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Hole pairing in the Hubbard model

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Abstract

The hole-pairing problem at the dilute limit on low-dimensional bipartite and non-bipartite lattices is studied by means of the generalized Hubbard model, in which on-site (U), nearest-neighbor (V), and assisted-hopping (Δt) terms are considered. The problem is addressed by mapping the original many-body problem onto a tight-binding one in a higher-dimensional space. It is found that there is a small region around $\Delta t/t_0 = 0.5$, where the pairing of holes is enhanced and non-pairing of electrons exists. Pairing phase diagrams are analyzed for linear, square and triangular lattices, in comparison with those results obtained from the extended Hubbard model. © 1998 Elsevier Science B.V. All rights reserved.

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For high-T_c cuprate superconductors, the pairing of holes (instead of electrons), the short coherence length of these pairs, and the low dimensionality of the system seem to be important elements to consider [1]. In recent years the real-space electronic correlation has been extensively studied by using the Hubbard model [2], which has the advantage of being simple and general, because it does not depend explicitly on the nature of interactions between particles. More recently, we have developed a mapping method [3], which consists of mapping the original many-body problem onto a tight-binding one with some ordered impurities in an nd-dimensional space, being n the number of electrons and d the dimensionality of original system. In this hyper-space lattice, the on-site (U) and the nearest-neighbor (V) interactions of the original Hamiltonian (Eq. (1)) become the self-energies of the impurities, whilst the assisted hopping terms (Δt) enhance the hopping parameter between these impurities, as shown in Fig. 1.

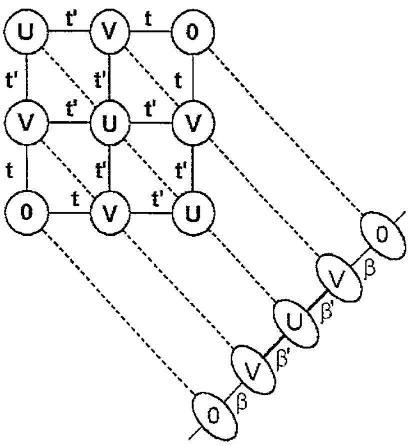

Fig. 1. Sketch of the mapping method for the 1D-GHH, where $\beta = 2t\cos(ka/2)$, $t = t_0 - 2\Delta t$, $t' = t + \Delta t$, k is the wave vector of pairs, and a is the lattice parameter.

The single-band generalized Hubbard-Hamiltonian (GHH) can be written as

$$H = -t_0 \sum_{\langle i,j\rangle,\sigma} c^+_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j + \Delta t \sum_{\langle i,j\rangle,\sigma} c^+_{i,\sigma} c_{j,\sigma}(n_{i,-\sigma} + n_{j,-\sigma}), \qquad (1)$$

where $\langle i,j\rangle$ denotes nearest-neighbor sites, $c^+_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ being $n_{i,\sigma} = c^+_{i,\sigma} c_{i,\sigma}$. When a particle–hole transformation is made in the GHH, i.e., electron operators are mapped onto hole's via $c^+_{i,\sigma} \to h_{i,\sigma}$,

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the Hamiltonian becomes

$$H = (U + 2ZV)(N - \sum_{i,\sigma} n^h_{i,\sigma}) + (t_0 - 2\Delta t) \sum_{\langle i,j\rangle,\sigma} h^+_{j,\sigma} h_{i,\sigma}$$
$$+ U \sum_i n^h_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n^h_i n^h_j$$
$$+ \Delta t \sum_{\langle i,j\rangle,\sigma} h^+_{i,\sigma} h_{j,\sigma}(n^h_{i,-\sigma} + n^h_{j,-\sigma}), \qquad (2)$$

where N is the total number of sites and Z is the lattice coordination number. The first term in Eq. (2) only contributes to a shift in the total energy, and then the holes also interact via a Hubbard model but with an effective hopping parameter $(t_0 - 2\Delta t)$. It is worth mentioning that U, V, and Δt are typically at about 20, 3, and 0.5 eV, respectively [4, 5].

In Fig. 2 the binding energies ($\Delta \equiv E_0 - E_0(U = V = \Delta t = 0)$ [6]) between two electrons and between two holes, for a linear chain (1D), a square and a triangular lattice, are comparatively analyzed as a function of $\Delta t/t_0$ for $U = 0$ and $V = 0$ and $3t_0$. The numerical calculations were performed on the same lattices but with impurities [6], obtained after a mapping procedure as shown in Fig. 1 for a linear chain. Note that for $0 \leqslant \Delta t/t_0 \leqslant \frac{2}{3}$ there is a strong hole-singlet pairing in all the three analyzed lattices and the pairing of electrons arises only for $\Delta t/t_0 \geqslant 2$, i.e., the pairing of holes requires a rather smaller Δt.

Shown in Fig. 3 is a phase diagram for two holes on the same three lattices of Fig. 2 for $V = 0$ and $3t_0$. We can see that for a small region around $\Delta t/t_0 = 0.5$ the pairs of holes survive even the on-site repulsion (U) is extremely high when $V = 0$. However, the pairing process is easily affected by the nearest-neighbor repulsion (V), in contrast with that occurring in the extended Hubbard model [6]. Finally, for $\Delta t/t_0 = 0.5$ we have a molecule-type problem and therefore, $\Delta = \frac{1}{2}[\sqrt{(U - V)^2 + 4Zt_0^2} - U - V]$, since $\beta = 0$.

In summary, we have shown that within the GHH the pairing of holes is suitable for small Δt. Furthermore, these pairing states are not sensitive to the on-site repulsion. These two facts could be relevant for the hole-pairing process in many real systems, in spite of $\Delta t \ll V \ll U$.

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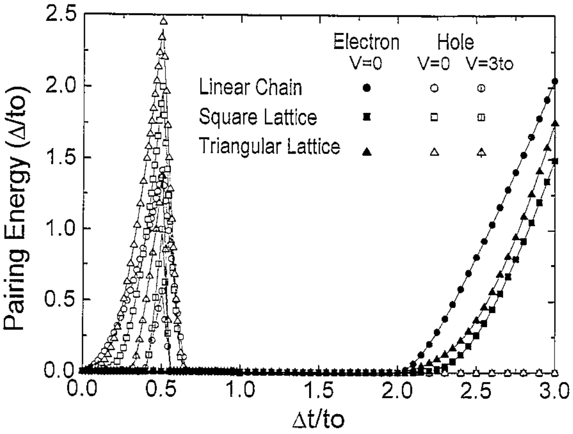

Fig. 2. Pairing energies of electron singlets and hole singlets for $U = 0$.

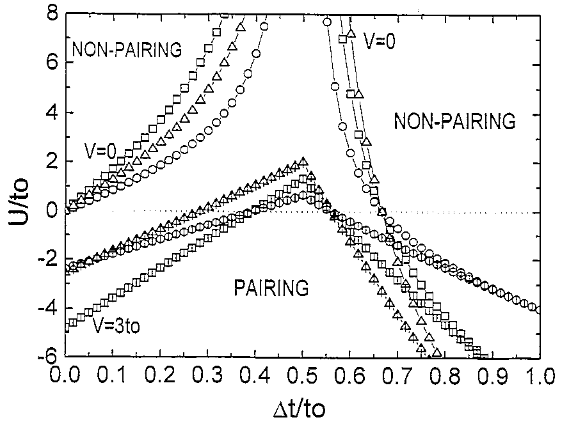

Fig. 3. Hole-singlet phase diagrams for $V = 0$ and $3t_0$ on the same lattices as in Fig. 2.

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