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Two-particle states in the generalized Hubbard model

L.A. Pérez, C. Wang*

Instituto de Investigaciones en Materiales, UNAM, A.P. 70-360, 04510, México D.F., Mexico

Abstract

The pairing between holes and between electrons at the dilute limit is studied by means of the generalized Hubbard model. The problem is addressed by mapping the original many-body problem into a tight-binding one in a higher-dimensional space. The results show a strong enhancement of the hole pairing around $\Delta t/t_0 = 0.5$, even though the on-site repulsion is extremely high. A significant reduction of the effective mass of pairs is also observed in this region, which could be important for the Bose–Einstein condensation of these pairs. Finally, pairing phase diagrams analyzed for linear, square, triangular and cubic lattices show a sensitive dependence on the nearest-neighbor interactions.

Keywords: Hubbard model; Singlet ground state; Bose–Einstein condensation

In spite of no general consensus on the high-T_c superconducting mechanism, the d-wave symmetry of the superconducting gap, the singlet pairing between holes (instead between electrons), and their short coherence length have been widely accepted [1]. It is suggested [2] that the transition temperature could be much less than that corresponding to the pairing process, and then a different scattering dynamics of the carriers is expected in this intermediate temperature regime. Certainly, an almost linear relationship between the T_c and n_s/m^* is observed [3], where n_s and m^* are the superconducting carrier density and their effective mass, respectively. Therefore, a detailed analysis of the hole pairing process and the dynamics of these pairs could be important to understand the high-T_c superconductivity.

Recently, we have mapped [4] the generalized Hubbard problem into a tight-binding one with "impurities" in an nd-dimensional space, n being the number of electrons and d the dimensionality of the original system. In this hyper-space, the onsite (U) and the nearest-neighbor (V) interactions become self-energies of the impurities, whilst the correlated hopping terms (Δt) of the generalized Hubbard model enhance the hopping parameter between these impurities [4]. In general, these three interactions have very different contributions, for example, for 3d electrons in transition metals U, V and Δt are typically about 20, 3 and 0.5 eV, respectively [5].

For a full-filled single band, we have previously found [4] hole-singlet pairing for $\frac{2}{3} \geqslant \Delta t/t_0 \geqslant 0$ in one- and two-dimensional systems, and for $0.613 \geqslant \Delta t/t_0 \geqslant 0.294$ in the simple cubic lattice, where $-t_0$ is the electron hopping parameter. However, the pairing of electrons arises only for $\Delta t/t_0 \geqslant 2$. An important parameter to analyze the dynamics of pairs is their effective mass, which has been calculated from the x-directional dispersion curve of the pairing ground state (m_p) and compared with the effective mass of the lowermost non-correlated state (m_{np}). The non-correlated states have a coherence length scaling with the system size. Fig. 1a shows a clear increase of the two-particle effective mass within the negative Hubbard model, being $V = \Delta t = 0$. Nevertheless, for the generalized Hubbard systems, a significant reduction of m_p/m_{np} around $\Delta t = 0.5t_0$ is observed, as shown in Fig. 1b for $U = V = 0$. This fact could be relevant, since the Bose–Einstein condensation temperature is proportional to $1/m^*$ [6].

The hole-singlet phase diagrams are shown in Fig. 2. Notice that at $\Delta t = 0.5t_0$, there is hole pairing with very large U. Finally, the transition lines for $V = 0$ in one- and

*Corresponding author. Fax: +52-(5)-6161251; e-mail: chumin@servidor.unam.mx.

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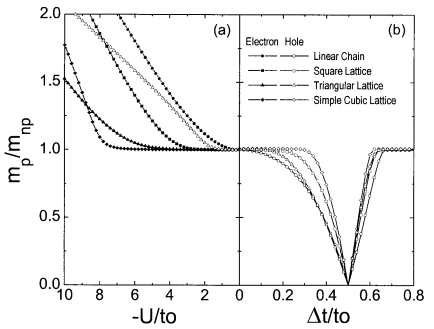

Fig. 1. Effective mass of two-particle ground state (m_p) in comparison with that corresponding to the lowermost non-pairing state (m_{np}), for (a) negative and (b) generalized Hubbard model. In (a) the effective masses of two electrons and of two holes are the same for bipartite lattices.

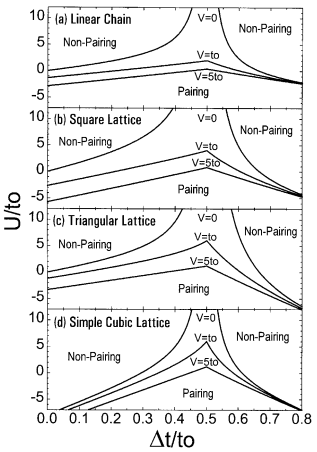

Fig. 2. Hole-singlet pairing phase diagrams for (a) a linear chain, (b) a square, (c) a triangular and (d) a simple cubic lattice.

two-dimensional systems always start from the origin, in contrast to the smaller pairing region in the three-dimensional case.

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