Using exact Lanczos diagonalizations we have shown that the pair-hopping model for negative $W$ exhibits a phase transition into $\eta$-superconducting state. The transition occurs at any band filling and the critical value $W_c$ varies between $W_c \simeq -1.75t$ at half-filling to $W_c \simeq -2t$ for two particles on the lattice.

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There is considerable interest in the pair–hopping model as a phenomenological model which captures some of the essential physics of the high–$T_c$ superconducting materials. The model was proposed ten years ago by Penson and Kolb as a model exhibiting the real–space pair formation mechanism. The Hamiltonian of the pair–hopping model contains, in addition to the usual one–electron hopping term, a term that hops singlet pairs of electrons from site to site and in the one–dimensional case is given by

$$
\mathcal{H} = -t \sum_{n,\alpha} (c_{n,\alpha}^\dagger c_{n+1,\alpha} + c_{n+1,\alpha}^\dagger c_{n,\alpha}) - W \sum_n (c_{n,\uparrow}^\dagger c_{n+1,\downarrow} c_{n+1,\uparrow} c_{n,\downarrow} + h.c.).
$$

(1)

Here $c_{n,\alpha}^\dagger$ ($c_{n,\alpha}$) is the creation (annihilation) operator for an electron with spin $\alpha$ at site $n$. Thus $t$ and $W$ are the single–electron and pair–hopping amplitudes respectively, and the competition between these two sources of delocalization leads to a rich phase diagram of the model. For $W = 0$, we have a system of free electrons, whose properties are exactly known. In the opposite limit $t = 0$ all sites are doubly occupied or empty, the model is superconducting by construction and equivalent to the XY model. The correspondence with the XY model can be seen by introducing $S = 1/2$ pseudospins $T_n$, with $T_n^x = c_{n,\uparrow}^\dagger c_{n,\downarrow}, T_n^z = c_{n,\uparrow}^\dagger c_{n,\uparrow} + c_{n,\downarrow}^\dagger c_{n,\downarrow} - 1)/2$. Then the Hamiltonian becomes

$$
\mathcal{H} = -W \sum_n (T_n^+ T_n^- + h.c.).
$$

(2)

This picture holds true for either sign of $W$, but it is important to note that $W \to -W$ is not a symmetry of the model and the way the system reaches its limiting behaviour at $|W| >> t$ is genuinely different for negative and positive $W$ cases. Moreover, as we show in this paper, if for positive $W$ a singlet superconducting state with order parameter $\Delta_{SS} = \langle c_{k,\uparrow}^\dagger c_{-k,\downarrow} \rangle$ corresponding to the usual Cooper pairs is realized, in the case of negative $W$, an $\eta$–superconducting state with order parameter $\Delta_{\eta} = \langle c_{k,\uparrow}^\dagger c_{-k,\downarrow} \rangle$ corresponding to the pairing with total momentum equal to $\pi$ is the ground state of the system at $W < W_c \approx -1.75t$.

The model was mainly studied in the case of half–filled band and $W > 0$. Penson and Kolb used exact diagonalizations data for chains up to 10 sites and found a phase transition into a superconducting state at which the spin gap (or single–particle excitation gap) opens for $W > W_c \approx 1.4t$. Later Affleck and Marston analysed the model within the framework of the weakly–coupling continuum limit approach. They found that for any $W > 0$ the spin excitation spectrum is gapped, while the charge excitation spectrum is gapless and the singlet superconducting instabilities are most divergent in the ground–state. In the case of $W < 0$ ($|W| << t$) at half–filling there is a gap in the charge excitation spectrum, the spin sector is gapless and the ground state corresponds to an insulator. Moreover Affleck and Marston argued the absence of any other transitions for $W > 0$ and the necessity of a phase transition into a sector with gapped spin excitations and gapless charge degrees of freedom for $-W \gg t$. This scenario of the ground–state phase diagram was recently confirmed by Sikkema and Affleck who used the Density Matrix Renormalization Group technique (DMRG) for chains up to 60 sites. For $W < 0$, they found a transition into a spin gapped phase at $W < W_c \approx -1.5t$.

In this paper we focus our attention on the transition into an $\eta$–superconducting state for negative $W$. This transition corresponds to a drastic change of the ground-state, after which the one particle hopping term is almost frozen out. To prove this, we used exact Lanczos diagonalizations. We have shown that the transition into $\eta$–superconducting state takes place at arbitrary filling and weakly depends on the band–filling. Our data suggests that the finite size effect are extremely small, that is why we restricted ourself to systems up to 10 sites.

As far as the main phenomenon characterizing the transition into an $\eta$–superconducting state takes place in the momentum space it is convenient to rewrite the Hamiltonian in this space

$$
\mathcal{H} = -2t \sum_{k,\alpha} c_{k,\alpha}^\dagger c_{k,\alpha} \cos(k) - 2W \sum_Q A_Q^\dagger A_Q \cos(Q)
$$

(3)

where $A_Q^\dagger = \frac{1}{\sqrt{L}} \sum k c_{k,\uparrow}^\dagger c_{k-Q,\downarrow}^\dagger$ is the creation operator of pair of electrons with opposite spins and total momentum.
$Q$, $L$ is the size of the system. As far as the total momentum of the system $Q_{tot}$ is conserved we can consider each sector of the Hilbert space for a given $Q_{tot}$ independently. It is clear that the ground state of the system belongs to the sectors $Q_{tot} = 0$ or $Q_{tot} = \pi$. States with $Q_{tot} \neq 0$ and $\pi$ exhibit a broken time reversibility symmetry and are excited states.

As it was shown by Yang, the general condition ensuring the possibility for $\eta$-pairing is

$$\epsilon(\vec{k}) + \epsilon(\vec{\pi} - \vec{k}) = \text{constant}$$

(4)

where $\epsilon(\vec{k})$ is the bare electron spectrum and $\vec{\pi} = (\pi, ..., \pi)$. The particularity of the pair-hopping model could be observed even in the case of two particles on a lattice. Below we consider the one-dimensional case, however the arguments are valid in any dimensions if the bare electron spectrum ensures the condition (3).

Let us first analyse the $W < 0$ case. For $W = 0$ the ground-state energy is $E_0 = -4t$ and the total momentum is $Q_{tot} = 0$. As we switch on $W$, it can be shown easily that the lowest energy in the $Q_{tot} = 0$ subspace goes to $-2W > 0$ (for $|W| \gg t$). On the other hand, the lowest energy in the $Q_{tot} = \pi$ sector is $2W < 0$. Thus there should be a transition at some critical value, from the unpaired state in the $Q_{tot} = 0$ sector into the $\eta$-pairing state in the $Q_{tot} = \pi$ sector. We can roughly estimate the critical value to be $W_c \approx -2t$. Indeed after the transition the ground-state corresponds to the wave function $A^\dagger_\pi |0\rangle$, which clearly describes an $\eta$-pair. It is clear that after the transition the one particle hopping term is completely frozen out (i.e. $<n_k> = \sum_a <c^\dagger_{ka}c_{ka}> = \text{constant}$).

In the opposite case $W > 0$, the ground-state always remains in the $Q_{tot} = 0$ subspace and its energy continuously goes from $-4t$ at $W = 0$ to $-2W$ for $W \gg t$. There is no more transition for $W > 0$ and the weight of Cooper pair continuously increases up to 1 when $W = +\infty$. In this limit the ground state wave function is $A^\dagger_0 |0\rangle$. Note that only for $W = \pm \infty$ the ground-states are equivalent up to a trivial $\pi/2$ shift of all momenta, reflecting the $W \rightarrow -W$ symmetry of the XY model.

As we show below using exact diagonalizations data the picture essentially remains in the case of many particle systems. Namely for $W < 0$, there is a phase transition (presumably of the first order) at the critical value of the pair-hopping amplitude from the insulating (1/2-filled case) or Luttinger–liquid state (lower filling) into a $\eta$-superconducting state. The transition occurs at any band filling and the critical value $W_c$ varies between $W_c \approx -1.75t$ at half-filling to $W_c \approx -2t$ for two particles on the lattice. The transition to $\eta$-pairing is characterized by the strong reduction of the one particle hopping term. However, it should be stressed that due to the quasi-bosonic character of the pairs, the weight of unpaired particles is extremely small but finite after the transition.

In the following part, we will present numerical data considering the lowest energy in the $Q = 0$ and $Q = \pi$ sectors. In Fig.1 we have plotted the lowest energy in each sectors at half-filling, as a function of $W$ for two different cases $L = 8$ and $L = 10$. In Fig.1a we clearly observe a different behaviour of the ground-state energy for $W > 0$ and $W < 0$. In the case $W > 0$ the ground state energy continuously goes to the XY model ground-state energy ($|W| = \infty$), and the ground-state always remains in the $Q = 0$ sector. There is no trace of any additional transition for $W > 0$, this is in complete agreement with the DMRG results. Let us now consider the $W < 0$ case. Below a critical value $W_c \approx -1.75t$ the energy is quasi linear in $W$ and becomes very close to the ground state energy of the XY model. Hence after the transition the one particle hopping term is almost frozen out. This transition can be observed more clearly in Fig.1b. Indeed before the transition the total momentum of the ground state is $0$ and it is $\pi$ after the transition. This transition from the $Q = 0$ to $Q = \pi$ subspace depends only on the parity of the number of pairs, therefore the transition is easily observed when this number is odd.

To distinguish superconducting phases corresponding respectively to $W > 0$ and $W < 0$, we calculated the distributions of $<n_k>$ and $<A^\dagger_\pi A_Q>$ in both cases (Fig.2). For $W > 0$ the $<n_k>$ distribution continuously goes to the limiting case $<n_k> = 1$ (i.e. $|W| = \infty$) and the distribution of $<A^\dagger_\pi A_Q>$ has a strong peak at $Q = 0$. In the opposite case, for $W < W_c$, $<n_k> \approx 1$ (reflecting the freezing out of one electron hopping term) and $<A^\dagger_\pi A_Q>$ shows a peak at $Q = \pi$. For $W > 0$, pairs with $Q = 0$ appear continuously in the system. On the other hand, when $W < 0$ the $Q = \pi$ pairs appear spontaneously when $W < W_c$. The competition between the $t$-term and the $W$-term leads to the total destruction of the old band structure at the critical point.

To show that $A_Q$ with $Q = 0$ or $\pi$ is a proper operator to describe the physics of the system we calculate,

$$Z_Q = \frac{|<N_e - 2|A_Q|N_e>|}{(<N_e|A^\dagger_\pi A_Q|N_e>)^{1/2}}$$

(5)

where $|N_e>$ is the ground-state with $N_e$ particles. This overlap measures the weight of quasi-particle with total momentum $Q$ in the ground-state. We checked numerically that $Z_Q$ is zero for all values of $Q$ except 0 and $\pi$. In Fig.3 we calculated this quantity for $Q = 0$ and $Q = \pi$. For $W > 0$, $Z_\pi = 0$ whilst $Z_0$ is finite and continuously approaches its limiting value. The jump at $W = 0$ is a finite size effect, it can be shown that it goes as $1/\sqrt{L}$. Thus the usual Cooper pairs appear continuously for $W > 0$.

In the opposite case $W < 0$, $Z_0 = 0$. Depending on the parity of the number of sites $Z_\pi$ is 0 or 1 for $W = 0^-$.

For $L = 6$, $Z_\pi = 0$ before $W = -1.5t$, the jump which appears at this point corresponds to a ‘crossing’ with some excited state, while the final transition corresponding to $\eta$-pairing occurs only at $W \approx -1.75t$, after this transition $Z_\pi \approx 1$. 
In the case of \( L = 8 \), \( Z_{\pi} = 1 \) for \( W = 0^- \) this is common when \( L = 4L_o \) due to the presence of electrons with momentum \( p_F = \pi/2 \). When we increase \( |W| \) the probability to find a particle on the Fermi surface is reduced, this is reflected by the reduction of \( Z_{\pi} \). After the transition to \( \eta \)-pairing \( Z_{\pi} \approx 1 \). This suggests that the \( \pi \)-pairs appear spontaneously in the ground-state after the transition. And \( A_0 \) and \( A_{\pi} \) are proper operators to describe the superconducting states for \( W > 0 \) and \( W < 0 \) respectively.

Another way to visualize this transition is to show the pairing phenomenon in real space. The corresponding quantity is given by,

\[
F(W) = \frac{1}{L} \sum_{i=1}^{L} < n_{i\uparrow} n_{i\downarrow} > - < n_{i\uparrow} > < n_{i\downarrow} > \tag{6}
\]

it is plotted in Fig.4a.

This picture shows that for \( W > 0 \) the pairs appear continuously in the system. In the opposite case \( W < 0 \), and \( |W| \ll t \) the tendency to pairing is reduced, this is in agreement with the effective repulsive character of the pair-hopping interaction in this limit. This effective repulsive character remains up to \( |W| < 0.5t \) after which a tendency to pairing appears. However the transition to \( \eta \)-state corresponds to the jump in \( F(W) \) at \( W \approx -1.75t \).

As it is clear from this figure that the finite size effects have only a weak influence on this value.

To show that the physics does not depend on the band filling, we analyse the model away from half-filling. In Fig.5 we plotted the lowest energy as a function of \( W \) in two particular cases. It is clear from this picture that the transition to \( \eta \)-state remains away from half-filling. To analyse the band-filling dependence of the critical value we calculated \( F(W) \) for a given size \( L = 10 \) and different number of particles (fig4b). This picture suggests that the critical value \( \eta \)-pairing weakly depend on the band filling. When we increase the band filling \( W_c \) goes from -2t (two particles) to -1.75t (half-filled case).

To conclude, in this paper we have shown that the pair-hopping model for \( W < 0 \) exhibits a phase transition into the \( \eta \)-superconducting state. The critical value at which the transition takes place weakly depends on the size of the system and on the band-filling, it varies between \(-2t < W_c < -1.75t \). For \( W > 0 \) our results are in agreement with previous work, and shows a continuous second-order transition to usual superconducting state at \( W = 0^+ \), with no additional transition for any \( W > 0 \). We argue that this phenomenon will remain unchanged in higher dimensions. Investigation of the 2D case is under consideration.

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