Pergamon

Solid State Communications, Vol. 108, No. 4, pp. 215–219, 1998

0038–1098/98 $ - see front matter

PII: S0038–1098(98)00347-0

ENHANCED HOLE PAIRING IN GENERALIZED HUBBARD SYSTEMS

L.A. Pérez and C. Wang*

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510, México D.F., Mexico

(*Received* 13 *May* 1998; *accepted* 13 *July* 1998 *by R.C. Dynes*)

The pairing between holes at the dilute limit is studied by means of a generalized Hubbard model, in which on-site (U), nearest-neighbor (V) and correlated-hopping (Δt) interactions are considered. 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 or nearest-neighbor repulsion is extremely high. A significant reduction of the effective mass of pairs in comparison with non-pairing ones is also observed in this region, which could be important in the Bose–Einstein condensation of these hole singlets. Finally, the pairing phase diagrams calculated in linear, square, triangular and cubic lattices show an enhanced hole pairing in low-dimensional systems. © 1998 Elsevier Science Ltd. All rights reserved

Keywords: A. high-T_c superconductors, D. electron–electron interactions, electronic states.

1. INTRODUCTION

The first decade of intensive investigations on the high transition temperature (T_c) superconductors has clarified important features, such as the *d*-wave symmetry in the superconducting gap [1], the singlet pairing between holes (instead between electrons) [2], and their short coherence length [3], in spite of no general consensus on the high-T_c superconducting mechanism. The normal state of these superconductors in the underdoped region is particularly interesting, where the in-plane resistivity as a linear function of temperature [4] and the appearance of a spin–gap well above T_c [5] have been observed. It is suggested [6] that the transition temperature T_c could be much less than the pairing temperature and then a different scattering dynamics of the carriers is expected in this intermediate temperature regime. Certainly, there is a linear relationship between the T_c and n_s/m^* [7], where n_s is superconducting carrier density and m^* their effective mass. Therefore, a detailed analysis of the pairing process and the dynamics of these pairs could be important to understand the high-T_c superconductivity.

A general way to analyze the electronic correlations in narrow-band systems might be worked out using the Hubbard model [8], because it is probably the *simplest* many-body model that considers the local electron–electron interactions in a general form. In spite of its simplicity rigorous results have been obtained only for one [9] and infinite [10] dimensions. In particular, the pairing problem has been studied by means of the extended [3] and the generalized Hubbard model [11]. Recently, we have developed a mapping method in which the original many-body problem is transformed into a tight-binding one with impurities in a higher dimensional space [12].

In this paper, we report an extension of the mapping method to the generalized Hubbard model and an analysis of the pairing between holes in comparison with the electron case. In Section II, the mapping method applied to generalized Hubbard electronic systems is discussed. The binding energy, the coherence length and the effective mass of the pairs are analyzed in Section III. Phase diagrams of the pairing ground states are also presented. Finally, some conclusions are given in Section IV.

* Corresponding author. E-mail: chumin@servidor.unam.mx

2. METHOD

The electronic correlation could be analyzed in general by means of the generalized Hubbard model, in which on-site (U), nearest-neighbor (V) and correlated-hopping (Δt) interactions are considered. Certainly, all these three interactions are present in a real solid, even their contributions could be very different, for example, for $3d$ electrons in transition metal U, V and Δt are typically about 20, 3 and 0.5 eV, respectively [8, 13]. Furthermore, the multiband problem of the CuO_2 plane in high-T_c superconductors could be reduced to a single-band one [14], since we are interested in their low-energy electronic excitations. Therefore, this effective one-band generalized Hubbard Hamiltonian can be written as

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

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 equation (1), i.e. electron operators are mapped onto hole's via $c^+_{i,\sigma} \rightarrow h_{i,\sigma}$, the Hamiltonian becomes:

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

where N is the total number of sites and Z is the lattice coordination number. The first term in equation (2) only contributes to a shift of the total energy and then, the holes also interact via a generalized Hubbard model but with an effective hopping parameter $t = t_0 - 2\Delta t$, instead of $-t_0$ for electrons.

When the correlated hopping interaction is introduced, the previously developed mapping method should be modified. As shown in Fig. 1 for the case of two holes in a linear chain, the projected hopping parameters β and $\beta_{\rm imp}$ are respectively given by $2t\cos(Ka/2)$ and $2t_{\rm imp}\cos(Ka/2)$, where $t_{\rm imp} = t + \Delta t$, K is the wave vector of the center of mass of the pair and a is the lattice constant. Notice that the hopping ($t_{\rm imp}$) between ''impurity states'' (with self-energies U or V) is enhanced by adding a Δt, since the correlated hopping interactions have contribution only on single-particle hopping processes into *or* from double occupied states.

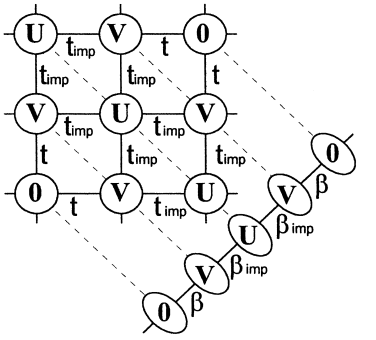

Fig. 1. Sketch of the one-dimensional generalized Hubbard hole-singlet states, represented by circles with self-energies and hopping-strengths indicated inside and in between, respectively. The projection procedure is shown by dashed lines. The final effective states are represented by ellipses and the effective hopping parameters are $\beta = 2t\cos(Ka/2)$ and $\beta_{\rm imp} = 2t_{\rm imp}\cos(Ka/2)$, where $t_{\rm imp} = t + \Delta t$, K is the wave vector of the pair and a is the lattice constant.

As we have demonstrated previously [12], within the extended Hubbard model the problem of electronic correlation is equivalent to a tight-binding one with impurities and the correlated states correspond to those impurity-states due to the negative self-energies U or V. In our case, for the generalized Hubbard model, the correlated electronic states are originated from the enhanced bonds (bond-impurities), with *or* without negative U or V. These two-particle correlated states will be analyzed in the following section.

3. RESULTS

In order to study the hole pairing ground state and the dynamics of these pairs, the binding energy, the coherence length and the effective mass of the pairs are analyzed. The binding energy has been calculated from the difference of energies between the lowermost pairing state ($K = 0$) and the lower-most non-correlated state, which is localized at the lower non-correlated band edge. In Fig. 2(a), the binding energies between two holes vs $\Delta t/t_0$, being $U = V = 0$, are shown for a linear chain, a square, a triangular and a simple cubic lattices, where the numerical diagonalizations are performed in their corresponding truncated projected lattices, as shown in Fig. 1, of 301, 3969, 5677 and 35937 effective states, respectively. The matrix sizes for numerical calculation are chosen as the minimum size so that the physical quantities have no important variation with the matrix size.

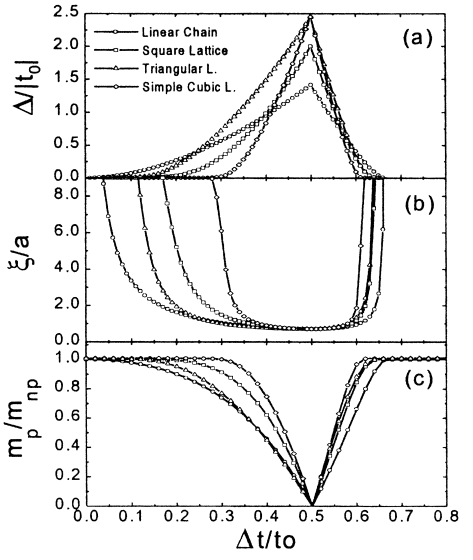

Fig. 2. Hole-singlet's (a) binding energy, (b) coherence length and (c) effective mass for a linear chain (open circles), a square (open squares), a triangular (open up-triangles) and a simple cubic lattice (open diamonds).

First, notice that there is a strong singlet-hole pairing for $0 < \Delta t/t_0 < 2/3$ in one- and two-dimensional systems and for $0.294 < \Delta t/t_0 < 0.613$ in the simple cubic lattice. These pairing intervals are in very good agreement with that obtained following the procedure introduced by Marsiglio and Hirsch [11]:

$$U(\Delta t, V) = 2E_0 \times \frac{G_0(0)[E_0V + 2Z\Delta t(2t + \Delta t)] - E_0V - 2Z(t + \Delta t)^2}{G_0(0)[E_0V - 2Zt^2] - E_0V}. \tag{3}$$

where E_0 is the singlet particle ground-state energy, $G_0(0) = (1/N)\Sigma_{\mathbf{k}} E_0/[E_0 - \epsilon(\mathbf{k})]$, and $\epsilon(\mathbf{k})$ is the dispersion relation of a single hole. For a simple cubic lattice, $G_0(0) \approx 1.51638$. However, for one- and two-dimensional lattices, $G_0(0) \rightarrow \infty$ [11] and then

$$U(\Delta t, V) = 2E_0 \frac{E_0V + 2Z\Delta t(2t + \Delta t)}{E_0V - 2Zt^2}. \tag{4}$$

Therefore, the pairing intervals are given by equations (3) and (4) evaluating for $U = V = 0$. On the other hand, the binding energy at $\Delta t = 0.5t_0$ is given by $(\sqrt{(U-V)^2 + 4Zt_0^2} - U - V)/2$ [15], which is determined by the coordination number Z, instead of the dimensionality, since in this case the problem can be reduced to a molecular-like one in the projected space, as shown in Fig. 1. It would also be worth mentioning that the pairing of electrons requires $\Delta t > 2t_0$ for one- and two-dimensional lattices and on the simple cubic lattice the requirement should be $\Delta t < 2.7136t_0$; both can be obtained from equations (3) and (4) by replacing t by $-t_0$ and evaluating for $U = V = 0$.

Another physical quantity to characterize a pair is its coherence length, which can be calculated as $\xi = \langle \mathbf{r}^2 \rangle^{1/2}$, where

$$\langle \mathbf{r}^2 \rangle = \frac{\sum_r \psi^*(\mathbf{r})\mathbf{r}^2\psi(\mathbf{r})}{\sum_r \psi^*(\mathbf{r})\psi(\mathbf{r})} \tag{5}$$

is the mean-square radius of the pair, $\psi(\mathbf{r})$ is the two-particle wave-function amplitude and $\mathbf{r}$ represents the internal coordinates of the pair. If this wave function has an exponential behavior with a characteristic length $\xi_0 \approx a$, the difference between ξ and ξ_0 is negligible. In fact, ξ would be reduced to the usual BCS coherence length by introducing a numerical factor of $2\sqrt{2}/\pi$ [17]. Figure 2(b) shows the coherence lengths for holes in the four analyzed lattices as Fig. 2(a). It can be observed that in general a short coherence length is always associated to a larger binding energy. However, an inverse proportionality between these two quantities, as in the BCS theory [18], is not found. Finally, the minimum coherence length ($\xi_{\min} = 1/\sqrt{2}$) is reached at $\Delta t = 0.5t_0$.

To study the dynamics of the pairs, a fundamental parameter is their effective mass, as discussed in [19]. For a three-dimensional gas of bosons, the Bose–Einstein condensation temperature is fully determined by the density of the gas (ρ) and their effective mass (m^*) in the following way [20]

$$T_{BE} = \frac{2\pi\hbar^2\rho^{2/3}}{1.897k_Bm^*}.$$

In this work, the x-directional effective mass of the pairs (m_p), calculated from the dispersion curve of the pairing ground state, is analyzed in comparison with the effective mass of the lowermost non-correlated state (m_{np}). Figure 2(c) shows a significant reduction of m_p/m_{np} around $\Delta t = 0.5t_0$. This is due to that in general the correlated hopping interaction enhances the mobility of the carriers, but the effective mass of single holes (m_{np}) becomes extremely large, since their effective hopping ($t = t_0 - 2\Delta t$) is very small in the region around $\Delta t = 0.5t_0$. It should be stressed that, even though the mobility of single holes is almost null in this region, the pair has a considerable mobility, which is proportional to the correlated hopping interaction (Δt) [15].

The hole–singlet ground-state diagrams for a linear chain, a square, a triangular and a simple cubic lattice are shown in Figs 3(a), 3(b), 3(c) and 3(d), respectively, for

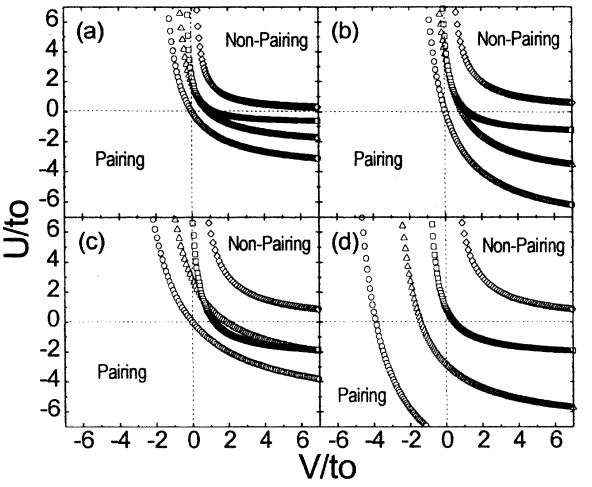

Fig. 3. Phase diagrams of hole-singlets on (a) a linear chain, (b) a square, (c) a triangular and (d) a simple cubic lattice, where the values of Δt are 0 (open circles), $0.2t_0$ (open triangles), $0.5t_0$ (open diamonds) and $0.6t_0$ (open squares).

$\Delta t = 0$ (open circles), $0.2t_0$ (open triangles), $0.5t_0$ (open diamonds) and $0.6t_0$ (open squares). First, observe the hyperbolic transition lines for $\Delta t = 0.5t_0$, which means that there is hole–singlet pairing even though U or V is very large, as shown in equations (3) and (4). Also, notice that the pairing region is increased when Δt goes from 0 to $0.5t_0$. However, an inverse process occurs when Δt is larger than $0.5t_0$, in agreement with Fig. 2(a). Finally, it can be seen that the transition lines for $\Delta t = 0$ (open circles) in one- and two-dimensional systems pass through the origin, in contrast to a smaller pairing region in the three-dimensional case, i.e. the low-dimensionality of the system in general enhances the pairing process. This is because the localization of the correlated states in the equivalent one-particle higher-dimensional space increases the kinetic energy of the system, known as the quantum confinement effect and then the existence of pairing states implies that the potential energies due to ''impurities'' must overcome the discussed increase of kinetic one. In this energy competition, the dimensionality of the system plays a crucial role [16].

4. CONCLUSIONS

We have studied the pairing problem between holes within the generalized Hubbard model, by extending the previously introduced mapping method to include the correlated hopping interactions, which appear as additional ''impurity bonds'' in the one-particle higher-dimensional space. This method has the advantage of giving a clear association between the binding and the impurity states. Also, the method provides an alternative and in some cases easier way to calculate real-space pairing properties, such as the coherence length. The results show a strong enhancement of the hole–singlet binding energy around $\Delta t = 0.5t_0$, instead of $\Delta t > 2t_0$ for electrons, which could be relevant since in real materials $\Delta t \ll U$. Also, a significant reduction of the effective mass of pairs in comparison with non-pairing ones is observed in this region, which could help the Bose–Einstein condensation of these hole singlets. Finally, the phase diagrams show a favored hole pairing in low-dimensional systems. This fact would not necessarily imply a higher superconducting transition temperature, since the superconductivity involves both the pairing and condensation processes and there is no Bose–Einstein condensation in *strict* two-dimensional systems at finite temperatures [21]. However, a ''local condensation'', i.e. phase coherence persists over a finite distance, could presumably become global when a small amount of interplane coupling is turned on [22].

Acknowledgements—This work was supported partially by CONACyT-25455E, DGAPA-IN101797 and UNAM-CRAY-SC008697. L.A.P. acknowledges the UNAM Ph.D. scholarship. Computations have been performed at the Cray Y-MP4/432 of DGSCA, UNAM.

REFERENCES

1. Wollman, D.A., Van Harlingen, D.J., Lee, W.C., Ginsberg, D.M. and Leggett, A.J., *Phys. Rev. Lett*., **71,** 1993, 2134; Tsuei, C.C. *et al*., *Phys. Rev. Lett*., **73,** 1994, 593.
2. Dagotto, E., *Rev. Mod. Phys.*, **66,** 1994, 763.
3. Micnas, R., Ranninger, J. and Robaszkiewicz, S., *Rev. Mod. Phys.*, **62,** 1990, 113.
4. Ando, Y., Boebinger, G.S., Passner, A., Wang, N.L., Geibel, C. and Steglich, F., *Phys. Rev. Lett.*, **77,** 1996, 2065.
5. Julien, M.-H., Carretta, P., Horvatic, M., Berthier, C., Berthier, Y., Segrasan, P., Carrington, A. and Colson, D., *Phys. Rev. Lett.*, **76,** 1996, 4238.
6. Emery, V.J., Kivelson, S.A. and Zachar, O., *Physica C*, **282–287,** 1997, 174.
7. Uemura, Y.J. *et al*., *Nature*, **364,** 1993, 605.
8. Hubbard, J., *Proc. R. Soc. London Ser*., **A276,** 1963, 238.
9. Lieb, E.H. and Wu, F.Y., *Phys. Rev. Lett.*, **20,** 1968, 1445.
10. Metzner, W. and Vollhardt, D., *Phys. Rev. Lett.*, **62,** 1989, 324.
11. Marsiglio, F. and Hirsch, J.E., *Physica C*, **171,** 1990, 554.
12. Navarro, O. and Wang, C., *Solid State Commun.*, **83,** 1992, 473.
13. Hirsch, J.E., *Phys. Rev.*, **B48,** 1993, 3327.
14. Schuttler, H.-B. and Fedro, A.J., *Phys. Rev.*, **B45,** 1992, 7588.

15. Hirsch, J.E., *Physica C*, **179,** 1991, 317.
16. Economou, E.N., *Green's Functions in Quantum Physics*, p. 112. Springer-Verlag, Berlin, 1983.
17. Hirsch, J.E. and Marsiglio, F., *Phys. Rev.*, **B39,** 1989, 11515.
18. Bardeen, J., Cooper, L.N. and Schrieffer, J.R., *Phys. Rev.*, **108,** 1957, 1175.
19. Hirsch, J.E. and Marsiglio, F., *Phys. Rev.*, **B45,** 1992, 4807.
20. Pathria, R.K., *Statistical Mechanics*, p. 180. Pergamon Press, London, 1972.
21. Hohenberg, P.C., *Phys. Rev.*, **158,** 1967, 383.
22. Huang, K., in *Bose–Einstein Condensation* (Edited by A. Griffin, D.W. Snoke and S. Stringari), p. 35. Cambridge University Press, 1995.