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Spinless fermion chains with weak interchain hopping

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Abstract

The linear renormalization-group transformation is used to study the thermodynamics of weakly coupled spinless fermion chains at half-filling. The model consists of a competing nearest-neighbour Coulomb repulsion and kinetic energy terms. The specific heat and the nearest-neighbour correlation function are studied as functions of temperature by varying the ratio of Coulomb repulsion to kinetic energy. The role of an interchain hopping is studied and the metal–insulator phase transition temperature as a function of hopping parameters is discussed.

1. Introduction

Studies of highly correlated electron systems are certainly one of the most important areas of condensed matter physics. A tremendous number of papers have been concerned with the investigation of heavy-fermion behaviour, magnetism of highly correlated systems, high-temperature superconductivity, or metal–insulator transitions and charge-ordering phenomena. In this paper, we investigate the effect of competing nearest-neighbour Coulomb repulsion and kinetic energy for a one-dimensional and for a two-dimensional spinless fermion model at half-filling and finite temperature. Generalizations of the model were used in the past for the description of the Verwey metal–insulator transitions and charge-ordering phenomena in Fe_3O_4, Ti_4O_7, LiV_2O_4 and other d-metal compounds [1–4]. For half-filling and zero temperature it is expected that a growth of the Coulomb interaction leads to a transition from a metallic to an insulating charge-ordered state. The evaluation of physical quantities at finite temperature poses serious difficulties even for one-dimensional integrable models since the whole eigenspectrum of the many-particle system has to be solved. Thermodynamics of quantum integrable systems have been discussed by the thermodynamic Bethe ansatz method [5]. The quantum transfer matrix approach was used to investigate the correlation length of the spinless fermion model [6, 7] at finite temperature. As an alternative approach, we apply in this paper the linear renormalization-group transformation (LRG) in order to study the temperature dependence of the specific heat of the spinless fermion model. Up to now, this approach was primarily applied to low-dimensional quantum spin systems.

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The paper is organized as follows. In the next section, we present the model in one dimension and discuss some basic properties which follow from particle–hole symmetry. In section 3, a brief review of the LRG transformation is presented and its region of validity is discussed. In section 4, the results for the one-dimensional model are presented. In section 5 the role of an additional interchain hopping is analysed.

2. The model

We start from the following one-dimensional spinless fermion model:

$$H = t\sum_{\langle ij\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - \mu\sum_i c_i^\dagger c_i. \tag{1}$$

Here $\hat{n}_i = c_i^\dagger c_i$ is the local occupation number operator and μ is the chemical potential. The first term describes the hopping between nearest neighbours and V is the Coulomb repulsion between fermions on neighbouring sites. In the sum $\langle ij\rangle$ over neighbouring sites each pair is to be counted only once.

By use of the Wigner–Jordan transformation it can be shown that the spinless fermion model (1) can exactly be transformed to the XXZ-spin chain in a magnetic field parallel to the anisotropy

$$H = \sum_{J=1}^{N}\{J_x(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + J_z S_j^z S_{j+1}^z - BS_j^z\} \tag{2}$$

where $\mathbf{S_j}$ are Pauli spin operators $S^z = \pm 1$, and $J_x = t/2$, $J_z = V/4$, and $B = (1/2)(\mu - V)$. It is well known that the XXZ chain (2) is a gapless system with no long-range order and an unbroken $U(1)$ symmetry as long as $-1 < J_z/J_x \leqslant 1$. Therefore, the system (1) has no gap as long as the ratio $t/(V/4)$ is larger than or equal to 2 and has a gap for $t/(V/4) < 2$. Note that in the following we are only interested in the case $V > 0$, that is in the electronic system (1) with repulsive Coulomb interaction between the electrons.

The spinless fermion model possesses an important particle–hole symmetry. For the purpose of this discussion we consider the following canonical transformation $c_i^\dagger \to c_i$ and $c_i \to c_i^\dagger$. For the occupation number operator the transformation reads $\hat{n}_i \to c_i c_i^\dagger = 1 - \hat{n}_i$ and for the Hamiltonian

$$H \to -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - (2V - \mu)\sum_i \hat{n}_i - (\mu - V)N. \tag{3}$$

The different signs of the hopping terms in (1) and (2) can be compensated by a further canonical transformation as follows. We divide the (one-dimensional) lattice into two sublattices A and B of even and odd sites in such a way that the hopping connects an A-site only to a B-site and vice versa. By formally replacing $c_i^\dagger \to -c_i^\dagger$ for $i \in A$ but not changing the operators $(c_i^\dagger \to c_i^\dagger)$ on sites B we obtain

$$H \to t\sum_{\langle ij\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - (2V - \mu)\sum_i \hat{n}_i - (\mu - V)N. \tag{4}$$

Thus the following symmetry relation for the free energy is found:

$$F(t, V, \mu) = F(t, V, -\mu + 2V) - (\mu - V)N. \tag{5}$$

The last term on the right-hand side is an additive constant. Thus, the temperature dependence of the free energy is the same when we replace the chemical potential μ by $-\mu + 2V$. By measuring the chemical potential relative to V, i.e., by introducing $x = \mu - V$, the relation

$$F(t, V, V + x) = F(t, V, V - x) - xN \tag{6}$$

shows that the free energy is symmetric around $\mu = V$ (except for the additive constant $-xN$).

For the average occupation number $n = \langle \hat{n}_i \rangle$ the particle–hole symmetry reads $n(t, V, \mu) = 1 - n(t, V, -\mu + 2V)$ or $n(t, V, V + x) = 1 - n(t, V, V - x)$. Thus, for the symmetric point $\mu = V$ one finds $n(t, V, \mu = V) = 1 - n(t, V, \mu = V)$ or $n(t, V, \mu = V) = 1/2$. The system is at half-filling if the chemical potential is equal to V.

3. Linear renormalization group transformation (LRG)

In order to formulate a renormalization transformation for the free energy it is helpful to absorb a factor $-\beta = -1/k_B T$ in the Hamiltonian (1). We define

$$\mathcal{H} = -\beta H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) - V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j + \mu \sum_i c_i^\dagger c_i. \tag{7}$$

Hereafter t, V, and μ denote βt, βV, and $\beta \mu$, respectively. The renormalization group transformation for the Hamiltonian $\mathcal{H}$ of the spinless fermion chain is defined by

$$\exp[\mathcal{H}'(\alpha)] = \mathrm{Tr}_c \, P(\alpha, c) \exp[\mathcal{H}(c)], \tag{8}$$

where the transformed Hamiltonian $\mathcal{H}'$ is a function of new fermion operators $\alpha^\dagger, \alpha$. The trace runs over the unitary space of the original fermions $c_i^\dagger, c_i$. The weight operator $P(\alpha, c)$ which couples the original to the new fermions is chosen in a linear form as follows:

$$P(\alpha, c) = \prod_{i=0} (1 + c_{mi+1}^\dagger \alpha_{i+1} + \alpha_{i+1}^\dagger c_{mi+1} + 2\hat{n}_{mi+1} \hat{\eta}_{i+1} - \hat{n}_{mi+1} - \hat{\eta}_{i+1}), \tag{9}$$

where $\hat{\eta}_i = \alpha_i^\dagger \alpha_i$ is the occupation number operator of the new fermions. Note that $P(\alpha, c)$ and thus the transformation depends on a chosen fixed integer m larger than 1, i.e., $m = 2, 3, \ldots$. The weight operator (8) is a product of local weights, $P(\alpha, c) = \prod_i p_i$. By performing the trace of p_i with local operators at site $mi + 1$ we find the following relations:

$$\begin{aligned} &\mathrm{Tr}_c \, p_i = 1 \\ &\mathrm{Tr}_c \, c_{mi+1}^\dagger p_i = \mathrm{Tr}_c \, p_i c_{mi+1}^\dagger = \alpha_{i+1}^\dagger \qquad \mathrm{Tr}_c \, c_{mi+1} p_i = \mathrm{Tr}_c \, p_i c_{mi+1} = \alpha_{i+1} \\ &\mathrm{Tr}_c \, \hat{n}_{mi+1} p_i = \mathrm{Tr}_c \, p_i \hat{n}_{mi+1} = \hat{\eta}_{i+1} \end{aligned} \tag{10}$$

($i = 0, 1, 2, \ldots$). In contrast, all traces formed with operators $c_j^\dagger$, c_j, or $\hat{n}_j$ at different sites $j \neq mi + 1$ vanish. Thus, the transformation (8) is a Suzuki–Takano [8, 9] decimation transformation. For instance, for $m = 2$ in the renormalization step only every other site survives, whereas for $m = 3$ every third site survives, and so on. In order to obtain effective interactions between the operators on surviving sites, for $m = 2$ at least a 3-site cluster has to be considered, and a 4-site cluster for $m = 3$. The relations (10) ensure that the partition function of the original Hamiltonian $\mathcal{H}(c)$ and the new Hamiltonian $\mathcal{H}'(\alpha)$ are the same, where in the latter case the trace has to be taken over the unitary space of the new fermions $\alpha^\dagger, \alpha$.

For the fully localized case, i.e., $t = 0$, the model (1) is equivalent to the Ising model with exchange interaction $J = V/4$ according to the equations (1) and (2). Therefore, in the case $t = 0$ the decimation transformation (8) can be carried out exactly. For a finite t, it is of course impossible to carry out the trace (8) exactly due to the non-commutativity of several terms of the Hamiltonian. Thus one has to make some approximation to obtain the explicit form of the LRG transformation. The simplest approximation is based on the Suzuki–Takano idea [8] to evaluate LRG transformation considering only a finite cluster and neglecting the effects of non-commutativity of several clusters. Finally, it should be emphasized that the procedure in which we confine ourselves to finite clusters is not very suitable for an itinerant fermion model. However, we expect that for $t < V$ and high temperatures it can be a reasonable approximation.

4. One-dimensional fermion system

In this section we discuss results for several thermodynamic quantities which were obtained within the LRG approach of section 3 for a single chain. Applying the transformation (8) for any m to the Hamiltonian (7) one obtains the transformed Hamiltonian $\mathcal{H}'(\alpha)$ in the same form as the original one for new fermion operators $\alpha^{\dagger}$, α and new parameters t', V' and μ',

$$\begin{aligned} t' &= \frac{1}{2}\ln\frac{f_0+f_\mu+f_t}{f_0+f_\mu-f_t}, \\ \mu' &= \ln\frac{(f_0+f_\mu)^2-f_t^2}{f_0^2}, \\ V' &= \ln\frac{f_0(f_0+2f_\mu+f_V)}{(f_0+f_\mu)^2-f_t^2}, \end{aligned} \tag{11}$$

with

$$\begin{aligned} f_0 &= \mathrm{Tr}_c(1-\hat{n}_1-\hat{n}_{m+1}+\hat{n}_1\hat{n}_{m+1})\exp[\mathcal{H}(c)], \\ f_t &= \mathrm{Tr}_c\, c_1^{\dagger}c_{m+1}\exp[\mathcal{H}(c)], \\ f_\mu &= \mathrm{Tr}_c(2\hat{n}_1+\hat{n}_{m+1}-2\hat{n}_1\hat{n}_{m+1}-1)\exp[\mathcal{H}(c)], \\ f_V &= \mathrm{Tr}_c(4\hat{n}_1\hat{n}_{m+1}-2\hat{n}_1-2\hat{n}_{m+1}+1)\exp[\mathcal{H}(c)]. \end{aligned} \tag{12}$$

We have evaluated numerically the renormalization transformation from the original set of coupling parameters (t, μ, V) to the set of renormalized parameters (t', μ', V') (8) where only one high-temperature fixed point ($t* = 0$, $V* = 0$) was found. Therefore, as expected, the system does not exhibit any finite-temperature phase transition. The free energy per site has been calculated by using the following formula:

$$f = \sum_{n=1}^{\infty}\frac{\ln f_0(t^{(n)}, \mu^{(n)}, V^{(n)})}{3^n}. \tag{13}$$

Figure 1 shows the specific heat c for the non-interacting fermion chain ($V = 0$) as function of temperature, as obtained from equation (13) for $m = 3, 5$, and 7. Of course, for $V = 0$ the Hamiltonian can be solved exactly (bottom line in figure 1). The different curves for several values of cluster sizes (4, 6, and 8) are due to the fact that the quantum effects are taken into account exactly only inside the cluster. As was already mentioned, the local LRG transformation (9) is not a suitable method for analysing the case $V = 0$. Nevertheless, the LRG procedure reproduces the exact result reasonably well, especially for higher temperatures. For this reason in figure 1 the low-temperature parts of the curves were excluded.

In figure 2 the specific heat for the interacting spinless fermion chain with the hopping parameter $t/(V/4) = 0.4$ (gapped system) as a function of temperature is presented for several values of the cluster size which are used in the LRG method. As is seen from the figure the results are very close to each other except for very low temperatures. For the smaller clusters a low-temperature maximum appears which is an artefact of neglecting quantum effects between adjacent clusters. For the 8-site cluster the temperature behaviour of the specific heat is found to be exponential-like down to a temperature of approximately $0.1V/4$, as expected for a gapped system. For comparison, in figure 3 the specific heat is shown for a simple two-site system at half-filling for different values of the hopping parameter t. As in the case of the 4- and 6-site clusters (compare figure 2), an additional peak is observed at low temperatures. The analytical expression for c is found from twice differentiating the free energy

$$F = -k_{\mathrm{B}}T\ln(2+\mathrm{e}^{-\frac{(V-2t)}{2k_{\mathrm{B}}T}}+\mathrm{e}^{-\frac{(V+2t)}{2k_{\mathrm{B}}T}}). \tag{14}$$

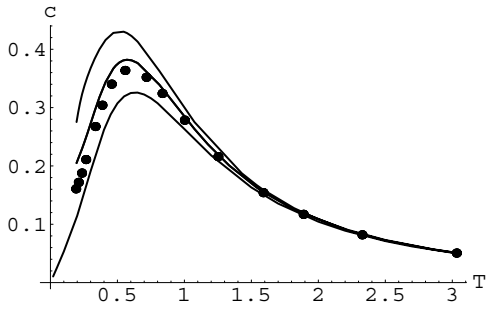

Figure 1. Temperature dependence of the specific heat for a non-interacting ($V = \mu = 0$) spinless fermion chain found from 4-site, 6-site, 8-site (points) clusters, and the exact result (from top to bottom). The temperature T is given in units of t.

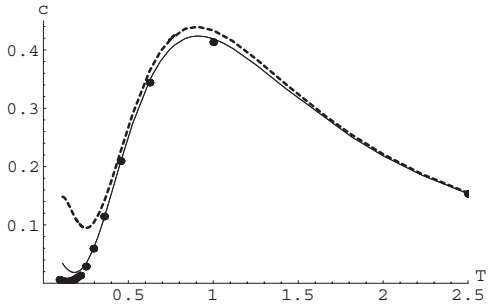

Figure 2. Temperature dependence of the specific heat for $t = 0.4$ at half-filling found from 8-site (points), 6-site (thin line), and 4-site (dashed) clusters (from bottom to top), where t and T are given in units of $V/4$.

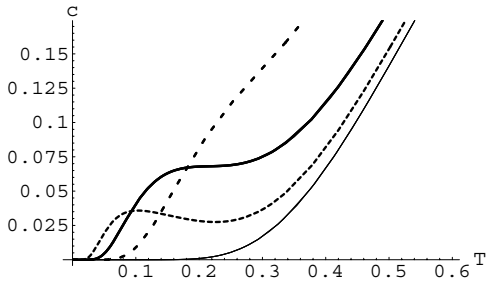

Figure 3. Specific heat as function of T for a two-site problem at half-filling for different values of t: $t = 0$ (thin line), $t = 0.08$ (dotted line), 0.15 (full line), $t = 0.3$ (dashed line) in units of $V/4$. The low-temperature peak is due to the hopping between the two possible singly occupied states.

One easily verifies that the low-energy peak scales with t^2 and originates from the coupling between the two possible singly occupied states in the two-site problem.

In figure 4 the temperature dependence of the specific heat of the chain system is presented for several values of the hopping parameter t in units of $V/4$, found from the 6-site cluster. Due to the restricted validity of our procedure at low temperatures the curves are only shown for temperatures $T > 0.2$. The characteristic temperature of the specific heat maximum T_{cmax} is shifted to higher values with increasing hopping and scales according to $T_{\mathrm{cmax}} \sim t^{1.67}$ for

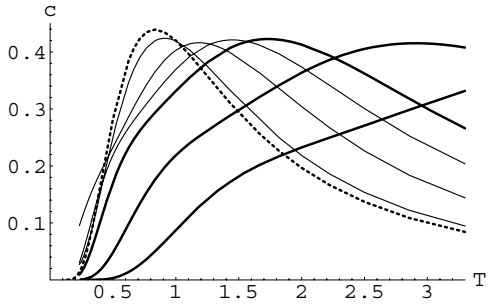

Figure 4. Temperature dependence of the specific heat for several values of the hopping parameter: $t = 0$ (dashed line), 0.4, 1, 1.5 (thin lines), and 2, 4, 8 (solid lines) from left to the right.

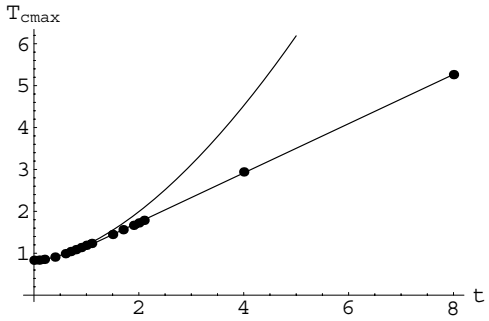

Figure 5. The characteristic temperature of the specific heat maximum as a function of the hopping parameter t in units of $V/4$. The upper curve indicates the power-law behaviour for small t.

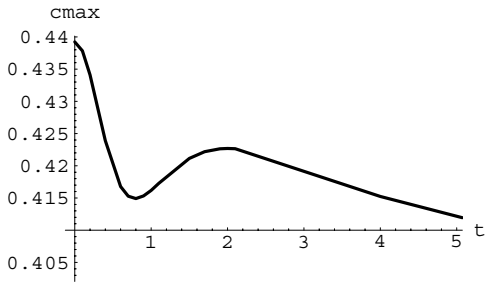

Figure 6. The height of the specific heat maximum as function of t.

small t and linearly for large t (figure 5). The height of the specific heat maximum, denoted by cmax, first decreases with increasing hopping and then increases again, thereby reaching a maximum for $t = 2$ at which the gap closes. For higher t, cmax decreases again, as shown in figure 6.

In figure 7 the average occupation number $n = \langle \hat{n}_i \rangle$ is shown as function of the chemical potential μ from the 4-site cluster LRG procedure for three different values of the hopping parameter t ($t = 0, 2$ and 3), and relatively low temperature $T = 0.2$. For all three cases $n = 1/2$ at $V = \mu$ (half-filling) is fulfilled, as is expected from section 1. Again, for $t = 0$ the procedure is exact. For $t > 0$ additional plateaus appear around $n = 1/4$ and $3/4$. This is of course a reflection of the trivial fact that in a 4-site cell all sites can be empty ($n = 0$)

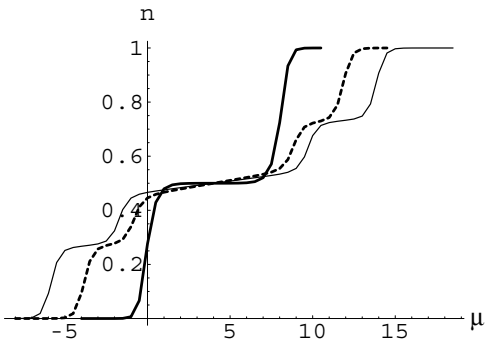

Figure 7. Average occupation number as a function of the chemical potential μ at fixed temperature $T = 0.2$ for $t = 0$ (solid curve), $t = 2$ (dashed), and $t = 3$ (thin), found from a 4-site cell. All energies are again given in units of $V/4$.

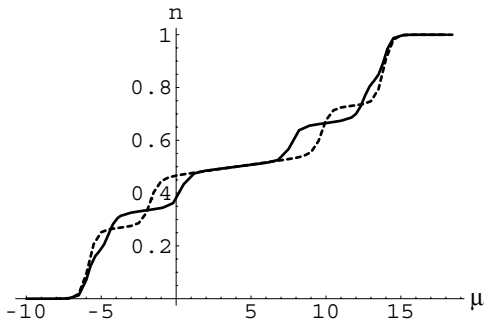

Figure 8. Average occupation number as function of the chemical potential μ at fixed temperature $T = 0.2$ and $t = 3$, found from a 6-site cell (solid curve) and 4-site cell (dashed).

or 1, 2, 3, or 4 sites can be occupied, which means $n = 1/4$, $1/2$, $3/4$, and 1, respectively. For a 6-site cell ($m = 5$) which admits periodicity 2, 3 or 6, the plateaus are visible around $n = 1/6$, $1/3$, $1/2$, $2/3$, and $5/6$ as expected (figure 8). It is obvious that a dependence of the average occupation number on the choice of the cell is a spurious effect of the cell method. In other words, the method can be applied only to the systems for which the occupation number is independent of the cell size. It is easy to see from figure 8 that such a condition is fulfilled for the systems around half-filling $\mu = 4$ ($\mu = V$) and of course for both trivial cases with all sites occupied or all sites empty.

Next, we use the LRG for a 6-site cluster to find the nearest-neighbour (NN) correlation function

$$G(i, i+1) = \langle \hat{n}_i \hat{n}_{i+1} \rangle. \tag{15}$$

In figure 9 its temperature dependence is shown for different values of the hopping t (in units of $V/4$). At high temperatures, $G(i, i+1)$ tends to $1/4$ for arbitrary values of t, which means $1/2$ particles per site, as expected. At low temperatures $G(i, i+1)$ goes to zero for $t = 0$ which means the fully ordered ground state with one particle at every other site. For increasing hopping the NN correlation function also increases since the neighbouring sites now become partially occupied. In contrast, for large temperatures the NN correlation function decreases with increasing hopping, which is also seen from figure 10. There, $G(i, i+1)$ is presented as a function of t for various values of the temperature. Note that all correlation functions

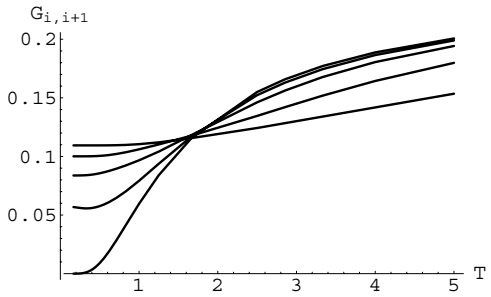

Figure 9. Temperature dependence of the NN correlation function for $t = 0, 1, 2, 4, 8$ (from top to bottom).

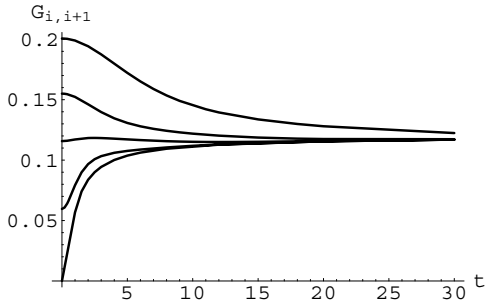

Figure 10. The NN correlation as a function of the hopping parameter t at $T = 0.167$, 1, 1.67, 2.5, and 5 (from bottom to top).

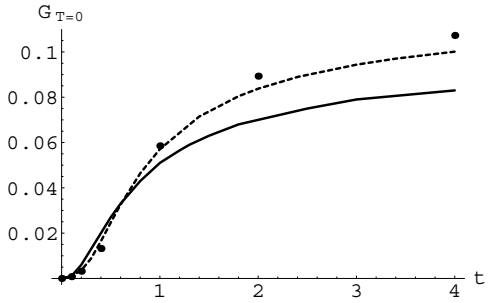

Figure 11. The NN correlation functions as function of t at half-filling in the limit $T \to 0$, as found from 4-site (solid line), 6-site (dashed line) and 8-site (points) clusters.

in figure 10 approach, for large t, the same value of approximately 0.13, where $t \gg T$ is always fulfilled. The value 0.13 should be compared with the exact value for $G(i, i+1)$ of $1/4 - 1/\pi^2 \approx 0.15$ for $T = 0$ and $t/V \to \infty$.

Though the LRG is not completely reliable for large hopping t and small temperature T it should make sense to extrapolate the NN correlation function values also to zero temperature, as can be seen from figure 9. The results from this extrapolation are shown in figure 11 for 4-, 6-, and 8-site clusters, plotted as function of hopping. Note that the curve for the 8-site cluster comes closer to the expected value of ≈ 0.15 for larger t than the smaller cluster curves.

5. Weakly coupled chains

As an attempt towards understanding the crossover from one to two dimensions, much attention has been focused on the problem of two chains coupled by a transverse hopping [10]. Of course, such a simplified model cannot be used to describe a phase-transition behaviour at finite temperatures which is expected for a system with an infinite number of chains. Below in this section, we shall use the LPRG (linear perturbation RG) [11] to study a system with an infinite number of spinless fermion chains at finite temperature, where the chains are coupled by a weak interchain single-particle hopping t_I.

The Hamiltonian of the spinless fermion model with nearest-neighbour intra-chain Coulomb repulsion V and hopping along (t) and between (t_I) the chains reads

$$\begin{aligned} H &= t\sum_{\langle ij\rangle}(c^\dagger_{i,j}c_{i+1,j}+c^\dagger_{i+1,j}c_{i,j}) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - \mu\sum_i c^\dagger_i c_i + t_\mathrm{I}\sum_{\langle ij\rangle}(c^\dagger_{i,j}c_{i,j+1}+c^\dagger_{i,j+1}c_{i,j}) \\ &= \mathcal{H}_0(c)+\mathcal{H}_\mathrm{I}(c) \end{aligned} \tag{16}$$

where the label i in the first and fourth term on the rhs refers to columns and j to rows. Let us separate the Hamiltonian (16) into a part $\mathcal{H}_0(c)$ containing the intra-chain interactions (t and V) and a remainder $\mathcal{H}_\mathrm{I}(c)$ containing the interchain hopping t_I. With the notation

$$\begin{aligned} \mathcal{Z}'_0(\alpha) &= \mathrm{Tr}_c\, P(\alpha,c)\exp\left[\mathcal{H}_0(c)\right] \\ &= j_0 + j_t(\alpha^\dagger_1\alpha_2+\alpha^\dagger_2\alpha_1) + j_\mu(\alpha^\dagger_1\alpha_1+\alpha^\dagger_2\alpha_2) + j_V\alpha^\dagger_1\alpha_1\alpha^\dagger_2\alpha_2, \end{aligned} \tag{17}$$

$$\begin{aligned} j_0 &= \frac{1}{f_0}, \qquad j_t = -\frac{f_t}{\Delta}, \qquad j_\mu = \frac{f_0+f_\mu}{\delta} - \frac{1}{f_0}, \\ j_V &= \frac{1}{f_0} - 2\frac{f_0+f_\mu}{\Delta} + \frac{1}{f_0+2f_\mu+f_V}, \\ \Delta &= f_0^2 - f_t^2 + 2f_0f_\mu + f_\mu^2, \end{aligned} \tag{18}$$

and

$$\langle A\rangle_0(\alpha) = \tfrac{1}{2}(\mathcal{Z}_0^{-1}\,\mathrm{Tr}_c\, AP(\alpha,c)\exp[\mathcal{H}_0(c)] + \mathrm{Tr}_c\, AP(\alpha,c)\exp[\mathcal{H}_0(c)]\mathcal{Z}_0^{-1}), \tag{19}$$

the transformation (8) for the Hamiltonian (16) can be written as

$$\mathcal{H}'(\alpha) = \mathcal{H}'_0(\alpha) + \ln\langle\exp[\mathcal{H}_\mathrm{I}(c)]\rangle_0 \tag{20}$$

with the standard cumulant expansion [12] for $\langle\exp[\mathcal{H}_\mathrm{I}(c)]\rangle_0$ and $\mathcal{H}'_0(\alpha) = \ln\mathcal{Z}'_0(\alpha)$.

To evaluate the transformation (20) one has to know the averages $\langle c^\dagger_i\rangle_0$, $\langle c_i\rangle_0$, and $\langle c^\dagger_i c_j\rangle_0$ which have closed but rather complicated expressions, for example:

$$\langle c^\dagger_1\rangle_0 = A_1\alpha^\dagger_1 + A_2\alpha^\dagger_2 + A_3\alpha^\dagger_2\alpha_2\alpha^\dagger_1 + A_4\alpha^\dagger_1\alpha_1\alpha^\dagger_2. \tag{21}$$

The coefficients A_i are given in the appendix.

As was explained in previous papers [11, 13], the LPRG transformation when applied on an infinite system generates an infinite number of new interactions. This is already the case in the second-order cumulant expansion which is the lowest non-trivial case for the present system. Thus in order to find the LPRG recursion relations we have to confine ourselves to a finite cluster. In a second-order calculation one has to consider three rows. We use a (4–6–4)-cluster with four, six, and again four sites for the first, second, and third row, respectively. In addition, for simplification we confine ourselves to only two-site interactions thereby neglecting 3- and 4-site interactions which appear for the (4–6–4)-cluster. Under these assumptions the LPRG transformation generates only one new interaction—an interchain diagonal hopping

$$t_\mathrm{D}\sum_{\langle ij\rangle} c^\dagger_{i,j}c_{i+1,j+1}.$$

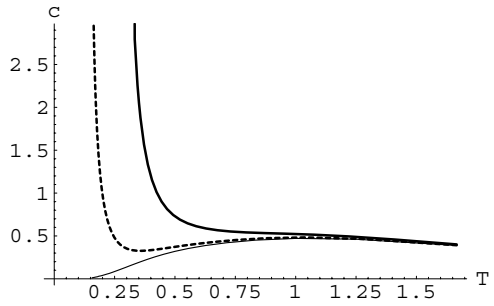

Figure 12. Temperature dependence of the specific heat for $t = 1$ and interchain hopping $t_\mathrm{I} = 0$ (thin line), 0.15 (dashed line), and 0.3 (solid line). All energies are given in units $V/4$.

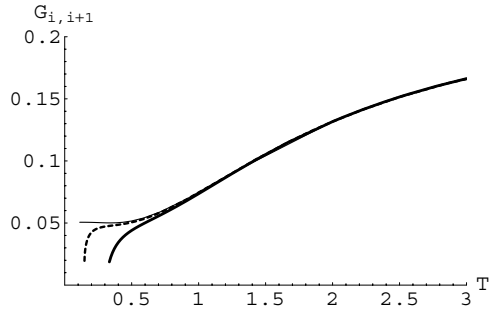

Figure 13. Temperature dependence of the NN correlation function for $t = 1$ and interchain hopping $t_\mathrm{I} = 0$ (thin line), 0.15 (dashed line), and 0.3 (solid line). All energies are given in units $V/4$.

We have evaluated numerically the renormalization transformation from the original set of five parameters (t, t_I, t_D, V, and μ) to the set of the renormalized parameters (t', t'_I, t'_D, V', and μ'). We have found two fixed points, which describe the behaviour of the system at $T = 0$ and ∞, and also the critical surface in a four-dimensional parameter space.

In figure 12 the specific heat for a system of spinless fermion chains is shown at half-filling for $t = 1$ with an additional weak interchain hopping $t_\mathrm{I} = 0.15$ and 0.3. For comparison, the curve for $t_\mathrm{I} = 0$ is also shown. Note that for finite t_I the specific heat diverges at a critical temperature T_c. The model characterized by the Hamiltonian (16) can exhibit only a charge ordering so the temperature T_c can be interpreted as a critical temperature between a charge-ordered and a metallic phase. This conjecture is supported by the temperature dependence of the NN correlation function $G(i, i+1)$, shown in figure 13. Similarly, as for a one-dimensional system, at high temperature $G(i, i+1)$ tends to $1/4$ for arbitrary values of t ($1/2$ particles per site); however, in the weakly coupled chains system, $G(i, i+1)$ clearly falls as T_c is approached.

In figure 14 the critical temperature T_c is shown as function of the interchain hopping t_I for the two cases $t = 1$ and 0.4 (at half-filling $V = \mu$). As is shown, the critical temperature increases with increasing t_I. At first sight an interchain hopping should destroy the charge order; however, in our model hopping is the only interaction which couples the chains. This is of course necessary to find long-range order at finite temperatures. In figure 15 the critical temperature is shown as function of the intra-chain hopping t for three values: $t_\mathrm{I} = 0.15$, 0.3, and 0.5. Because there is no interchain Coulomb repulsion, charge ordering at finite temperatures is only possible for finite values of t. For $t = 0$ the chains are

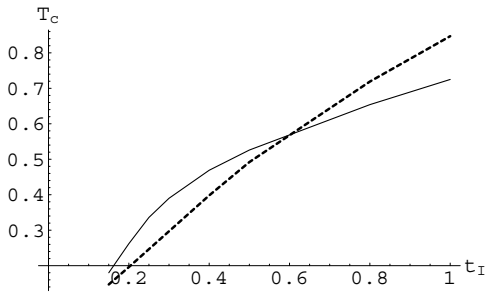

Figure 14. Critical temperature T_c as function of the interchain hopping t_I for intra-chain hopping $t = 0.4$ (thin line) and $t = 1$ (dashed line).

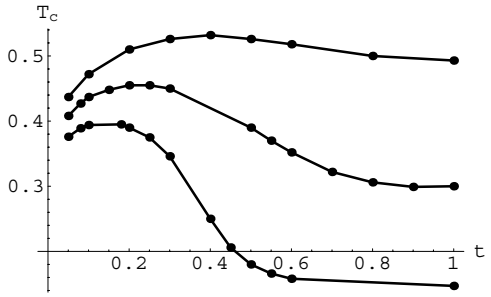

Figure 15. Critical temperature as function of the intra-chain hopping t for interchain hopping $t_I = 0.15$, 0.3, and 0.5, from bottom to top.

effectively decoupled. Note that for large enough t the critical temperature decreases again with increasing t.

6. Summary

First, the one-dimensional spinless fermion model with hopping term and intersite Coulomb repulsion at half-filling has been studied by means of the LRG transformation. We have applied the LRG method based on a 4-, 6-, and 8-site cluster calculation. Only for $t = 0$ the transformation can be carried out exactly. For t not too large we believe that the method should lead to reasonable results, especially at high temperatures. The temperature dependence of the specific heat and the nearest-neighbour correlation function has been discussed. In the limit $T = 0$ the increase of the correlation function with t shows that the hopping term tends to destroy long-range order.

The role of a small interchain hopping for systems with an infinite number of the spinless fermion chains has also been investigated. We have employed the LPRG method on a (4–6–4)-cluster by confining ourselves to two-site interactions only. We have assumed in our model that the chains are coupled by a single-particle hopping. A possible Coulomb repulsion between neighbouring chains was neglected. As one would expect, such hopping can lead to a phase transition from a metallic to a charge ordered phase. The transition temperature increases with increasing interchain hopping t_I. For a fixed value of t_I the system undergoes the phase transition only if the intra-chain hopping t is finite. For $t = 0$ the chains are effectively decoupled in our approximation. As expected, for a sufficiently strong intra-chain hopping

t the critical temperature decreases with increasing t. We also have found the temperature dependence of the specific heat. The specific heat curves exhibit anomalies associated with the charge ordering transition for all values of the interchain hopping. Finally, it should be emphasized once more that the present approach is valid only for not too small temperatures. For very small interchain parameter t_I the description of the phase transition leads to very low transition temperatures and is thus less reliable. Note (figure 12) that for $t_\mathrm{I} = 0.3$ the transition takes place at a temperature for which our method should be applicable.

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Appendix. Evaluation of expectation values

In this appendix we present as an example one of the averages necessary to evaluate the transformation (19).

$$\langle c_1^\dagger \rangle_0(\alpha) = A_1\alpha_1^\dagger + A_2\alpha_2^\dagger + A_3\alpha_2^\dagger\alpha_2\alpha_1^\dagger + A_4\alpha_1^\dagger\alpha_1\alpha_2^\dagger, \tag{A.1}$$

where

$$\begin{aligned} A_1 &= j_0 o_1 + \tfrac{1}{2} j_t o_2 + + \tfrac{1}{2} j_\mu o_1, \\ A_2 &= j_0 o_2 + \tfrac{1}{2} j_t o_1 + \tfrac{1}{2} j_\mu o_2, \\ A_3 &= j_0 o_3 - j_t(o_2 + \tfrac{1}{2} o_4) + j_\mu(o_1 + \tfrac{3}{2} o_3) + \tfrac{1}{2} j_V(o_1 + o_3), \\ A_4 &= j_0 o_4 - j_t(o_1 + \tfrac{1}{2} o_3) + j_\mu(o_2 + \tfrac{3}{2} o_4) + \tfrac{1}{2} j_V(o_2 + o_4), \end{aligned} \tag{A.2}$$

and

$$\begin{aligned} o_i &= \tfrac{1}{2}\,\mathrm{Tr}_c[(c_1^\dagger g_i + g_i c_1^\dagger)\exp[\mathcal{H}_0(c)], \\ g_1 &= c_1 - c_1 n_4, \qquad g_2 = c_4 - c_4 n1, \\ g_3 &= 2c_1 n_4 - c_1, \qquad g_4 = 2c_4 n_1 - c_4. \end{aligned} \tag{A.3}$$

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