The generalized Hubbard model in one dimension: a renormalization group study

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Abstract. We have modified an existing real space renormalization group scheme to remove some physically inconsistent features and used the rectified method to study the ground state of the one-dimensional Hubbard model with nearest-neighbour repulsion and the bond–charge interaction for half filling. For the nearest-neighbour interaction we find a phase diagram which agrees nicely with the Monte Carlo results. For the case of bond–charge interaction we have reproduced some available exact results and found some interesting information in the parameter regime where no exact solution is available.

1. Introduction

Since the discovery of high-temperature superconductivity in layered perovskites [1] the studies on the role of electron–electron interaction in different electronic systems have become extremely important [2]. In this context the simplest model one can think of is the Hubbard model [3] where only the on-site electronic correlation has been taken into account. But often the range of the interaction is comparable to the lattice spacing. Consequently, the inclusion of the nearest-neighbour correlations is required. In general an interacting electronic system can be described by a tight-binding Hamiltonian of the form [3]

$$H = \sum_{ij,\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{ijkl,\sigma\sigma'} \langle ij|\frac{1}{r}|kl\rangle c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma'} c_{k\sigma} \tag{1}$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a particle with spin σ in a Wannier orbital located at site i; the corresponding number operator is $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. T_{ij} is the Fourier transform of the band energy and $\langle ij|1/r|kl\rangle$ denotes the matrix element of the Coulomb interaction with respect to the Wannier orbitals located at sites i, j, k, l. Assuming for simplicity that only nearest-neighbour overlap terms are important compared to the longer-range overlaps we are left with the following relevant matrix elements of the Coulomb interaction:

$$U = \langle ii|1/r|ii\rangle$$
$$V = \langle ij|1/r|ij\rangle$$
$$W = \langle ij|1/r|ji\rangle = \langle ii|1/r|jj\rangle \tag{2}$$
$$X = \langle ii|1/r|ij\rangle$$

where i and j are nearest neighbours.

The basic approximation introduced by Hubbard was to neglect all other interaction terms apart from U, the on-site Coulomb repulsion. The basis of such an approximation was justified by Hubbard [3] on the following grounds. For 3d electrons in transition metals $U \sim 20$ eV while the next important term $V \sim 6$ eV though actually V is reduced to 2—3 eV due to the screening effect of the conduction electrons. Other terms are even smaller e.g. $X \sim 0.5$ eV and $W \sim \frac{1}{40}$ eV. This simplified model containing only the kinetic energy term and the on-site U term is believed to bear the essential physics of narrow-energy-band systems. But it is always interesting to note the physical consequences of the inclusion of other interactions because they may not be of negligible magnitude in other systems e.g. 1D polyene chains [4]. Though it is physically expected that $U > V > X > W$ should hold in general it is not always expected that, in particular, V and X be much smaller than U. As an example, for benzene, $U \simeq 17$ eV, $V \simeq 9$ eV, $X \simeq 3.3$ eV and $W \simeq 0.9$ eV [5]. So we retain the nearest-neighbour interaction V and the so-called bond–charge interaction X and obtain the following one-band generalized Hubbard Hamiltonian in 1D:

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1}$$
$$+ X \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} (n_{i-\sigma} + n_{j-\sigma}) - \mu \sum_i n_i \tag{3}$$

with $t = -T_{ij}$ for i, j nearest neighbours (denoted by a sum over $\langle ij \rangle$) and $U, V, X, t \geqslant 0$. Here $n_i = n_{i\sigma} + n_{i-\sigma}$; μ is the chemical potential.

In its simplest form containing the nearest-neighbour hopping t and the on-site Coulomb repulsion U, the Hamiltonian (3) is exactly solvable only in one dimension (1D) [6]. The more generalized versions, e.g. one including the nearest-neighbour repulsion term V or the bond–charge interaction X, are investigated by using different approximate methods [4, 7–10].

Here we apply a real space renormalization group (RG) technique [7, 11, 12] to explore this generalized Hubbard model in 1D for a half-filled band. The present RG scheme being well suited for a particle–hole (p–h) symmetric model we apply this method at present only for $X = 0$ and $X = t$ for which the Hamiltonian (3) is p–h symmetric. The motivation behind using this method is that this relatively simple method works over the whole range of couplings U and V due to its non-perturbative nature and also that it includes some fluctuations beyond the mean-field level and this is of absolute necessity owing to the low dimensionality of the system.

For $X = 0$ the available RG scheme [7] is found to suffer from a drawback. We have suggested here a remedy to this trouble and used this modified scheme for both $X = 0$ and $X = t$. We find that the phase diagram obtained by our scheme for $X = 0$, the extended Hubbard model, is in nice agreement with the Monte Carlo results. It is also found that this method reproduces all the known exact results [13] for $X = t$. Moreover, the present RG scheme gives some interesting information in the parameter regime where no exact solution is available.

In section 2 we present the difficulties of the available RG method [7] and their origin. Sections 3 and 4 are devoted to a discussion on the removal of these odd features in RG and its application for the $X = 0$ case. In section 5 we discuss the application of RG in the case of bond–charge interaction for $X = t$. In section 6 we present the RG results for bond–charge interaction along with a summary of the known exact solution. Section 7 summarizes the present work.

2. Trouble with the existing RG scheme

In the absence of the bond–charge interaction term X the Hamiltonian (3) reduces to the so-called one-band extended Hubbard model. This model has been already investigated by means of real space RG [7] by Fourcade and Spronken (hereinafter referred to as FS); this method was an extension of the methodology originally developed by Hirsch [11] and Dasgupta and Pfeuty [12].

This real space RG method works in the following way. The 1D lattice is partitioned into blocks of finite size. The block Hamiltonian is solved exactly and only four suitable low-lying states are retained. Then the intrablock part of the Hamiltonian as well as the interblock part are projected onto this truncated basis to renormalize the coupling constants in the Hamiltonian.

The major difficulty in handling the present model on a 1D lattice is that in spite of a global p–h symmetry this Hamiltonian does not possess this symmetry for a finite-size block due to the end effect. This forces one to recast the Hamiltonian in a form which contains an 'effectively p–h symmetric' interblock part of the Hamiltonian [14]. This is precisely what FS did in rewriting the Hamiltonian in the following way [7]:

$$
H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i \left(\frac{1}{2} - n_{i\uparrow} \right) \left(\frac{1}{2} - n_{i\downarrow} \right) + V \sum_i (1 - n_i)(1 - n_{i+1}) + D \sum_i \mathbf{1}_i
$$

(4)

where the chemical potential $\mu = U/2 + 2V$ is partly absorbed in the interaction terms and $D = -\mu/2$. The constant D accounts for the renormalization of vacuum energy. The Hamiltonian has several conserved quantities: total number of particles N, total spin S and the z component S_z of the total spin besides the p–h symmetry (on a bipartite lattice) pointed out earlier.

Using a three-site block FS retained the following four states of the block Hamiltonian: the lowest-energy states in the subspaces $\{N = 2, \ S = S_z = 0\}$, $\{N = 3, \ S = S_z = \frac{1}{2}\}$, $\{N = 3, \ S = -S_z = \frac{1}{2}\}$, $\{N = 4, \ S = S_z = 0\}$.

Of these states, the first and the fourth are connected by p–h symmetry while the second and the third by spin reversal symmetry. This led to the following RG equations [7] which relate the renormalized parameters (primed quantities) to the original parameters (unprimed ones) in the Hamiltonian:

$$
\begin{aligned}
U' &= 2(E_2 - E_3) \\
D' &= 3D + (E_2 + E_3)/2 \\
t' &= \lambda^2 t \\
V' &= \rho^2 V
\end{aligned}
$$

(5)

where E_2 and E_3 are the lowest eigenvalues of the subspaces $\{N = 2, \ S = S_z = 0\}$ and $\{N = 3, \ S = S_z = \frac{1}{2}\}$ respectively; and

$$
\begin{aligned}
\lambda &= \langle N = 2, \ S = S_z = 0 | c_{\uparrow}^b | N = 3, \ S = S_z = \tfrac{1}{2} \rangle \\
\rho &= (1 - \langle N = 2, \ S = S_z = 0 | n^b | N = 2, \ S = S_z = 0 \rangle).
\end{aligned}
$$

(6)

The superscript b refers to the boundary site of a block. The form of this Hamiltonian remains preserved in the RG iterations.

This scheme reproduces the ground state energy correctly in the atomic limit ($t = 0$). In the presence of t one can also find out the spin density wave (SDW)/charge density wave (CDW) phase boundary from this scheme. FS also studied several other quantities like the

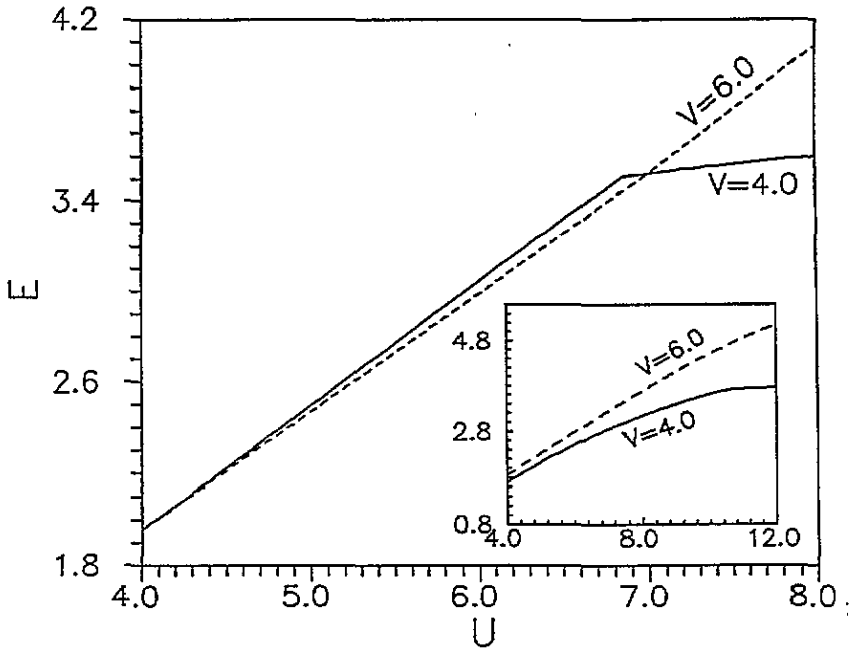gap in the single-particle excitation spectrum, the local moment and the average value of double occupancies.

Figure 1. Plot of the ground state energy/site E against U as calculated in the FS scheme. The inset shows the same calculated in the present modified prescription ($t = 1.0$).

But this RG scheme, being an approximate one, suffers from some difficulties which are not apparent in the work of FS. These problems, as we try to point out in the present work, are by-products of the approximate renormalization prescription of V, the nearest-neighbour Coulomb interaction. In order to realize this trouble let us refer to figure 1 which shows a plot of the ground state energy/site E against U (parametrized by different V) as obtained from the RG of FS. It is very strange that the curves for large (compared to hopping t) V values intersect each other. This suggests that in the intermediate range of the values of U it is possible to lower the energy by increasing a repulsive interaction (V)! But this does not happen for small V ($V \sim t$) and again in the atomic limit there appears no trouble. This indicates that there might be some trouble in the renormalization in V which shows up in the 'non-atomic, large-V' regime.

Let us now look back critically at the root of this discrepancy. The way the Hamiltonian (3) is rewritten by FS for the case $X = 0$ requires that the interblock Hamiltonian be written as

$$H_{int} = -t \sum_{j,\sigma}(c^\dagger_{j,3\sigma}c_{j+1,1\sigma} + \text{HC}) + V \sum_j (1 - n_{j,3})(1 - n_{j+1,1}) \qquad (7)$$

where j is the block index and 3 and 1 refer to the two adjacent terminal sites of the jth and $(j + 1)$th blocks respectively. Now we see that since we have absorbed the chemical potential term in the U and V parts of the Hamiltonian, the interblock part automatically contains a part ($\sim V$) of the intrablock term. This part gets estimated in terms of V', the renormalized quantity for V, rather than V itself. It is noteworthy that the intrablock part creeping into the interblock term comes originally from the chemical potential which is compensated at the end of the calculation and one uses $\mu = U/2 + 2V$ at this point. So

an error $\sim(V - V')$ is introduced in the ground state energy. As V' falls off compared to V this error tends to show up. Up to a range $V \sim t$ this offset is smeared out by the band energy (this was the regime FS studied) but in the case of large (compared to t) V this gives rise to an odd behaviour found in figure 1. It is, however, interesting to see that this problem does not show up in the atomic limit; the reason is discussed in the following section.

3. Remedy for the RG scheme: a possible way

Now let us consider the atomic limit of the RG scheme of FS. The recursion relations are [7]

$$
\begin{array}{llll}
U' = U & V' = V/9 & \text{for } U > 2V & \\
U' = 3U - 4V & V' = V & \text{for } V < U < 2V & \quad(8) \\
U' = U - 2V & V' = V & \text{for } U < V &
\end{array}
$$

where we see $V' < V$ only for $U > 2V$. In the atomic limit $U > 2V$ corresponds to a highly degenerate wave function with singly occupied sites. Therefore the V part in the interblock (as well as in the intrablock) Hamiltonian reduces to zero since $(1 - n_{j,3})$ and $(1 - n_{j+1,1})$ are identically zero; consequently the precise value used for V' does not play any role in the calculation. So in this case there is no error in the ground state energy due to the renormalization of V. For the other regime of the parameter space $V' = V$ and thus, again, there is no problem.

It is worthwhile to note that in the atomic limit this scheme yields the exact ground state energy $E = U/2$ for $U < 2V$ and $E = V$ for $U > 2V$. But while calculating the energy the renormalization of V does not explicitly enter the calculation for the $U > 2V$ region (where $V' < V$) but it does in the other regime, $U < 2V$. In other words, obtaining the correct value of E for $U < 2V$ does not impose any stringent requirement on the renormalization of V (any value of V' will do) within the prescription of FS. Therefore, if there is any inconsistency in the renormalization of V it is not apparent in the atomic limit.

To see it in detail we try to give an alternative way of visualizing this renormalization procedure for the $U > 2V$ limit. We use our knowledge that in this limit (for $t = 0$) all the sites are singly occupied. Instead of writing the Hamiltonian in the way FS did we put it in the form

$$
H = U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1}. \quad(9)
$$

Now, it is clear that at each iteration the blocks are in three-particle states with all sites singly occupied with an energy $2V$. So to get the ground state energy/site we just accumulate the three-particle energy at the nth stage scaled down by a factor of 3^n up to infinite terms. This gives

$$
E = \frac{2V}{3} + \frac{2V'}{3^2} + \frac{2V''}{3^3} + \cdots. \quad(10)
$$

If we have $V' = \alpha V$ then for all iterations $V^{(n+1)} = \alpha V^{(n)}$ (n being any stage of iterations) since wave functions are identically the same at all stages. Then from (10),

$$
E = \frac{2V}{3 - \alpha}. \quad(11)
$$

But we know that to get the correct result we have to have $E = V$. Using this in equation (11) we see that this demands $V' = V$ unambiguously.

So, it seems that even in the atomic limit FS prescription is not adequate over the whole range of the parameter space and in fact $V' = V$ is the unique renormalization of V anywhere in the atomic limit. If hopping is introduced V' is expected to fall off (but definitely in a manner slower than that in the FS scheme). But unfortunately there is no way (at least right now) to find that out. Instead we take this atomic limit renormalization of V for the $t \neq 0$ case too and proceed to see what happens.

This prescription neglects only the effect of single-particle hopping in renormalized V; otherwise it is perfect in the atomic limit. Satisfactorily enough, this has removed the odd behaviour shown in figure 1. This means that still there is an approximation in the renormalization of V but it is not as severe as in the FS scheme. Now this error is $\sim t$ (due to neglect of the effect of t in V') at worst and does not spoil the scheme at large V. After all the present model has an intrinsic trouble of losing p–h symmetry in the finite block which forces some difficulty in the renormalization of V to appear at some stage or other; it is better to choose that approximate scheme which does not give rise to any physical inconsistency as in figure 1.

4. Application of the RG: extended Hubbard model

As a test of the proposed modification of the RG of FS we apply it to the 1D extended Hubbard Hamiltonian (4). Apart from the routine calculations of energy and local moment one might be interested in finding out the phase diagram.

Now, as in the original FS scheme, one should be thinking of drawing an SDW/CDW boundary by the zeros of the quantity $(U_\infty - 2V_\infty)$ where U_∞ and V_∞ are the values of U and V respectively after iterations converge to a fixed point. This also turns out to be the line where the local moment L_0 goes over from a value $> \frac{3}{8}$ to a value $< \frac{3}{8}$ in FS calculation ($L_0 = \frac{3}{8}$ corresponds to the free fermionic value). Now in our prescription it is not meaningful to study the zeros of $(U_\infty - 2V_\infty)$ simply because we have not renormalized U and V on the same footing; the effect of t enters in U' but not at all in V'. Rather we should use the expectation value of a suitable operator that changes from one phase to another. We take the local moment for this purpose. This is expected to be less erroneous because its estimation is solely dependent on the wavefunction constructed iteratively.

Using the criterion that L_0 crosses the value $\frac{3}{8}$ we draw the SDW/CDW boundary in figure 2. $L_0 > \frac{3}{8}$ corresponds to SDW phase while $L_0 < \frac{3}{8}$ corresponds to a CDW state since in the CDW phase pairs start forming more and more while the SDW state favours single occupancies to hold a spin modulation. The phase boundary thus obtained shows a spectacular agreement with the available Monte Carlo data [9] which is not the case for the boundary drawn within the FS scheme (figure 2).

So, at this point, it seems more reliable to proceed with this kind of prescription to investigate similar Hamiltonians with further generalizations. In the next section we shall see the effect of the bond–charge interaction on the extended Hubbard model within this RG framework.

5. Application of the RG: bond–charge interaction

The generalized model (3) with bond–charge interaction X has been considered in several contexts like electron correlation effects in polyacetylene [4] or in problems regarding hole superconductivity [10]. Recently it has been solved exactly for $X = t$ over a wide range of parameter space for the half-filled band [13]. Since t is typically ~ 0.2–2 eV the values of
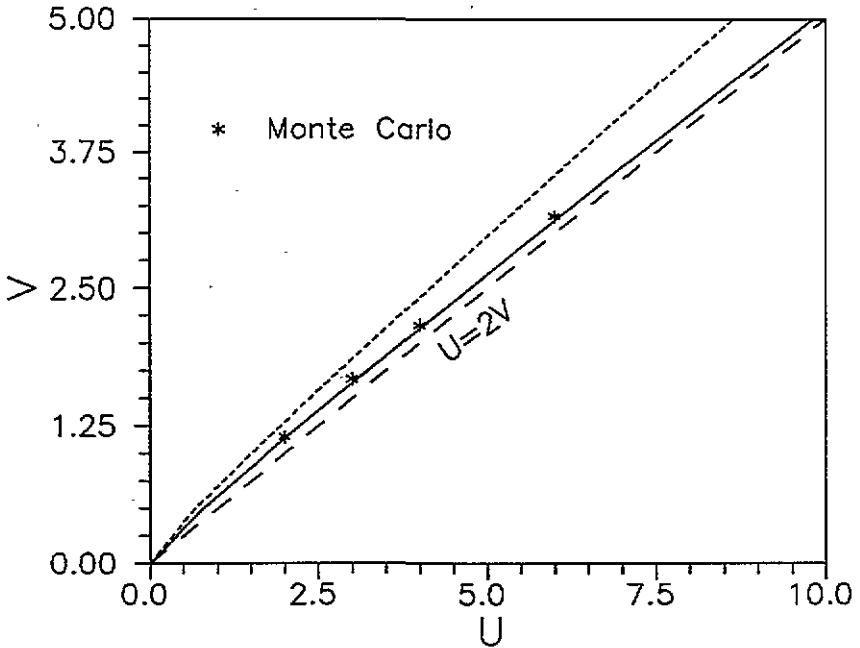
Figure 2. Phase diagram of the extended Hubbard model. The phase boundary obtained in the present scheme (solid line) is compared with that obtained in the FS scheme (dotted line) and the Monte Carlo results. The dashed line $U = 2V$ gives the phase boundary in the atomic limit ($t = 0$) between a singly occupied paramagnetic phase and a CDW region.

X and t are quite comparable. So it is reasonable to look at the special case $X = t$ where some exact results are also available.

Since for half filling the chemical potential $\mu = U/2 + 2V$ for this model and we are considering the case $X = t$ we can rewrite the Hamiltonian (3) in the following form:

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} (1 - n_{i-\sigma} - n_{j-\sigma}) + U \sum_{i} \left(\frac{1}{2} - n_{i\uparrow} \right) \left(\frac{1}{2} - n_{i\downarrow} \right)$$
$$+ V \sum_{i} (1 - n_i)(1 - n_{i+1}) + D \sum_{i} 1_i. \tag{12}$$

The diagonal quantities are renormalized [7] by the relations

$$U' = 2(E_2 - E_3) \tag{13a}$$
$$D' = 3D + \tfrac{1}{2}(E_2 + E_3) \tag{13b}$$

as they were in in equation (5).

To diagonalize the off-diagonal terms one needs to evaluate the matrix elements of operators corresponding to the boundary site of a cell. The first term in (12) appears like a constrained hopping term of amplitude t. To renormalize this we require the matrix element of c_σ^b, the annihilation operator of spin σ at the boundary site b between renormalized cell states. As in equation (6),

$$\langle v = 2, S = S_z = 0 | c_\downarrow^b | v = 3, S = S_z = \tfrac{1}{2} \rangle = \lambda$$

so that we can identify [11, 12] the renormalized annihilation operator c_σ' by $c_\sigma^b = \lambda c_\sigma'$. We

also require the matrix element of $c_\sigma^b n_{-\sigma}^b$ where $n_\sigma^b = c_\sigma^{b\dagger} c_\sigma^b$. This is

$$\langle \nu = 2, S = S_z = 0 | c_\uparrow^b n_\downarrow^b | \nu = 3, S = S_z = \tfrac{1}{2} \rangle = \lambda'$$

where λ and λ' both are real. Matrix elements for operators of reversed spin are the same in magnitude (apart from the sign) due to spin flip symmetry of the Hamiltonian. Putting all these together we obtain the renormalized hopping:

$$t' = \lambda(\lambda - 2\lambda')t. \tag{13c}$$

For the renormalization of V we use the relation $V' = V$, as discussed in section 3.

In the present scheme the ground state energy per site E is calculated from the converged value of the constant term D in (12) whose value at the nth stage of iteration is $D^{(n)}$. E is obtained from the limit

$$E = \lim_{n \to \infty} \frac{D^{(n)}}{3^n} \tag{14}$$

while the local moment is obtained by the relation

$$L_0 = \tfrac{3}{4}\langle (n_\uparrow^c - n_\downarrow^c)^2 \rangle \tag{15}$$

where n_σ^c is the number operator of spin σ at the central site of a block. The recursion relation for L_0 turns out to be of the form

$$L_0 = \alpha + \beta L_0' \tag{16}$$

where α and β are functions of t, U, V. We also compute the q transform of the density–density autocorrelation function defined by

$$N(q) = \frac{1}{N} \sum_{lm} (1 - n_l)(1 - n_m) \exp[iq(R_l - R_m)] \tag{17}$$

where R_l and R_m are positions of lth and mth sites respectively. Recursion of this type of correlation function is straightforward [11].

6. Bond–charge interaction: RG results

Before discussing the results obtained by this method let us summarize the exact results known so far [13]. It is shown for half filling and for $X = t$ that the ground state energy E_0 is given by

$$E_0 = LVZ/2 \qquad \text{if } U \geqslant (4t + V)Z \tag{18a}$$
$$E_0 = LU/2 \qquad \text{if } U \leqslant (-4t + V)Z \tag{18b}$$

where Z is the coordination number of the lattice containing L sites. The ground state is a 2^L-fold-degenerate (all sites singly occupied) paramagnetic insulator in the first case while it is a chess-board-type CDW on a bipartite lattice in the second case. Now in our case $Z = 2$. So we have energy/site $E = V$ for $U \geqslant 8t + 2V$ and $E = U/2$ for $U \leqslant 8t + 2V$. In the first case, all sites are singly occupied and the probability $P_\uparrow$ ($P_\downarrow$) that a site be occupied by an $\uparrow$ ($\downarrow$) spin is $\tfrac{1}{2}$. The probability $P_{\uparrow\downarrow}$ (P_0) that a site be doubly occupied (empty) is zero. So the local moment $L_0 = \tfrac{3}{4} = 0.75$ (the $\tfrac{3}{4}$ factor comes from the fact that S^2 for a spin-$\tfrac{1}{2}$ object is $\tfrac{1}{2}(\tfrac{1}{2} + 1) = \tfrac{3}{4}$). In the second case $P_\uparrow = P_\downarrow = 0$ and $P_{\uparrow\downarrow} = P_0 = \tfrac{1}{2}$. Therefore the CDW state possesses a local moment $L_0 = 0$. Apart from these exact results there is nothing known exactly in the region where $2V - 8t < U < 2V + 8t$. With this in hand we proceed to explain the real space RG results.
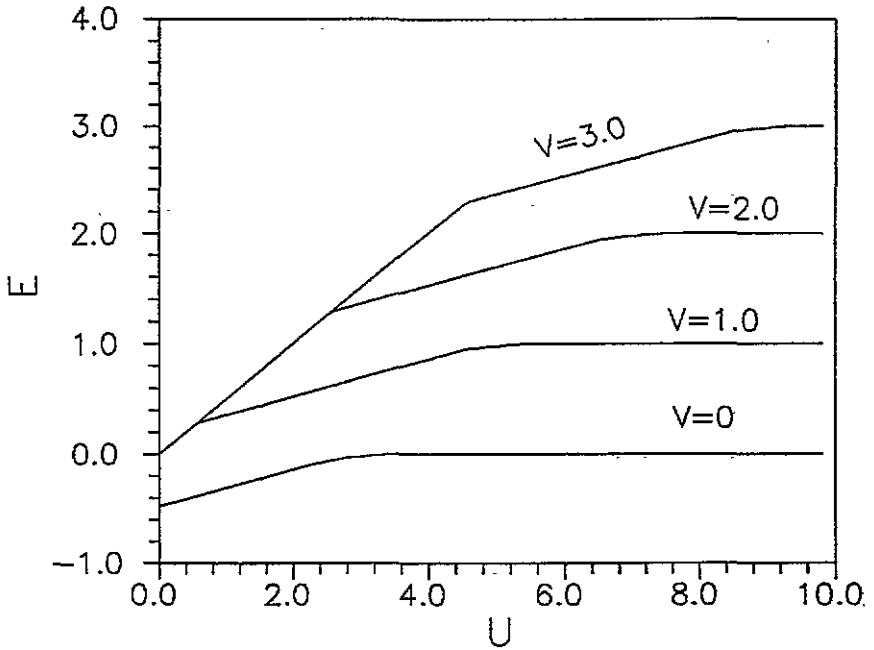
Figure 3. Plot of the ground state energy/site E against U for different V for the bond–charge interaction $X = t$ ($t = 1.0$).

The ground state energy per site E is plotted against U for different V in figure 3. The local moments also plotted against U and parametrized by V are shown in figure 4. It appears that the energy curve consists of two linear regions, one for $U \leqslant U_{c_1}$ where $E = U/2$ and the other for $U \geqslant U_{c_2}$ where $E = V$. Correspondingly in figure 2 we see that $L_0 = 0$ for $U \leqslant U_{c_1}$ while $L_0 = 0.75$ for $U \leqslant U_{c_2}$. Now, for each V, $U_{c_1} > 2V - 8t$ and $U_{c_2} < 2V + 8t$. Thus for the regions where exact results are available, the RG method reproduces the exact values of energy and local moment. We also conclude that the 2^L-fold paramagnetic region with $E = V$ extends up to $U \sim U_{c_2}$, well below the lower bound [13] $U = 2V + 8t$ and that the CDW state with $E = U/2$ extends up to $U \sim U_{c_1}$, well above the upper bound $U = 2V - 8t$. It is notable that U_{c_1} and U_{c_2} gradually increase with the increase of V which is also expected naively.

The most striking result is that in between U_{c_1} and U_{c_2} there appears a wide plateau-like structure with $L_0 = 0.375$ in the plot of the local moment. Now for the case when $P_\uparrow = P_\downarrow = P_0 = P_{\uparrow\downarrow} = \frac{1}{4}$ we obtain $L_0 = \frac{3}{8} = 0.375$. Usually this happens for the free-fermion metallic case. But it may appear that this kind of a model cannot have a metallic ground state in 1D for the following reason. Let us recall the fact that the special kind of restriction on single-particle hopping considered here has the property of conserving the number of double occupancies. Consequently, whenever a double occupancy and an empty site come side by side single-particle hopping gets quenched. Again, if two electrons of opposite spins come at adjacent sites further hopping stops (the term $(1 - n_{i-\sigma} - n_{j-\sigma})$ of (12) is zero in both cases). Therefore, in such a half-filled case, no long-range hopping seems possible in a truly infinite chain because at some place or other this kind of situation occurs. From RG point of view the lattice must contain (renormalized) single particles side by side or an adjacent empty site and doubly occupied site at some renormalized length scale—resulting in the blockade of long-range hopping. Moreover in this region
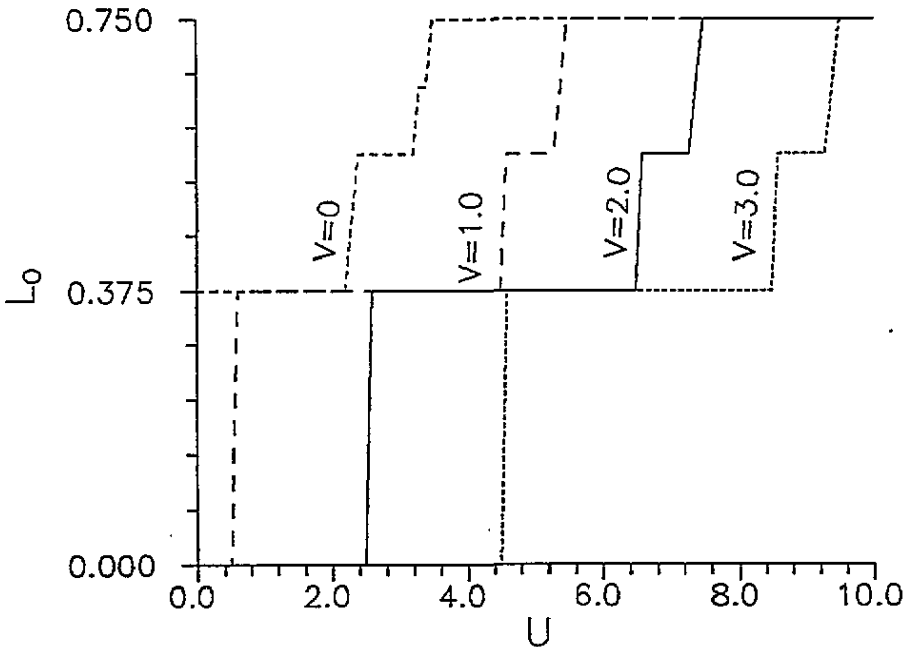
Figure 4. Plot of the local moment L_0 against U for different V for the bond–charge interaction $X = t$ ($t = 1.0$).

($L_0 = 0.375$) if one starts from a non-zero value of U/t, however small, the RG iterations of U/t flow to ∞; this also gives an indication that this phase is not metallic. But equal probabilities of all the four configurations (as suggested by $L_0 = 0.375$) indicate that the electrons are freely mobile over a finite length scale. Therefore, from the present RG point of view, this is a non-metallic phase with a free-fermionic local moment, although a recent work [15] identifies this phase as a metallic one for the $V = 0$ case.

In figure 5 we have plotted the density–density autocorrelation function $N(q)$ defined in (17) for $q = \pi$. We see that for $U \leqslant U_{c_1}$, where $L_0 = 0$, this quantity sharply diverges pointing out a CDW state. Other q branches do not show a sizeable value. This indicates that the CDW is chess-board type. This is also in perfect agreement with the available exact result [13].

7. Conclusion

In conclusion, we have investigated the problems with an existing real space RG scheme for the extended Hubbard model and tried to find a reasonable solution for it. Then we apply this modified RG method to study the extended Hubbard model with and without the bond–charge interaction (for a special value of the interaction) for the 1D half-filled case.

For the case without the bond–charge interaction we obtain a CDW/SDW phase boundary which agrees excellently with the available Monte Carlo results. In the case of the bond–charge interaction we have reproduced some exact results in one region of the parameter space (only where the exact solution [13] is known). We find that the two limiting phases, namely the single-occupancy paramagnetic phase and the CDW one, extend well inside the parameter space where exact results are not available. Moreover we find an intersecting non-metallic phase (for small and intermediate values of V) with metallic
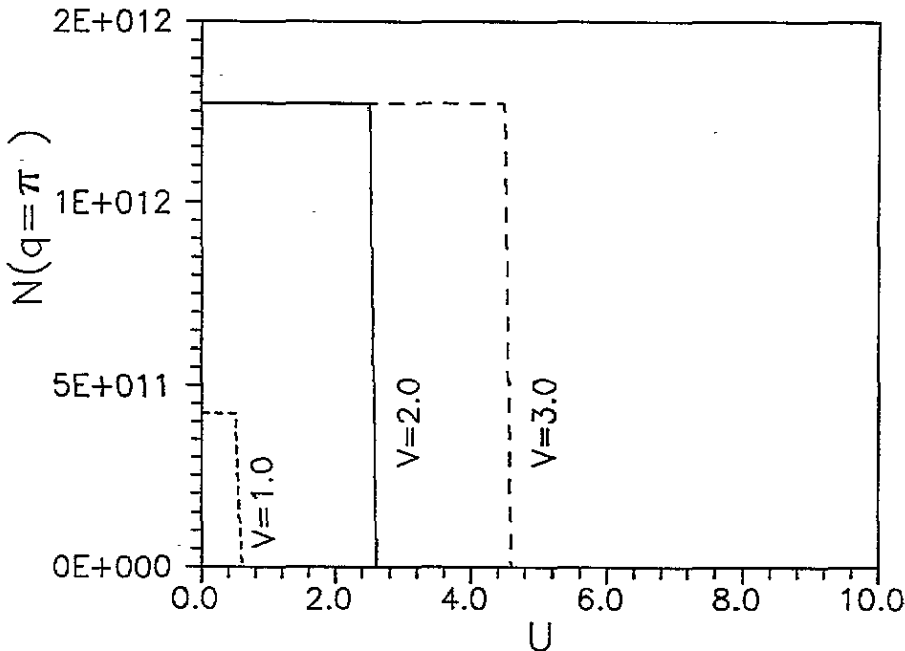
Figure 5. Plot of the density–density autocorrelation functions $N(q)$ against U (for different V) for $q = \pi$ for the bond–charge interaction $X = t$ ($t = 1.0$).

(free-fermionic) local moment.

It is worthwhile to study this model with larger cell size to achieve numerical reliability in the intermediate region (since there is no exact result) and observe the fate of the small structures in the local moment plot (with L_0 other than 0, 0.375 and 0.75) as well as the precise positions of U_{c_1} and U_{c_2}. The interesting phase of the $L_0 = 0.375$ plateau requires some attention and a proper order parameter, if any, could be identified for the same. It would be interesting to study the cases where $X \neq t$. This, of course, will change the physics e.g. the 2^L-fold-degenerate paramagnetic phase will then be pushed towards antiferromagnetic ordering. This and the non-half-filled case may have an effect especially on the $L_0 = 0.375$ phase. A problem with using such a method directly in these cases is the lack of p–h symmetry which may be bypassed by using a suitable approximate scheme [16]. The present RG scheme is often found to bring out the essential physical features correctly; however, it is well known that this scheme cannot claim a very high degree of accuracy in the numerical results. The reason behind this drawback has recently been addressed by White [17] and an alternative approach to the RG scheme has been developed. This apparently promising method, known as density matrix RG [17], can as well be an alternative tool for these investigations; however, this requires heavy computation. Finally, it may be fruitful to study this model in higher dimensions for its obvious utilization [10].

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