Nonperturbative results for attractive Hubbard pairings in triangular lattices

L. A. Pérez, O. Navarro, and C. Wang
Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510, Distrito Federal, Mexico

(Received 2 November 1995; revised manuscript received 9 February 1996)

The electron pairing problem is studied by means of the extended Hubbard Hamiltonian. The original many-body problem is mapped onto a tight-binding one in a higher dimensional space, where the problem can be solved in an exact way. In a triangular lattice, the effects of the frustration of antibonding states on the electronic correlation are analyzed in detail. It is found that the hole pairing is always stronger than the electron case, in contrast with the bipartite lattices, where there is a complete symmetry between electron and hole pairings. The ground state of two holes, when the attractive nearest-neighbor interaction is dominant, is surprisingly triplet and its wave function has directional nodes. A pairing phase diagram for holes in triangular lattices is also presented. [S0163-1829(96)08124-6]

It has been almost ten years since the discovery of high-T_c cuprate superconductors.[1] Although some important aspects of the physical origin of their superconductivity remain controversial, a set of characteristic features has been established. It has been found that pairing exists, between holes rather than electrons, and that superconductivity occurs at low carrier concentration with a short coherence length.

Theoretical models which consider the local interactions seem appropriate to describe the short-range electron or hole pairings. The Hubbard model is one of the simplest and general models expressed in terms of local interactions and it is used to study the many-body aspects of electronic properties in solids. Recently, the Hubbard model has been the subject of renewed interest due to the fact that it contains the basic ingredients to investigate the narrow-band electronic correlation and the dynamics of electron pairs, which are believed to be relevant for explaining not only unconventional types of superconductivity but also unusual normal-state properties.[2]

The single-band extended Hubbard Hamiltonian (EHH) can be written as

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

where $\langle i,j\rangle$ denotes nearest-neighbor sites, $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma=\downarrow$ or $\uparrow$ at site i, and $n_i=n_{i,\uparrow}+n_{i,\downarrow}$ being $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$. It is important to mention that in principle U and V are positive because they are direct Coulomb integrals. However, U and V could be negative if attractive indirect interactions through phonons or other bosonic excitations are included and they are stronger than the direct Coulomb repulsion.

When a particle-hole transformation[3] is made in the EHH, $c^{\dagger}_{i,\sigma}\rightarrow h_{i,\sigma}$, the Hamiltonian becomes

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

where N is the total number of sites, Z is the lattice coordination number, $h^{\dagger}_{i,\sigma}$ ($h_{i,\sigma}$) is the hole creation (annihilation) operator, and $n^{h}_{i}=n^{h}_{i,\uparrow}+n^{h}_{i,\downarrow}$ with $n^{h}_{i,\sigma}=h^{\dagger}_{i,\sigma}h_{i,\sigma}$. The first term in Eq. (2) only contributes to a shift in the total energy, and so holes also interact via a Hubbard model. However, there are two crucial differences between the electron and hole cases: the density of holes is $1-n$ in terms of the electron density (n) and the signs of the hopping parameter are opposite, which is irrelevant for the band structure of a bipartite lattice.

The effects of lattice symmetry on electronic correlation is an interesting and not very widely studied subject. There are peculiar behaviors of electronic instabilities on nonbipartite lattices. For instance, a strong-coupling analysis on triangular lattices indicates that the charge density wave state cannot be formed for any band filling due to frustration.[4] In particular, the two-particle problem is the simplest case in which electronic correlation can be analyzed in a nonperturbative way. Historically, the problem has been extensively studied in bipartite lattices.[5] In this paper, pairings between electrons and between holes in a triangular lattice are analyzed. The analysis is done following a mapping method previously reported[6] and its extension to triangular lattices is given in Ref. 7.

For the case of two spin-half particles, the total spin could be one (spin triplet) or zero (spin singlet). In the latter case, the spatial part of the wave function is symmetrical under interchange of the particles because the spin part is antisymmetrical. In the former, the spatial wave function is antisymmetrical, which is equivalent to being antisymmetrical under reflection through the central site (with self-energy U) on the mapped network of states [e.g., see Fig. 1(b)]. It is worth mentioning that spin-triplet pairing is independent of the on-site interaction U since the amplitude of the wave function is always null at the center impurity. Finally, it is important to remember that the noninteracting hole ground state is doubly degenerate. Its wave functions are shown in Fig. 1, where the amplitudes a and b are determined by the normalization condition and they are related by $b=\sqrt{3}a$. Notice that the wave functions in Figs. 1(a) and 1(b) have totally different spatial

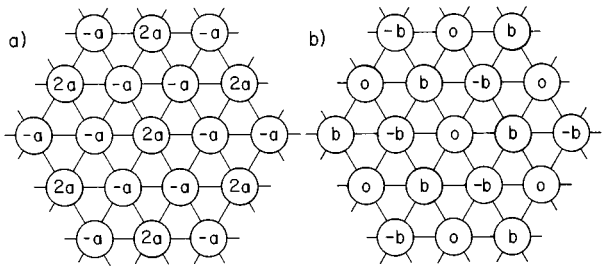

FIG. 1. Doubly degenerate noninteracting ground states for holes in triangular lattices: (a) spatially symmetrical and (b) antisymmetrical wave functions.

symmetry, the former being symmetrical under the interchange of particles and the latter being antisymmetrical. It can also be observed that the wave function in Fig. 1(b) is not isotropic and it has nodes along several directions.

In order to analyze the pairing state we look at the binding energy (Δ) and the coherence length (ξ) for both electron and hole cases. The essential difference between these two cases is that the sign of the hopping parameter t in the EHH, has been taken to be equal to -1 for electrons and $+1$ for holes. The numerical diagonalizations in the mapped lattice were performed on a truncated triangular lattice of 2269 effective states. The matrix sizes for numerical diagonalization were chosen as the minimum size so that the physical quantities have no important variation with matrix size.

The binding energy has been calculated from the difference of energies between the lowermost pairing state (zero center-of-mass linear momentum) and the original lower band edge when there is no electron-electron interaction. The coherence length is defined[8] as $\xi=\langle \mathbf{R}^2\rangle^{1/2}$, where

$$\langle \mathbf{R}^2\rangle = \frac{\sum_R \psi^*(\mathbf{R})\mathbf{R}^2\psi(\mathbf{R})}{\sum_R \psi^*(\mathbf{R})\psi(\mathbf{R})} \tag{3}$$

is the mean-square radius of a pair and $\psi(\mathbf{R})$ is the amplitude of the pair wave function when the vector of internal coordinates of the pair is $\mathbf{R}$. In fact, ξ would be reduced to the usual BCS coherence length by introducing a numerical factor of $2\sqrt{2}/\pi$.[8]

In Figs. 2(a) and 2(b), the binding energy and the coherence length as functions of U (for $V=0$) for singlets of electrons and of holes in a triangular lattice are compared with those in a linear chain and in a square lattice. Notice first that, for a given U, the binding energy between electrons increases as the coordination number (Z) is reduced because the kinetic energy is proportional to Z. In general, $\Delta \approx U-2Zt$ for a very strong interaction regime, when frustration is absent. For triangular lattices, it is noted that the pairing strength between holes is always stronger than the electron case. This asymmetry is caused by the frustration of antibonding states. In fact, the enlarged binding energy between holes could be understood by considering its behavior in the strong interaction regime where the pairing-state energy for both electrons and holes goes like U while the noninteracting lower band edge is reduced for holes due to the

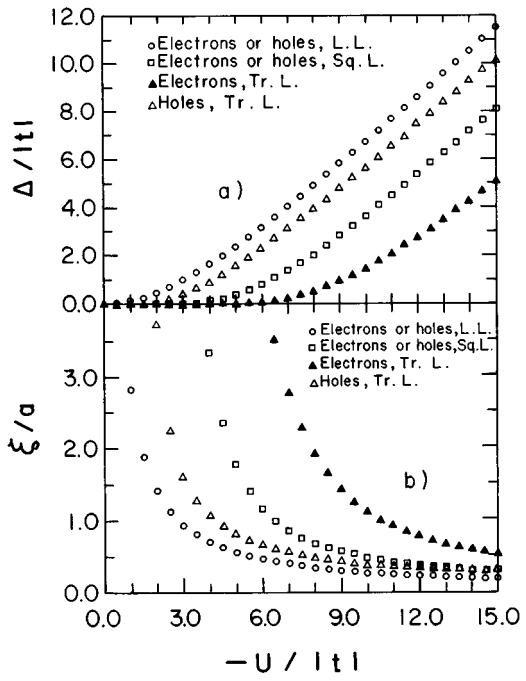

FIG. 2. Binding energy (Δ) and coherence length (ξ) vs $U/|t|$, being $V=0$, for singlets of holes and of electrons in a linear chain (L.L.), a square lattice (Sq.L.), and a triangular one (Tr.L.).

frustration, therefore enhancing the hole binding energy. For the other extreme of interactions, this asymmetry is also expected since it is well known in both BCS theory[9] and in the single impurity in the tight-binding scheme[10] that $\Delta \approx C\exp[-1/(|U|\rho_d)]$ for small U, where C is a positive constant and ρ_d is the density of states at the band edge. Therefore the binding energy Δ is larger for holes, since the ρ_d for holes is larger than that of the electrons due to frustration. Finally we mention that in Fig. 2(a) an exponential increase of Δ as a function of U is observed in the weak interaction regime.

In Figs. 3 and 4 the binding energy and the coherence length versus V (for $U=0$) are shown for singlets and triplets, respectively. Notice that in triangular lattices the pairing asymmetry between holes and electrons is still present for nearest-neighbor interactions, being stronger for hole pairing. Furthermore, the hole-singlet ground state has a two-dimensional behavior in the weak interaction regime and a linear chain behavior in the other extreme. This change of behavior is due to a change of the nature of the ground state, i.e., in the weak interaction regime the ground state has a wave function like that shown in Fig. 1(a) and a new one containing a node at the central site (self-energy U in Fig. 1 of Ref. 7) for strong interactions. This singlet wave function containing a central node becomes the ground state since the appearance of the central node increases the amplitudes significantly at its first neighbors when the interaction V is strong enough. Therefore, the linear-chain behavior of the binding energy is mainly due to the ring-like localization of the wave function in the space of states.

On the other hand, it can be observed in Fig. 4 that the hole triplets in triangular lattices have a very large binding energy, even larger than the linear-chain case and hole-singlet case (see Fig. 3). In order to analyze the nature of

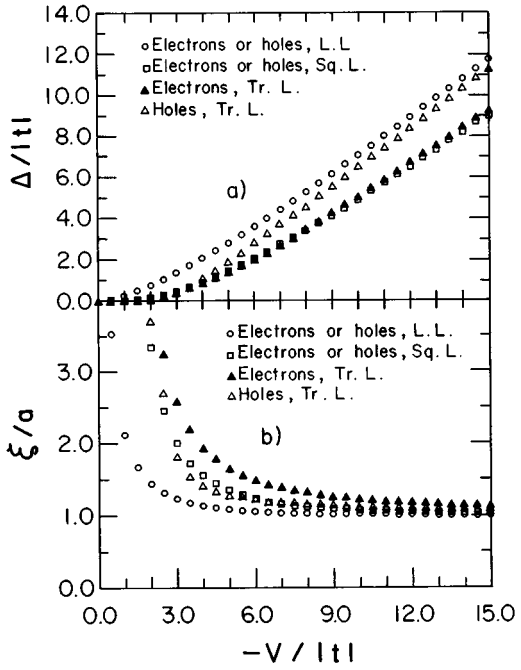

FIG. 3. Binding energy (Δ) and coherence length (ξ) vs $V/|t|$, being $U=0$, for the same systems of Fig. 2.

hole pairing, a pairing phase diagram of the two-hole ground state for all interaction regimes is shown in Fig. 5. We can see that the hole pairs are singlets when U is dominant, while they are triplets in the V-dominant region. The transition between singlet and triplet bound states in the strong interaction regime can be obtained analytically by evaluating the ground-state energies corresponding to both spatially symmetric and antisymmetric wave functions, which are similar

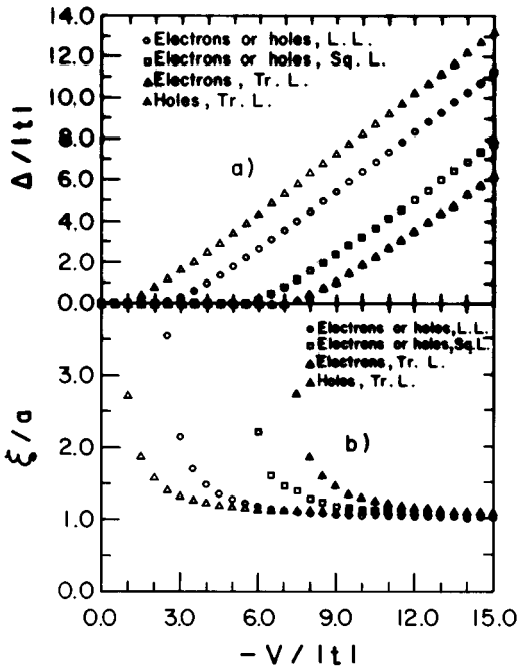

FIG. 4. Plots of (a) the binding energy (Δ) and (b) coherence length (ξ) vs $V/|t|$, being $U=0$, for triplets of holes and electrons in the same lattices as Fig. 2.

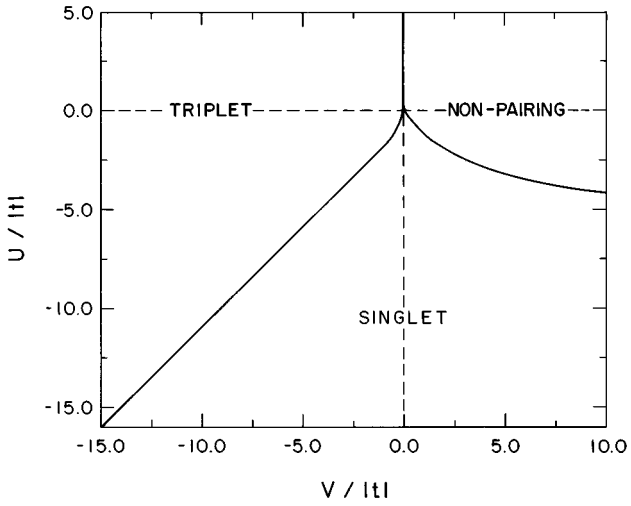

FIG. 5. Pairing phase diagram showing the nature of the two-hole ground state in a triangular lattice. There are three sorts of ground states, nonpairing, singlets, and triplets, depending on the regime of interactions.

to those shown in Fig. 1, except that the amplitudes of the wave functions decay rapidly with **R**, i.e., only the states with self-energies U and V (see Fig. 1 of Ref. 7) have amplitudes significantly different from zero. Hence, it is assumed that in the strong interacting limit the ground-state wave function for singlets ($|s\rangle$) has an amplitude C at the central site, A at its nearest neighbors, and zero at the other sites. Likewise, the triplet wave function ($|a\rangle$) has zero amplitude at all sites except at the mentioned nearest neighbors where alternating amplitudes B and $-B$ along the nearest-neighbor ring are found.

The ground-state energy for both symmetric and antisymmetric cases are given by $E_s=\langle s|H|s\rangle=UC^2+6VA^2+24tAC+24tA^2$ and $E_a=\langle a|H|a\rangle=6VB^2-24tB^2$, respectively. The normalization condition gives $C=\pm\sqrt{1-6A^2}$ and $B^2=\frac{1}{6}$. Therefore, at the singlet-triplet phase transition ($E_s=E_a$) we have $-U+V-4t-6A^2(V-U+4t)\pm 24tA\sqrt{1-6A^2}=0$. The condition to obtain a solution for A in real space is $U=V-t$. This result is in very good agreement with the numerical results shown in Fig. 5. Finally, the transition between triplet and nonpairing states occurs exactly at $V=0$ because there is no influence of U on the triplet formation.

In summary, we have studied the pairing problem between electrons and between holes in a triangular lattice by means of an attractive Hubbard Hamiltonian. The original many-body problem has been mapped onto an equivalent impurity tight-binding one. The pairing behavior in triangular lattices has been investigated by analyzing the binding energy, the coherence length, and the phase diagram for the ground state. It is observed that the pairing strength of holes is always stronger than the electron case, due to the frustration of antibonding states. It means that a simple geometrical modification could enhance the hole-pairing process. Furthermore, in a wide region where attractive nearest-neighbor interaction is dominant, hole ground states are triplets, instead of singlets. Although no triplet superconductivity has been observed until recently, triplet fermion pairing is well

known. For instance, the superfluid state of ^3He[11] where the fermionic ^3He atoms form p-wave spin-triplet pairs.

Another interesting result is that the triplet ground state has directional nodes, i.e., the corresponding wave function of pairs has a null amplitude along several directions. This result could be important since the observation of d-wave pairing symmetry has been reported recently,[12] where directional nodes or a phase shift of π predicted by the $d_{x^2-y^2}$ pairing state is found. It is important to stress that in spite of the similitude between the triplet hole ground state in triangular lattices and d-wave pairing symmetry observed in cuprate superconductors they have essential differences. First, the hole ground state pairing in cuprate superconductors is a spin-singlet instead of a spin-triplet found in the present work. Furthermore, the number of directional nodes is three for the triangular-lattice case and two for the $d_{x^2-y^2}$ pairing state since the value of the center-of-mass angular momentum must be even for singlets and odd for triplets. Finally, the appearance of the directional nodes in the triangular lattice is caused by the triplet pairing and the frustration of antibonding states, while the origin of d-wave superconductivity is not completely clear yet.

The present work could be extended to analyze systems containing more than two particles. The effects of the frustration of antibonding states on the pairing asymmetry between electrons and between holes could be also investigated on other lattices, for example, the face-centered-cubic lattice. Moreover, since the mapping method is a completely real space procedure, it allows us to analyze disordered lattices, where the localization of the wave function could be essential in the pairing process. These studies are currently in progress.

This work was partially supported by the DGAPA-UNAM (Grant No. IN-104595) and the CONACyT of Mexico (Grant No. 0205P-E). Numerical calculations were performed at the Cray Y-MP4/432 of DGSCA-UNAM (Project No. SC-005096).

[1] J.G. Bednorz and K.A. Müller, Z. Phys. B **64**, 189 (1986).
[2] R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).
[3] M.W. Long, in *The Hubbard Model (Recent Results)*, edited by M. Rasetti (World Scientific, Singapore, 1991), p. 1.
[4] R.R. dos Santos, Phys. Rev. B **48**, 3976 (1993).
[5] D.C. Mattis, Rev. Mod. Phys. **58**, 361 (1986); L. Chen and C. Mei, Phys. Rev. B **39**, 9006 (1989); M. Fabrizio, A. Parola, and E. Tosatti, *ibid.* **44**, 1033 (1991).
[6] O. Navarro and C. Wang, Solid State Commun. **83**, 473 (1992).
[7] O. Navarro, L.A. Pérez, and C. Wang, Physica C **235-240**, 2167 (1994).
[8] J.E. Hirsch and F. Marsiglio, Phys. Rev. B **39**, 11 515 (1989).
[9] J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[10] E.N. Economou, *Green's Functions in Quantum Physics* (Springer-Verlag, Berlin, 1983), p. 110.
[11] P. Schiffer and D.D. Osheroff, Rev. Mod. Phys. **67**, 491 (1995).
[12] D.A. Wollman *et al.*, Phys. Rev. Lett. **71**, 2134 (1993); C.C. Tsuei *et al.*, *ibid.* **73**, 593 (1994).