correlated squeezing effect by the generator \( R_5 \) with \( \beta_{ij} \) as the variational parameter. We assume that the effect of the nearest-neighbour correlated squeezing is much smaller than the onsite squeezing so that we can neglect the fluctuation in the correlated squeezing and consider only density-independent correlated squeezing of the phonon state. Also the next-nearest-neighbour correlated squeezing is neglected and we choose, \( \beta_{ij} = \beta \), when \( i \) and \( j \) are nearest neighbors and \( \beta_{ij} = 0 \), otherwise. Finally the generator \( R_6 \) with the variational parameter \( \Delta \) makes sure that the coherence is maintained in the phonon subsystem. Whether it is really necessary for the phonons to be in a coherent state is finally determined by the variational calculation. A many-phonon state \( |\Phi\rangle \) with \( A_{n} \) as the variational parameters is chosen as the final averaging phonon state. One may notice that we have assumed \( A_{n} \) to be independent of sites. This is a plausible approximation because the system is considered uniform. It may be noted that \( m = 0 \) gives the usual zero-phonon state: \( \prod_i |0_i\rangle \). For \( m = 1 \), \( |X\rangle = \prod_i (A_0 |0_i\rangle + A_1 |1_i\rangle) \) is a many-phonon state which is a linear combination of different phonon states with the restriction that no site can contain more than one phonon. We shall call it a Restricted many-phonon state. For \( m = 2 \), the averaging many-phonon state:

\[
|X\rangle = \prod_i \left( A_0 |0_i\rangle + A_1 |1_i\rangle + \frac{A_2}{\sqrt{2!}} |2_i\rangle \right)
\]

is a linear superposition of different phonon states in which a particular site can be occupied at most by three phonons. Thus equation (9) is the most general many-phonon
state in which a particular site can contain any number of phonons. The effective electronic Hamiltonian $H_{\text{eff}}$ is given by

$$H_{\text{eff}} = \langle \Phi | H | \Phi \rangle$$

$$= -J \sum_{i} n_{i\sigma} + U_{\text{eff}} \sum_{i} n_{i\uparrow} n_{i\downarrow} - t_{\text{eff}} \sum_{i,j} \epsilon_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \omega_{0} h^2$$

$$+ \Delta e^{i\beta} e^{2\alpha_{+} + 2\alpha_{-}} \sum_{\sigma} n_{\sigma} \left( 2h + \Delta e^{2\alpha_{+} + 2\alpha_{-}} \sum_{\sigma} n_{\sigma} \right) + K$$

$$+ \frac{\omega_{0}}{2} \left[ (e^{i\beta})_{00} \cosh \left( 4\alpha_{i} + 4\alpha_{d} \sum_{\sigma} n_{\sigma} \right) - 1 \right],$$

where $J$ is the ground state polaron self-energy, $t_{\text{eff}}$ is the renormalized hopping integral, $U_{\text{eff}}$ is the effective onsite Coulomb correlation energy, $K$ is a constant and $\beta_{ij}$ are the elements of $\beta$ matrix (for a chain of $N$ atoms) whose elements are denoted by $\beta_{ij}$. As already mentioned earlier, $\beta_{ij}$ is given by: $\beta_{ij} = \delta_{j,i+1} \beta$. The expressions for $J$, $U_{\text{eff}}$, $t_{\text{eff}}$, and $K$ are given by

$$J = Q + P [Me^{2\alpha}(2A_{0}A_{1} + 2A_{1}A_{2} + 2A_{2}A_{3}) - 2\Delta] - 2h],$$

$$U_{\text{eff}} = U + 2(\sqrt{\pi} \eta) \omega_{0} - 4(\sqrt{\pi})^{2} h,$$

$$t_{\text{eff}} = t \{ 1 + 2\sqrt{2} \alpha A_{2}(A_{0} \xi - \sqrt{2} A_{2}) \xi - 2\alpha_{i} \kappa + 6A_{1} \sqrt{6} \alpha \tau + \alpha^{2}(0.5A_{1}^{2} - 1.63A_{2} + 3A_{3}) \}$$

$$\times e^{-\alpha_{i} e^{-\beta_{ij}}},$$

$$K = \frac{1}{4}Me^{4\alpha_{i}} \{ 2\sqrt{2} A_{2}A_{3} + (2\sqrt{2} A_{2}A_{3} + 2\sqrt{6} A_{2}A_{3} + 4\Delta) \}

+ PMe^{2\alpha_{i}}(2A_{0}A_{1} + 2A_{1}A_{2} + 2\sqrt{3} A_{2}A_{3} - 2\Delta) \times (2\alpha_{d} + 3\alpha_{i}^{2})$$

$$- Mhe^{2\alpha_{i}}(2A_{0}A_{1} + 2\sqrt{2} A_{2}A_{3} - 2\Delta) \times (2\alpha_{d} + 3\alpha_{i}^{2})$$

$$- hMe^{2\alpha_{i}}(2A_{0}A_{1} + 2\sqrt{2} A_{2}A_{3} - 2\Delta) \times (2\alpha_{d} + 3\alpha_{i}^{2})$$

$$+ \frac{1}{4} e^{4\alpha_{i}}(1 + 4\beta_{i}^{2})(4\alpha_{d} + 12\alpha_{i}^{2})(1 + 2A_{1}^{2} + 4A_{2}^{2})$$

$$+ 2\sqrt{2} A_{2}A_{3} + 2\sqrt{6} A_{2}A_{3} + 6A_{3}^{2} + 4\Delta)$$

$$\times \frac{1}{4} e^{-4\alpha_{i}}(1 + 4\beta_{i}^{2})(4\alpha_{d} - 12\alpha_{i}^{2})(1 + 2A_{1}^{2} + 4A_{2}^{2})$$

$$- 2\sqrt{2} A_{2}A_{3} - 2\sqrt{6} A_{2}A_{3} + 6A_{3}^{2}$$

$$- \frac{1}{4} Me^{-4\alpha_{i}}(2\sqrt{2} A_{2}A_{3} + 2\sqrt{6} A_{2}A_{3}) \}$$

where

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

$$Q = (\sqrt{\pi} \eta) \omega_{0} - 2\sqrt{\pi} \eta g, \quad P = g - \sqrt{\pi} \eta \omega_{0}$$

$$\xi = \eta\{ 1 - 6\alpha_{d} + 36\alpha_{i}^{2} \} \{ 1 + 2\beta + 4\beta^{2} + 4\beta^{3} \} e^{4\alpha_{i}},$$

$$\kappa = \eta\{ 1 - 6\alpha_{d} + 36\alpha_{i}^{2} \} \{ 1 + 2\beta + 4\beta^{2} + 4\beta^{3} \} e^{4\alpha_{i}},$$

$$\zeta = \eta\{ 1 - 36\alpha_{d} \} \{ 1 + 4\beta^{2} - (2\beta + 4\beta^{3}) \} e^{-8\alpha_{i}};$$

$$\gamma = \eta\{ 1 - 36\alpha_{d} \} \{ 1 + 4\beta^{2} + (2\beta + 4\beta^{3}) \} e^{-8\alpha_{i}};$$

$$\sigma = \eta\{ 1 - 198\alpha_{d} \} \{ 1 + 4\beta^{2} + (2\beta + 4\beta^{3}) \} e^{-12\alpha_{i}};$$

$$\nu = \eta\{ 1 - 6\alpha_{d} + 36\alpha_{i}^{2} \} \{ 1 + 2\beta + 4\beta^{2} + 4\beta^{3} \} e^{-4\alpha_{i}}.$$

It is interesting to note that a close-form exact analytical expression could be obtained for $(e^{\beta})_{0i}$ which is given by

$$(e^{\pm\beta})_{0i} = \sum_{i=0,1,2,\ldots} \frac{(-\beta^{2i+j})}{i! (i+j)!},$$

where ‘0’ refers to a representative atom and $j$ refers to the $j$th atom counted from the representative 0th atom.
The exact ground state energy per site of $H_{\text{eff}}$ is obtained by using Bathe-Ansaz method [6] as

$$
\varepsilon_{\text{e}} = -J + \omega_{\text{e}} \left[ h^2 + \frac{(\text{e}^{2\alpha})_{\text{e}} \cosh (4\alpha_{\text{e}})}{2} - 1 \right] + \frac{1}{4} [U_{\text{eff}} - |U_{\text{eff}}|] + \omega_{\text{e}} M \Delta \text{e}^{2\alpha_{\text{e}}} (2h + \Delta \text{e}^{2\alpha_{\text{e}}}) + K = 4t_{\text{eff}} \int_{0}^{\infty} \frac{J_{0}(x) J_{1}(x)}{x \left[ 1 + \exp \left\{ \frac{x |U_{\text{eff}}|}{2t_{\text{eff}}} \right\} \right]} \, dx,
$$

where $J_{0}(x)$ is the Bessel functions of zeroth order and $J_{1}(x)$ is that of first order.

### 3. Results and explanations

The ground state energy has been minimized with respect to the variational parameters $\eta$, $h$, $\alpha_{\text{e}}$, $\alpha_{\text{d}}$, $\beta$, $\Delta$, and $A_{\text{d}}, A_{\text{d}}, A_{\text{d}}, A_{\text{d}}, \ldots$. In figure 1 we have shown the results for the ground state energy. The dotted line refers to the result obtained by TC who used the variational parameters $\eta$ and $h$. The dotted-dashed line corresponds to the results obtained by KC who used the variational wave function with the parameters $\eta$, $h$, $\alpha_{\text{e}}$, $\beta$, $\Delta$. The dashed line represents the results obtained by MMC by using an additional variational parameter $\alpha_{\text{d}}$. Finally the solid line refers to the present results where we have used a many-phonon state as the final averaging state. As we can see from the figure, the present results for the ground state energy are only marginally better than those of the previous variational calculations. Later we shall show that this marginal improvement in the energy can have significant effect on the phase diagram. This often happens with a variational calculation, as a small error of order $\delta$ in the wave function causes only an error of order $\delta^2$ in the energy.

In figure 2, we plot the effective hopping parameter $t_{\text{eff}} / t$ with respect to the onsite Coulomb correlation energy $U$. The figure shows for small $U$, and a reasonable value of electron-phonon coupling constant $\alpha$, $t_{\text{eff}}$ is small. Hence in this limit the band is narrow and massive bipolarons can form. This is the insulating CDW state in which case peierl’s instability occurs and the probability of double occupancy becomes large. For large $U$, the e-p interaction becomes irrelevant and then one has just the Hubbard model and ground state becomes an antiferromagnetic Mott insulator. This is the SDW state. One can see that as in [5, 15, 18], here too, between SDW and CDW states, some interesting features are visible.

To understand these features more critically, we investigate, as earlier, the behaviour of the derivative of the renormalized hopping integral ($d t_{\text{eff}} / dU$) with respect $U$. This behaviour is shown in figure 3. Interestingly, $d t_{\text{eff}} / dU$ exhibits a double-peak structure. As we have already pointed out, at small $U$, the system is in a CDW phase and at large $U$, the ground state of the system would be in an SDW phase. It appears that the minimum of
the valley between the two peaks corresponds essentially to $U_{\text{eff}} = 0$ which is the crossover point from CDW phase to SDW phase. One can get the value of $U_{\text{eff}}$ from $U$ using equation (14). Since the minimum of the valley corresponds essentially to $U_{\text{eff}} = 0$, the existence of a valley between the two peaks suggests that the CDW-SDW transition as $U$ is increased is not direct but it goes through a different phase. It would certainly be interesting to uncover the nature of this phase. For $t = 0.2$, we find that for a particular value of $\alpha$, there exists a pair of values of $U$ ($U_1$ and $U_2$) at which $(dU_{\text{eff}}/dU)$ shows the peaks, $U_1$ corresponding to the first peak and $U_2$ to the second peak. Thus we can plot the phase diagram: $(U_1, U_2)$ versus $\alpha$ for a range of $\alpha$ values. This phase diagram is shown in figure 4. It is well known that for a system to show a metallic behaviour it is necessary that

![Figure 2](image1.png)

**Figure 2.** Variation of $t_{\text{eff}}/t$ as a function of $U$.

![Figure 3](image2.png)

**Figure 3.** Derivative of $t_{\text{eff}}$ as a function of $U$. 
the band-width $2zt$, where $z$ is the coordination number and $t$ is the hopping parameter, is larger than or equal to the Holstein-Hubbard gap $U$, which is the onsite Coulomb correlation energy. Thus for our effective one-dimensional Holstein-Hubbard system, the metallicity criterion should be given by: $4t_{\text{eff}} / U_{\text{eff}} \geq 1$. Interestingly, we observe that in the phase diagram, for a given $\alpha$, the region between the $U_1 -$ line and the $U_2 -$ line, does satisfy the criterion: $4t_{\text{eff}} / U_{\text{eff}} \geq 1$. Thus we can conclude that the region between the $U_1$ and $U_2 -$ lines in figure 4 is in a metallic phase. One can easily see that above the $U_1 -$ line, strong correlation would prevail and the system would be in an SDW phase, while below the $U_2 -$ line, the e-p interaction wins and the system would be in a CDW phase. Thus $U_1 -$ and $U_2 -$ lines describe the phase boundaries. The $U_1 -$ line separates the SDW phase and the metallic phase, while the $U_2 -$ line separates the metallic phase and the CDW phase.

We also compare, in figure 4, our results with the previous results obtained by TC [6], KC [15] and MMC [18]. In the figure, ‘Many phonon’ refers to the results obtained by considering the state $|X\rangle = \prod_i (a_0|0\rangle + a_1|1\rangle)$. It is analogous to the many-Cooper pair state of the BCS theory or the Gurary wave function of the intermediate coupling theory of the polaron problem. We improve the calculation by increasing the value of $\gamma$ in (9) and find that the phase diagram does not change beyond $\gamma = 3$. The corresponding phonon state can be referred to as the generalized many-phonon state. One can see that the present calculation shows a wider metallic phase as compared to those of TC, KC and MMC. That the successive improvements in the variational calculation widen the metallic phase imparts a fair amount of confidence in our conjecture on the existence of a metallic phase at the crossover region of the CDW-SDW transition. The calculation performed here can be considered as semi-exact, since the most generalized phonon state has been chosen and the effective electronic problem has been solved exactly by the Bethe ansatz method. However, still the method is not exact because the total wave function is taken as an outer product of electronic state and the phonon state (which of course depends on electron variables).

To obtain an additional evidence for the existence of a metallic state at the CDW-SDW transition region, we next calculate the average local spin moment $L_0$ per site which we define as

$$L_0 = \frac{1}{N} \sum_i \langle S_i^z \rangle,$$

where $S_i$ is the electronic spin at the $i$-th site. We have

$$S_i^z = S_{\alpha}^z + S_{\beta}^z + S_{\gamma}^z,$$

Figure 4. Phase diagram in the $\alpha$, $U$—plane determined by the peaks in $dt_{\text{eff}} / dU$. The corresponding phase diagrams obtained by TC, KC, MMC are also shown for comparison.
Defining $S_i^\pm = S_{i\sigma} \pm i S_{i\bar{\sigma}}$, where

$$
S_i^+ = c_i^\dagger \sigma_i^+, \quad S_i^- = c_i^\dagger \sigma_i^-, \quad S_{i\sigma} = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}),
$$

we can write

$$
S_i^z = \frac{1}{2}(S_i^+ S_i^- + S_i^- S_i^+) + S_i^{z2} = \frac{3}{4} - \frac{3}{2N} \sum_{i}(n_{i\uparrow} n_{i\downarrow}).
$$

From equations (12), (21) and (24), we can immediately obtain

$$
L_0 = \frac{3}{4} - \frac{3}{2} \frac{d\varepsilon_0}{dU}
$$

For a particular value of $L_0$, we can determine a set of $(U, \alpha)$ values and plot a $L_0 -$ line in the $(U, \alpha)$-plane. Thus we can draw contour plots for different values of $L_0$. Figure 5 shows these contour plots, as mentioned, in the $(\alpha, U)$-plane. If the motion of the electrons is completely uncorrelated as we have in a gas of non-interacting electrons, then equation (19) yields: $L_0 = 0.375$, which is more or less the value we see in intermediate state. This gives one more indication of the presence of an intermediate metallic phase at the CDW–SDW transition region.

4. Conclusion

The 1D HH model has been investigated variationally using a series of unitary transformations and a generalized many-phonon state to obtain an effective electronic Hamiltonian which is finally solved exactly by the method of Bethe ansatz to obtain the ground state energy of the system. It is shown that the present semi-exact treatment yields a broader metallic phase at the crossover region of the CDW-SDW transition as compared to the previous variational calculations and thus lends credence to the original conjecture of Takada and Chatterjee [5]. It is to be noted that it is not important by how much amount the metallic phase widens in an improved variational calculation, rather what is important is that the metallic phase does widen and does not shrink in an improved variational calculation. The issue of the existence of a metallic phase in the HH model is not only important from the point of view of high temperature superconductivity but also from the fundamental physics related to the existence of different phases in strongly correlated Fermi systems.

Figure 5. Contour plots of the local moment $L_0$ in $\alpha$, $U$ plane.
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