Pair correlation functions in one-dimensional correlated-hopping models

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Abstract. We investigate ground-state properties of two correlated-hopping electron models, the Hirsch and the Bariev model. Both models are of recent interest in the context of hole superconductivity. Applying the Lanczos technique to small clusters, we numerically determine the binding energy, the spin gaps, correlation functions, and other properties for various values of the bond-charge interaction parameter. Our results for small systems indicate that pairing is favoured in a certain parameter range. However, in contrast to the Bariev model, superconducting correlations are suppressed in the Hirsch model, for a bond-charge repulsion larger than a critical value.

Since the discovery of high-$T_c$-superconductivity strong efforts have been made to explain the pairing mechanism with the aid of microscopic models for strongly correlated fermions, the Hubbard and $t$-$J$ model being the most popular among them. In one dimension, exact results can be derived for the Hubbard model and for the supersymmetric $t$-$J$ model by applying the Bethe ansatz [1]. The main interest is the question whether and how collective behaviour can lead to a compensation of the Coulomb repulsion between the electrons. As a possible explanation, models with correlated-hopping interactions are a subject of current research [2–18].

In 1989, Hirsch [2] proposed a model for the description of oxide superconductors by considering the holes in a nearly filled band as the charge carriers. The Hamiltonian contains among other contributions a correlated hopping interaction, i.e. a bond-charge repulsion. A modified version of Hirsch’s model, the Bariev model, has been solved by Bethe ansatz [3]. Although it only contains one half of the bond-charge interaction terms of the original model, it is expected to maintain its basic qualities because it also takes into account the modification of the hopping amplitude by the presence of a particle with opposite spin. Considered as an electron model, the bond-charge repulsion leads to the formation of Cooper pairs of holes, a process which is favoured at small hole density [4].

In this paper we compare exact diagonalization results for the two models obtained by using the Lanczos technique [19]. Although the systems treated are small (up to 16 sites) and despite the finite size effects which render the interpretation of
the results difficult, comparison with some exact results for the Bariev model (in the thermodynamic limit), obtained from the Bethe ansatz solution, shows good agreement.

In the following we shall consider a one-dimensional system consisting of \( N = N_\uparrow + N_\downarrow \leq 2L \) itinerant electrons on a closed chain of \( L \) sites with periodic (PBC) or antiperiodic (ABC) boundary conditions. Electron hopping is possible between nearest neighbour sites, but the hopping matrix element is modified by the presence of electrons with the opposite spin direction on the sites involved in the hopping process.

The Hamiltonian of the Hirsch model reads

\[
\mathcal{H}_H(\Delta t) = -\sum_{j=1}^{L} \sum_{\sigma=\pm 1} \left( c_{j,\sigma}^+ c_{j+1,\sigma} + c_{j+1,\sigma}^+ c_{j,\sigma} \right) \left( 1 - \frac{\Delta t}{2} (n_{j,-\sigma} + n_{j+1,-\sigma}) \right),
\]

and the Bariev model is described by the Hamiltonian

\[
\mathcal{H}_B(\Delta t) = -\sum_{j=1}^{L} \sum_{\sigma=\pm 1} \left( c_{j,\sigma}^+ c_{j+1,\sigma} + c_{j+1,\sigma}^+ c_{j,\sigma} \right) \left( 1 - \Delta t n_{j+1,\mp\sigma} \right),
\]

where \( c_{j,\sigma}^+ \) and \( c_{j,\sigma} \), respectively, denote the creation and annihilation operators of an up-electron (\( \sigma = 1 \)) or down-electron (\( \sigma = -1 \)) at site \( j \). \( n_{j,\sigma} \) (which equals 0 or 1) is the number of particles with spin \( \sigma \) at site \( j \). As can easily be seen, the interaction parameter \( \Delta t \) is positive in the repulsive model \( H \) because it leads to a decrease of the hopping probability (for \( \Delta t < 2 \)), if an electron with opposite spin direction is present. In this sense there is an additional correlation between the up-spin and down-spin hopping processes.

We start our exact diagonalization study with the discussion of the ground-state energy. The energy difference between the Hirsch and the Bariev model is very small for small \( \Delta t \). As shown in fig. 1, the energy curves, as functions of the particle number \( N \), coincide for \( \Delta t = -0.2 \) and \( \Delta t = 0.2 \). They are also in good agreement for \( \Delta t = -1 \), but the curves spread apart for \( \Delta t = 1 \), where
the difference between the bond-charge interaction terms in the two models becomes relevant. The figure also indicates that the energy difference is small at low electron and low hole density for all values of the interaction parameter $\Delta t$. For comparison, we included the exact result \[6\] for the Bariev model at $\Delta t = 1$ as a full line, which is $\frac{E}{L} = -\frac{2}{\pi} (1 + \frac{n}{2}) \sin \left( \frac{n \pi}{1+\frac{n}{2}} \right)$. The exact diagonalization results for $L = 12$ all lie on this curve.

In the following, we discuss properties of the Hirsch and Bariev model for small hole filling. In the case of quarter filling of holes (i.e. electron filling $n = 3/2$), we can compare results for systems with $L = 4, 8, 12, 16$ sites.

The spin excitation energy is defined as $\Delta_s = E(S^z = 1) - E(S^z = 0)$, where $E(S^z)$ is the ground-state energy in the subspace with fixed $S^z$; it corresponds to the lower critical magnetic field $h_c$ which is necessary to create a non-zero magnetization in the system. In the absence of a spin excitation gap, $h_c$ vanishes, as is the case in the repulsive Hubbard model and the supersymmetric $t$-$J$ model. On the contrary, the attractive Hubbard model and the Bariev model have a gap in the spin excitations (see \[4, 8, 20\] and references therein).

In fig. 2 we show the results for $\Delta_s$ for both models. We choose PBC for $L = 16$ and 8 and ABC for $L = 12$ and 4, because the results facilitate the extrapolation into the thermodynamic limit if the Fermi wavenumber $k_F = n\pi/2$ of the free infinite system is one of the possible $k$ numbers of the finite system \[21\]. We verified that there is already good agreement between the exact diagonalization results for $L = 12$ and the analytic solution $\Delta_s = \frac{2}{\pi} \sin \left( \frac{n \pi}{1+\frac{n}{2}} \right) - \frac{4n}{2+n} \cos \left( \frac{n \pi}{1+\frac{n}{2}} \right)$ \[6\] for the Bariev model at $\Delta t = 1$. The results strongly suggest that the spin gap is maximal at $\Delta t = 1$ in both models and that the spin gap is vanishing in the Hirsch model for $\Delta t \gtrsim 1.5$ in contrast to the Bariev model where it remains non-zero. The vanishing of $\Delta_s$ at $\Delta t = 2$ in the Hirsch model is evident for any system size and boundary condition and a large range of densities. It is due to the high degeneracy at that parameter value where the Hirsch model can be treated analytically and the ground-states are of the $\eta$-pairing type \[8, 11\]. Moreover, results for other hole densities indicate that the vanishing of the spin gap in the Hirsch model is not
Figure 3: Spatial singlet pair correlations $G_0$ (○), $G_1$ (□), and triplet pair correlations $G_2$ (△) of the Hirsch model at $\Delta t = 1$ (left) and $\Delta t = 1.7$ (right) for $L = 16$, $n = 3/2$.

Figure 4: Same as in fig. 3 for the Bariev model.

restricted to the band filling of $n = 3/2$.

Whenever there is a gap in the spin excitation spectrum, spin correlations decay exponentially so that other correlations, such as pair correlations are more likely to dominate. We calculate the singlet pair correlation functions for on-site and next-neighbour pairs and the triplet pair correlation function, defined as

\[
G_0(r) = \langle P_0^+(r)P_0(0) \rangle, \\
G_1(r) = \langle P_s^+(r)P_s(0) \rangle, \\
G_2(r) = \langle P_t^+(r)P_t(0) \rangle,
\]

with the pairing operators

\[
P_0^+(r) = c_{r\uparrow}^+c_{r\downarrow}, \\
P_s^+(r) = \frac{1}{\sqrt{2}}(c_{r\uparrow}^+c_{r+1\downarrow}^+ - c_{r\downarrow}^+c_{r+1\uparrow}^+), \\
P_t^+(r) = \frac{1}{\sqrt{2}}(c_{r\uparrow}^+c_{r+1\downarrow}^+ + c_{r\downarrow}^+c_{r+1\uparrow}^+).
\]

When the number of doubly occupied sites is reduced in the ground-state of the interacting system—as compared to free fermions—$G_1(r)$ is expected to be
larger than $G_0(r)$, although both functions should be equivalent with respect to their decay in the infinite system. We compare results for both models for $\Delta t = 1$ and $\Delta t = 1.7$. Fig. 3 shows that at $\Delta t = 1$ both singlet correlation functions of the Hirsch model decay slowly to a non-zero value (which nevertheless can be zero in the infinite system, when finite size effects are absent). The triplet correlations decay very rapidly to zero. On the other hand, all pair correlations decay fast to zero at $\Delta t = 1.7$ where there is no spin excitation gap. This is different for the Bariev model where the decay is slower (fig. 4). We mention that the spin operator $\hat{S}^2$ does not commute with the Hamiltonian $H_B$ so that $S$ is no good quantum number in the Bariev model, in contrast to the Hirsch model.

To gain some insight into the dependence of the pair correlation functions on the bond-charge interaction parameter $\Delta t$, we also show their Fourier transform $\tilde{G}_j(k) = \frac{1}{L} \sum_r G_j(r) \cos(kr)$ for $k = 0$ which is simply the sum of the correlations over all spatial distances. Although it is not possible to discuss the decay by means of this function only, it helps to determine at which values of the interaction pair correlations are favoured. Fig. 5 indicates that singlet pairing is strong at $\Delta t \approx 1$ in both models, i.e. where the spin gap is large. This tendency is diminished drastically in the Hirsch model at parameters $\Delta t \gtrsim 1.1$. On the other hand, these functions are decreasing more slowly in the Bariev model. The curves of $\tilde{G}_0$ and $\tilde{G}_1$ have a similar shape and only differ by magnitude. Triplet correlations are small in both models and vary little as functions of $\Delta t$.

To complete the comparison of the two models, we calculate the binding energy $E_B(N) = E(N+2) + E(N) - 2E(N+1)$. To suppress the finite size effects, we choose twisted boundary conditions (TBC), which means that the wavefunction at site 0 and site $L$ is related by $\Psi(L) = e^{i\varphi}\Psi(0)$, and take the average of $E_B$ over various values of the twisting angle $\varphi$. To estimate the finite size effects, we also show the maximum/minimum $E_B$ obtained in this way (fig. 6). The binding energy is negative in the Hirsch model for $\Delta t < 1.4$, but becomes positive for larger values of $\Delta t$. In the Bariev model, the averaged $E_B$ is zero at $\Delta t = 0$ and $\Delta t = 2$ and negative for all other $\Delta t$, with minimum at $\Delta t = 1$. For $\Delta t > 1.7$, the finite size effects in the Bariev model are too large to decide if binding occurs or
Figure 6: Binding energy of the Hirsch model (left) and Bariev model (right), $n = 20/12$, averaged over TBC (full line). The broken lines estimate the finite size deviations.

not, but we have strong evidence that binding is suppressed in the Hirsch model for $\Delta t > 1.5$.

We conclude that our calculation of various ground-state properties of finite clusters at small hole doping indicates that the Bariev model and the Hirsch model show similar behaviour as long as the bond-charge repulsion $\Delta t$ is small. Pair correlations are strongest in both models for $\Delta t \approx 1$. For $\Delta t \gtrsim 1.5$, there is a change in the ground-state properties of the Hirsch model, and superconducting correlations are strongly suppressed for large $\Delta t$, which is in accordance with mean field results [9]. In the Bariev model, there is no such evident change.

We finally propose a simple argument which might help to understand why the parameter of $\Delta t \approx 1.5$ can be a phase boundary in the Hirsch model: The analytic diagonalization of the local interaction (acting only on two neighbouring sites) of (1) shows that (for $1 < \Delta t < 2$) $|\Psi_1\rangle = |\sigma 2\rangle + |2\sigma\rangle$ and $|\Psi_2\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |20\rangle + |02\rangle$ ($0$, $\sigma$, $2$ denoting the empty, singly, and doubly occupied site) are local eigenvectors with eigenvalues $E_1 = 1 - \Delta t$ and $E_2 = -2 + \Delta t$ [12]. Since $E_1 = E_2$ for $\Delta t = 3/2$, there is a level-crossing in the local ground-state at that parameter, whereas this effect is absent in the Bariev model. This criterion might be of importance for the global ground-state, too.

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