Eur. Phys. J. B **36**, 519–523 (2003)
DOI: 10.1140/epjb/e2004-00007-3

THE EUROPEAN PHYSICAL JOURNAL B

Anisotropic pairing with repulsive interactions in a model with different orbitals per site

F. Guinea[a]

Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain

Received 6 October 2003 / Received in final form 1st December 2003
Published online 30 January 2004 –

Abstract. An extension of the Hubbard model, with two orbitals of different symmetry per site is studied. When the two orbitals are hybridized by crystal field effects, the BCS approximation shows that the model has an instability towards anisotropic superconductivity. The competition between superconductivity and antiferromagnetism, and the relevance of other pairing mechanisms, like the Kohn-Luttinger instability, are also analyzed.

PACS. 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 74.20.Mn Nonconventional mechanisms

1 Introduction

The emergence of superconductivity in systems of strongly correlated electrons with only repulsive interactions is a subject of extensive study. It was established, using the formulation of the BCS theory, but computing higher orders in the screened repulsive interaction, that the metallic state is unstable towards anisotropic superconductivity, due to the angular dependence of the dielectric constant [1]. This Kohn-Luttinger instability is greatly enhanced when the Fermi surface in anisotropic [2–4]. By using RPA or model dielectric functions, it can also be shown that isotropic Fermi surfaces can give rise to anisotropic superconductivity [5]. Nowadays, there is ample numerical evidence suggests that models with purely repulsive interactions can lead to anisotropic superconductivity [6–9].

An alternative scheme which leads to a superconducting ground state starting from models with repulsive interactions was proposed in [10,11]. This model includes an assisted hopping term which is a natural extension of the Hubbard model when many non degenerate orbitals per ion are considered. The consideration of a single orbital per site in the Hubbard model is justified when the energies of other ionic states are much higher than the conduction electron bandwidth, determined by the intersite hopping, and the onsite Coulomb repulsion. General arguments, however, show that the typical intraionic level spacing and the Coulomb repulsion are usually of the same order of magnitude [10,11]. This assisted hopping term strongly favors the existence of a superconducting ground state [10–12]. In its standard version, this model leads to isotropic superconductivity for small hole concentrations, and for a moderate value of the onsite repulsion. The superconducting gap is finite throughout the entire Fermi surface, although with a strong energy dependence.

We study in this work a simple variation of the Hubbard model, which includes: i) Two non degenerate orbitals of different symmetries per ion, ii) an intraionic repulsion term, and, iii) an anisotropic distortion of the crystal lattice, which leads to a weak hybridization of the two ionic orbitals. In order to simplify the analysis, we assume that the energy difference between the two ionic levels is the largest parameter in the problem. If this parameter is strictly taken to be infinity, the model reduces to the standard Hubbard model. Although the main features of the model have been inspired by the phenomenology of the cuprate superconductors, the model has been simplified on purpose, so that the calculations can be carried out analytically.

Following general arguments [10,11], we show that the consideration of a second orbital leads naturally to assisted hopping terms in an effective low energy Hamiltonian. The main difference with previous work is that the induced superconductivity is anisotropic, and the gap presents nodes at the Fermi surface. The existence of anisotropic pairing, moreover, implies that superconductivity exists for arbitrary on site Hubbard repulsion, and doping levels, at least within the BCS theory. Using the similitude to the standard Hubbard model, we argue that the only alternative phase antiferromagnetism. Then, we analyze the competition between superconductivity and antiferromagnetism, which prevails near half filling.

The next section presents the model, Then, we analyze the main features of the superconducting solution, within BCS theory. Section 4 discusses the phase diagram of the model. Some concluding remarks, highlighting the most general properties of the model are discussed in Section 5.

[a] e-mail: paco.guinea@icmm.csic.es

2 The model

We assume a crystal with one atom per unit cell, in a two dimensional square (tetragonal) lattice with a weak distortion, which destroys the equivalence of the two main axes. It will be clear form the discussion, however, that the main features of the calculated superconducting phase can be easily generalized to similar situations. We assume that this distortion is small, and we will treat its effects as a perturbation. Using the tetragonal symmetry of the undistorted lattice, we take the lowest lying orbital to be $d_{x^2-y^2}$, and the second orbital to be s or $d_{3z^2-r^2}$. In the following, we will denote these two orbitals s and d. We define $\Delta = \epsilon_s - \epsilon_d$ as the difference between the energy of these levels. Without loss of generality, we set $\epsilon_d = 0$. For simplicity, we assume that there is only repulsion between electrons in the more localized d orbital, U, although the calculations can be easily extended to other types of on site interactions. Hopping can take place only between nearest neighbors, with amplitudes t_{ss}, t_{sd} and t_{dd}. Finally, the orthorhombic distortion implies that the crystal field can induce an hybridization between the s and d in the same site, V_{CF}, which is forbidden in an orthogonal lattice. The Hamiltonian is:

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_{ion} + \mathcal{H}_{tunn} \\
\mathcal{H}_{ion} &= \sum_{\sigma i} \Delta c^\dagger_{s\sigma i} c_{s\sigma i} + U n_{d\uparrow i} n_{d\downarrow i} \\
&\quad + \sum_{\sigma i} V_{CF} c^\dagger_{s\sigma i} c_{d\sigma i} + \text{h.c.} \\
\mathcal{H}_{tunn} &= \sum_{ij\sigma} t_{dd} c^\dagger_{d\sigma i} c_{d\sigma j} + t_{ss} c^\dagger_{s\sigma i} c_{s\sigma j} \\
&\quad \pm t_{sd} c^\dagger_{s\sigma i} c_{d\sigma j} + \text{h.c.}
\end{aligned} \tag{1}$$

We emphasize that this is a very simple extension of the one band Hubbard model. We expect, however, that the qualitative features of this solution can be generalized to more complex models.

We are neglecting in equation (1) possible differences between the hoppings in the two directions due to the asymmetry of the lattice [19], which is included through the crystal field potential V_{CF} only. Note that, due to the different symmetries of the two orbitals, the hopping between an s and a d orbital has opposite sign along the two axes of the lattice (see Fig. 1). As discussed in the following, this change of sign is crucial in stabilizing d-wave superconductivity. In many metallic oxides the bandwidth, determined by the hoppings which we take to be of similar order of magnitude, as there is no simple argument to estimate their relative strength, $|t_{dd}| \sim |t_{sd}|$. We assume that the bandwidth is comparable to the Coulomb repulsion U, and to the spacing between the atomic levels Δ. The crystal field splitting introduced here arises from the existence of an orthorhombic distortion, and it can show large variations in similar compounds.

In order to make possible an analytical treatment, we assume that $V_{CF} \ll U, |t_{ss}|, |t_{sd}|, |t_{dd}| \ll \Delta$. As mentioned above, there is no a priori justification for this inequality.

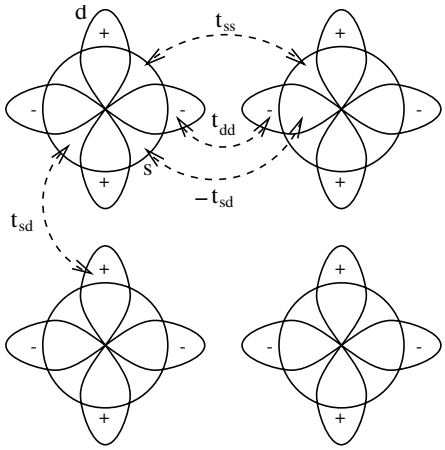

Fig. 1. Sketch of the hopping terms between the two orbitals in the unit cell.

Note, however, that a large separation between ionic levels is an assumption required in order to derive any single band model. In particular, the standard Hubbard model can be obtained in the limit $\Delta \to \infty$. In this regime, the effects due to the second atomic orbital can be neglected. In the following, we will use Δ^{-1} as an expansion parameter, so that we analyze small deviations from the Hubbard model.

The lowest lying eigenstates of the single ion Hamiltonian, $\mathcal{H}_{ion}$, for zero electrons, one electron with spin σ, and double occupancy, can be approximated as:

$$\begin{aligned}
|0\rangle &= |0\rangle \\
|1\rangle_\sigma &\approx \left(c^\dagger_{d\sigma} + \frac{V_{CF}}{\Delta} c^\dagger_{s\sigma} \right) |0\rangle \\
|2\rangle &\approx c^\dagger_{d\uparrow} c^\dagger_{d\downarrow} |0\rangle + \frac{V_{CF}}{\Delta - U} \left(c^\dagger_{d\uparrow} c^\dagger_{s\downarrow} + c^\dagger_{s\uparrow} c^\dagger_{d\downarrow} \right) |0\rangle
\end{aligned} \tag{2}$$

with energies:

$$\begin{aligned}
E_0 &= 0 \\
E_1 &\approx -\frac{V_{CF}^2}{\Delta} \\
E_2 &\approx U - 2\frac{V_{CF}^2}{(\Delta - U)}.
\end{aligned} \tag{3}$$

Other ionic states lie at higher energies, the energy difference being of order Δ. In the limit $\Delta \to \infty$, we can truncate the number of possible electronic states to those described in equation (2). The Hilbert space of the model is equivalent to that of a system with a single orbital per site, whose occupancy can be zero, one, or two. Hence, this truncation defines a single band system, as in the standard Hubbard model.

We can define an effective Hamiltonian using this restricted basis, and neglect the matrix elements which involve other states at higher energies, $\sim \Delta$. The only terms which remain are a site diagonal contribution which gives the renormalized one particle level, an effective hopping term, and a renormalized on site repulsion. The hopping

term, however, depends on the occupancy of the sites involved in the process. States with different number of electrons are described by different combinations of $|s\rangle$ and $|d\rangle$ orbitals (see Eq. (2)), so that the associated hoppings involve different contributions from t_{dd} and t_{ss}. After some algebra, using equations (1) and (2), we obtain:

$$\begin{aligned}
\langle 0_i|\langle 1_{\sigma j}|\mathcal{H}_{tunn}|1_{\sigma i}\rangle|0_j\rangle &\approx t_{dd} \pm 2t_{sd}\frac{V_{CF}}{\Delta} \\
\langle 1_{\uparrow i}|\langle 1_{\downarrow j}|\mathcal{H}_{tunn}|2_i\rangle|0_j\rangle &\approx t_{dd} \pm t_{sd}\left(\frac{V_{CF}}{\Delta}+\frac{V_{CF}}{\Delta-U}\right) \\
\langle 1_{\sigma i}|\langle 2_j|\mathcal{H}_{tunn}||2_i\rangle 1_{\sigma j}\rangle &\approx t_{dd} \pm 2t_{sd}\frac{V_{CF}}{\Delta-U}. \qquad (4)
\end{aligned}$$

These matrix elements define the new hoppings. They include a correction to the initial value of t_{dd}, due to transitions involving intermediate states. In these processes, an electron in a given d orbital jumps into a virtual state in where in the s orbital of a neighboring site with amplitude proportional to t_{sd}, and then moves to the low energy d orbital at that site via the hybridization provided by the crystal field splitting, V_{CF}. The energy difference associated to this virtual process is either Δ or $\Delta - U$, depending on the occupancy of the d orbital not involved in the hopping. Hence, the generated hopping is proportional to $t_{sd}V_{CF}$, and it depends on the occupancy of the sites. As the sign of t_{ds} is different along the two axes of the lattice, these corrections also are of opposite sign along the axes. The final effective Hamiltonian can be written as:

$$\begin{aligned}
\mathcal{H}_{eff} = &\sum_{\sigma ij} \tilde{t}_{\pm}\tilde{c}^{\dagger}_{\sigma i}\tilde{c}_{\sigma j} \pm \delta t(\tilde{n}_{\sigma i}+\tilde{n}_{\sigma j})\tilde{c}^{\dagger}_{-\sigma i}\tilde{c}_{-\sigma j} + \text{h.c.} \\
&+\sum_i \tilde{U}\tilde{n}_{i\uparrow}\tilde{n}_{j\downarrow} \qquad (5)
\end{aligned}$$

where we have shifted the origin of energies by $-V_{CF}^2/\Delta$, see equation (3). We define in equation (5):

$$\begin{aligned}
\tilde{c}_{\sigma i} &\approx c_{d\sigma i} + \frac{V_{CF}}{\Delta}c_{s\sigma i} \\
\tilde{t}_{\pm} &\approx t_{dd} \pm 2t_{sd}\frac{V_{CF}}{\Delta} \\
\delta\tilde{t} &\approx 2t_{sd}\frac{V_{CF}U}{\Delta^2} \\
\tilde{U} &\approx U - 2\frac{UV_{CF}^2}{\Delta^2}. \qquad (6)
\end{aligned}$$

As mentioned earlier, the effective Hamiltonian, equation (5), reduces to the standard Hubbard Hamiltonian if the value of Δ is taken to be strictly infinity.

Note that, as we are expanding to first order in V_{CF}/Δ, we can neglect normalization terms in the definition of the electron operators $\tilde{c}_{\sigma i}$. For the same reason, $\delta\tilde{t}$ has the same absolute value along the two axes of the lattice. The symmetries of the orbitals involved imply that, to first order, there are no next nearest neighbor assisted hopping terms.

3 Superconducting solution

We now study the properties of the normal state of the effective Hamiltonian, equation (5), in mean field theory. Replacing the operators $\tilde{n}_{\sigma i}$ by their average values, the energy bands of the effective Hamiltonian are:

$$\epsilon_{k_xk_y} = \left(\tilde{t}_+ + \frac{n}{2}\delta\tilde{t}\right)\cos(k_x) + \left(\tilde{t}_- - \frac{n}{2}\delta\tilde{t}\right)\cos(k_y) \qquad (7)$$

where n is the number of electrons in the unit cell.

The Hamiltonian in equation (5) has two terms which describe electron-electron interactions, the onsite repulsion, and the assisted hopping. From them, we can write an interaction term in momentum space [10]:

$$\begin{aligned}
V_{k_xk_yk'_xk'_y} = &\Big\{\tilde{U} \\
&+\delta\tilde{t}\left[\cos(k_x)-\cos(k_y)+\cos(k'_x)-\cos(k'_y)\right]\Big\} \\
&\times \tilde{c}^{\dagger}_{\uparrow k_xk_y}\tilde{c}^{\dagger}_{\downarrow -k_x-k_y}\tilde{c}_{\uparrow k'_xk'_y}\tilde{c}_{\downarrow -k'_x-k'_y}. \qquad (8)
\end{aligned}$$

This pairing interaction allows us to define a self consistent gap equation, within the BCS theory, in the usual way. Because of the explicit dependence of the pairing interaction on k_x and k_y it can easily be shown[10] that, if there is a superconducting gap, $\Delta_{sc\,k_xk_y}$, it must be of the form:

$$\Delta_{sc\,k_xk_y} = a + b\left[\cos(k_x)-\cos(k_y)\right]. \qquad (9)$$

The superconducting gap is specified by the coefficients a and b. Near the transition temperature, the gap equation can be expanded in powers of the gap itself, and one obtains an eigenvalue equation. The parametrization of the gap given in equation (9) implies that this linearized equation near T_c can be written as a linear equation for the coefficients a and b. This equation is [10]:

$$\begin{aligned}
a &= a\Big[\tilde{U}I_0 - \delta\tilde{t}(I_x-I_y)\Big] + b\Big[\tilde{U}(I_x-I_y) \\
&\quad +\delta\tilde{t}(I_{xx}-2I_{xy}+I_{yy})\Big] \\
b &= a\delta\tilde{t}I_0 - b\delta\tilde{t}(I_x-I_y) \qquad (10)
\end{aligned}$$

where:

$$\begin{aligned}
I_0 &= \int_{k_xk_y}^{\epsilon_{k_xk_y}<\epsilon_F} \frac{n(\epsilon_{k_xk_y}/T)}{\epsilon_{k_xk_y}-\epsilon_F} \\
I_x &= \int_{k_xk_y}^{\epsilon_{k_xk_y}<\epsilon_F} \frac{\cos(k_x)n(\epsilon_{k_xk_y}/T)}{\epsilon_{k_xk_y}-\epsilon_F} \\
I_{xx} &= \int_{k_xk_y}^{\epsilon_{k_xk_y}<\epsilon_F} \frac{\cos^2(k_x)n(\epsilon_{k_xk_y}/T)}{\epsilon_{k_xk_y}-\epsilon_F} \qquad (11)
\end{aligned}$$

and similar expressions for I_y, I_{xy} and I_{yy}. The function $n(\omega/T)$ is the Fermi-Dirac distribution, and ϵ_F is the Fermi energy.

From equations (10), the critical temperature is given by:

$$\begin{aligned}
0 = 1 + \tilde{U}I_0 - 2\delta\tilde{t}(I_x-I_y) + \delta\tilde{t}^2\Big[&(I_x-I_y)^2 \\
&-I_0(I_{xx}-2I_{xy}+I_{yy})\Big]. \qquad (12)
\end{aligned}$$

As usual in BCS theory, the integrals in equations (11) diverge as $-\log[(N(\epsilon_F)T]$ at low temperatures, where $N(\epsilon_F) \sim \tilde{t}^{-1}$ is the density of states at the Fermi level, and $\tilde{t} = (\tilde{t}_+ + \tilde{t}_-)/2$. As we are assuming a weak orthorhombic distortion, $I_x \approx I_y$. Hence, the r.h.s. in equation (12) diverges as $-\log^2[N(\epsilon_F)T]$ at low temperatures, and there is always a solution. In the cases considered previously [10], this $\log^2$ divergence in the gap equation is exactly cancelled, due to the different symmetry of the gap. Then, the counterpart of equation (9) has no solution for sufficiently large values of the on site repulsion.

The critical temperature is given, approximately, by:

$$T_c \sim c_1 \tilde{t} e^{-(c_2 \tilde{U})/[N(\epsilon_F)\delta \tilde{t}^2]} \sim c_1' t e^{-(c_2 \Delta^4)/[t^2 N(\epsilon_F) V_{CF}^2 U]} \tag{13}$$

where we assume $t_{dd} \sim t_{sd} \sim t$. The coefficients c_1 and c_2 are numerical constants. The expression in equation (13) implies that the superconductivity is suppressed as $\Delta \to \infty$. It is enhanced by the the lattice asymmetry, described by V_{CF}, and by the existence of a finite U, as the assisted hopping term requires the presence of electron-electron interactions. Near half filling, the van Hove singularity in the density of states implies $T_c \propto t e^{-c\sqrt{\lambda}}$, where $\lambda = \Delta^4/(t V_{CF}^2 U)$ [13–15]. The expression in equation (13) ceases to be valid near the band edges, as $I_{xx} - 2I_{xy} + I_{yy} \to 0$. It can be shown that, in this limit:

$$\lim_{n \to 0} I_{xx} - 2I_{xy} + I_{yy} \propto n \tag{14}$$

where n is the number of carriers per unit cell. Then:

$$\lim_{n \to 0} T_c \sim c_1' t e^{-(c_2 \Delta^4)/[n t V_{CF}^2 U]} \to 0. \tag{15}$$

We can also calculate:

$$\frac{a}{b} \sim \frac{\delta \tilde{t}^3 N^2(\epsilon_F)}{U I_0} \sim \frac{t^3 N^2(\epsilon_F) U^2 V_{CF}^3}{\Delta^6} \tag{16}$$

so that $a/b \to 0$ as Δ becomes the largest energy in the problem. In this limit, the gap, equation (9), will have $d_{x^2-y^2}$ symmetry.

The present calculation does not consider other mechanisms which can lead to a superconducting state. The screened on site repulsion alone suffices to induce superconductivity, by means of the Kohn-Luttinger instability [1]. Hence, it is interesting to compare the value in equation (13) with the critical temperature predicted in this case for the Hubbard model without assisted hopping terms, T_{cKL}. The effective coupling constant arises from the screened interaction, and, to lowest order in U, it goes as $U^2 N(\epsilon_F)$. Hence, $T_{cKL} \sim d_1 t e^{-d_2/(UN(\epsilon_F))^2}$. Thus, within the perturbative approach used here, we find $T_c \gg T_{cKL}$, at least in the weak coupling regime, $UN(\epsilon_F) \ll 1$.

4 Phase diagram

So far, we have only considered the superconducting instability. Near half filling, it is well known that the Hubbard Hamiltonian in a bipartite lattice has nesting properties, and antiferromagnetism is favored. The corresponding Néel temperature is proportional to the antiferromagnetic gap, so that [16]:

$$T_N \sim b_1 t e^{-b_2/\sqrt{UN(\epsilon_F)}}. \tag{17}$$

As mentioned earlier, when $V_{CF} \ll \Delta$, the full Hamiltonian being considered here, equation (1), is reduced to the Hubbard model. Near half filling, the superconducting temperature calculated in the previous section satisfies $T_c \ll T_N$, so that the system will be antiferromagnetic instead of superconducting. As the doping is increased, the Néel temperature is reduced, and the antiferomagnetic phase disappears at densities, measured from half filling, $n^* \sim e^{-b_2/\sqrt{UN(\epsilon_F)}}$. It is likely that phase separation, or some kind of inhomogeneous order may take place at these fillings [17,18]. Alternatively, Hartree-Fock studies of the Hubbard model suggest that an orthorhombic distortion favors the formation of stripes [19]. The analysis presented here does not include the role of quantum fluctuations beyond the mean field approximation. These fluctuations will suppress the antiferromagnetic instability. Higher order terms in $V_{CF}/\Delta, U/\Delta$, not considered here, will break the electron-hole symmetry shown in Figure 2 [10,11], and, in general, they will tend to reduce the region where antiferromagnetism prevails. At densities higher than n^*, the superconducting state discussed in the previous section is most stable low temperature phase. It is interesting to note that the lattice distortion considered here can be due to an intrinsic electronic instability of the Hubbard model in a square lattice [20].

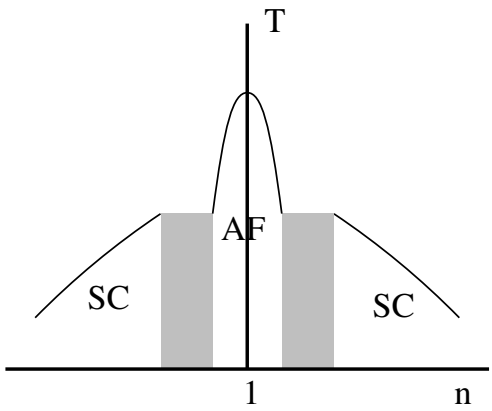

Fig. 2. Sketch of expected phase diagram for the model described by equation (1), see text for details. The present analysis is insufficient to characterize the intermediate regions between the antiferromagnetic and superconducting phases, shown shaded in the figure.

A sketch of the expected phase diagram is shown in Figure 2.

5 Conclusions

We have studied an extension of the standard Hubbard model, which includes, in a simple way, the effect of other atomic levels.

As extensively discussed [10,11], virtual processes which involve these levels induce an effective assisted hopping term (see also [21]). The two atomic levels considered in the present work have different symmetry, and are mixed by crystal field effects. This condition leads to a change in the sign of the assisted hopping term along the two crystallographic axes, which makes the model differ from the previous cases where assisted hopping has been discussed [10,11].

We have avoided the difficulties associated to intermediate coupling situations by restricting the study to a well defined weak coupling case, where the BCS theory is valid (for a similar approach to another problem involving assisted hopping, see [22]).

The main difference between our work and previous studies of Hamiltonians with assisted hopping terms [10–12] is that the assisted hopping interaction is not proportional to the non interacting hopping terms. The assisted hopping interaction gives rise to a separable kernel in the BCS equations, which fixes the form of the possible gap at the Fermi surface. If the assisted hopping is proportional to the hopping, this gap must be uniform at the Fermi surface. A uniform gap is unfavorable in the presence of strong electron-electron interactions, and the superconductivity is suppressed. When the assisted hopping is not proportional to the hopping, the superconducting gap is not uniform at the Fermi surface. Then, solutions with changes of sign become possible, which are stable even in the presence of a significant electron-electron repulsion.

The existence of anisotropic superconductivity, in the case studied here, is related to the induced assisted hopping terms, which, in turn, are determined by the symmetries of the orbitals involved. Thus, the nature of the superconducting phase is directly related to the orbitals which form the bands. In more conventional models, the existence of anisotropic superconductivity is related to the shape of the Fermi surface (which can be highly anisotropic, even if the orbitals involved are isotropic), or to the anisotropies in the screened interaction, like in the Kohn-Luttinger instability.

In the weak coupling regime, the value of the critical temperature arising from the assisted hopping term tends to be larger than that due to the Kohn-Luttinger mechanism. In addition, the BCS equations admit a superconducting phase for arbitrary values of the doping, and, within the limitations of the BCS method, for arbitrary values of the onsite repulsion.

The only low temperature phase which may prevail over the superconducting state considered here is antiferromagnetism near half filling. Thus, a combination of weak coupling techniques give a qualitative understanding of the model for the whole range of dopings. The model analyzed here can be considered as an extension of the ordinary Hubbard model. As, most likely, the dominant instability of the Hubbard model away from half filling is towards d-wave superconductivity, there is no competition with the pairing mechanism considered here. It seems plausible that this enhancement will also take place in the intermediate coupling regime. It would be interesting to check this possibility using techniques valid in this regime.

Finally, the present results can be extended to other systems where assisted hopping terms are likely to arise. In quantum dots, where the sign of these terms can be random [22], they can enhance the tendency towards local pairing.

I am grateful to J.E. Hirsch, for sharing his insights in the nature of assisted hopping effects, and for many other helpful discussions. The hospitality of the Kavli Institute for Theoretical Physics, where this work was done, is gratefully acknowledged. The KITP is supported by NSF through grant PHY99-07949. Additional funding comes from MCyT (Spain) through grant PB96-0875.

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