

NON PERTURBATIVE TREATMENT OF ATTRACTIVE INTERACTIONS IN THE METALLIC LIMIT OF Cu - O HUBBARD HAMILTONIAN.

R. Medina^(1,4), M. Di Stasio⁽²⁾, W. Geertsma⁽³⁾,
U. Maini-Bettolo⁽⁴⁾, L. Pietronero⁽²⁾, and S. J. Scütto^(2,5)

- (1) *Centro de Física, Instituto Venezolano de Investigaciones Científicas, P. O. Box 21827, 1020A Caracas, Venezuela.*
- (2) *Dipartimento di Fisica, Università Degli studi di Roma "La Sapienza", Piazzale Aldo Moro 2, I-00185 Roma, Italy.*
- (3) *Solid State Physics Laboratory, University of Groningen, 9718-EP, Groningen, The Netherlands.*
- (4) *Dipartimento di Fisica, II Università di Roma, Tor Vergata, Via O. Raimondo, 00173 Roma, Italy.*
- (5) *Laboratorio de Física Teórica, Departamento de Física, Universidad Nacional de La Plata, C. C. 67 - 1900 La Plata, Argentina.*

We study, by non perturbative methods, the nature of the attractive interaction via oxygen superexchange in the Cu - O Hubbard-type Hamiltonian. The approach is based on a comparison with an effective Hamiltonian and shows that the attractive interaction can be large and eventually overcome the effective repulsion in the metallic phase.

1.- Introduction and General Discussion.

The aim of this paper is to investigate, by non perturbative methods, the possibility of effective attractive interactions in the Hubbard-type Hamiltonian for the Cu - O plane. Our approach is different than the usual ones in the sense that we will be looking for an attractive interaction in limits in which the Hubbard problem corresponds to non magnetic *metallic* behaviour. We start with a brief discussion of the Hamiltonian, the usual approach and our new method.

The Hubbard-type Hamiltonian for the Cu - O plane is

$$H = E_d \sum_{i,\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} + E_p \sum_{j,\sigma} p_{j,\sigma}^\dagger p_{j,\sigma} + \sum_{\langle i,j \rangle} t_{ij} (p_{i,\sigma}^\dagger d_{i,\sigma} + \text{h.c.}) + U_d \sum_i n_{d,i,\uparrow} n_{d,i,\downarrow} + U_p \sum_j n_{p,j,\uparrow} n_{p,j,\downarrow} \quad (1.1)$$

with usual notations ($t_{ij} = \pm t$ according to symmetry). The states considered correspond to the $(x^2 - y^2)$ d orbital of Copper and one p orbital for each oxygen. As far as the range of parameters, one can gain information from the large amount of studies of materials of this type.⁽¹⁾ Interpreting the Hamiltonian of Eq. (1.1) for the description of holes, these parameters can be estimated to be

$$\begin{aligned} \Delta &= E_p - E_d \simeq 1 \text{ eV} \\ t &\simeq 1 \div 2 \text{ eV} \\ U_d &\simeq 6 \div 8 \text{ eV} \\ U_p &\simeq 2 \div 4 \text{ eV} \end{aligned} \quad (1.2)$$

Sometimes a nearest neighbour Cu - O repulsion is included (U_{pd}). However it is easy to see from microscopic arguments that U_{pd} should be substantially smaller than both on-site repulsions and in general we will neglect it. For simplicity we also neglect the possible direct hopping between oxygens.

(a) *Usual approach.* A standard way to study this Hamiltonian, in order to get an attractive interaction, is by two canonical transformations, as shown in the scheme below⁽²⁾

$$H(\text{Cu} - \text{O}) \longrightarrow H(t_{\text{eff.}}, U_{\text{eff.}}) + \dots \longrightarrow H_{\text{Heisenb.}}(J) + \dots \quad (1.3)$$

This consists in a perturbative scheme in which, in a first step, the oxygen sites are eliminated and an effective single band Hubbard Hamiltonian is derived. Then, in a second step, by taking the limit of large $U_{\text{eff.}}$, one can reduce this to a Heisenberg Hamiltonian whose J can be interpreted as an attraction. One should note that in this procedure, the attractive interaction J is naturally related to an insulating state in view of the large $U_{\text{eff.}}$ limit.

(b) *Present approach.* We intend to focus on the possibility that, contrary to the result of the usual approach, an effective attraction may be present also in the metallic

state. Of course, such an interaction can be derived perturbatively in the limit $t \ll \Delta$. This gives rise to an additional J term (of order t^4/Δ^3) in the effective Hamiltonian. Usually, however, such a term is neglected and the only J considered is the one of the Heisenberg Hamiltonian obtained in the limit $U_{\text{eff.}} \rightarrow \infty$. In addition, we want to go beyond the perturbative point of view (i.e., $t \ll \Delta$) since the correct parameters for this problem (Eq. 1.2) show that $t/\Delta \approx 1$. This calls for an analysis of the terms that have been neglected in the first step of the scheme of Eq. (1.3). The corresponding new scheme is therefore

$$H(\text{Cu} - \text{O}) \longrightarrow H(t_{\text{eff.}}, U_{\text{eff.}}; J) \quad (1.4)$$

If this could be achieved a new possibility could arise; namely one could have a situation in which $t_{\text{eff.}}$ and $U_{\text{eff.}}$ correspond to a metallic state and still have an attractive superexchange-type interaction, J . In such a case, given a suitable combination of $U_{\text{eff.}}$ and J , one could then obtain pairing and superconductivity within a BCS scheme.

In order to study this question we consider a non perturbative mapping of the original problem into an effective Hamiltonian containing explicitly a J term. In practice this can be done in various ways and in this paper we are going to show the first results for various methods.

In sect. 2 we start with the simplest possible search of an attraction based just on the analysis of total energies of small systems.

In sect. 3 instead, we perform a mapping into an effective Hamiltonian by comparison of the spectra. This allows a detailed identification of the various terms.

In sect. 4 we show the results of this mapping for an extended two dimensional system.

In sect. 5 we include some general remarks and conclusions.

2.- Simplest Way to Look for an Attraction.

As a preliminary step, we consider the possibility of a total attraction by comparing the ground state energies of various configurations for small systems. This is similar to what has already been done by various authors.^(3,4) As we shall see, however, this approach presents serious problems. First of all the required condition of total attraction is sufficient but not necessary for pairing. In addition, the extraction of an effective interaction is unreliable in view of various effects like kinetic contributions, boundary and finite size effects.

The idea is to compare the total ground state energies of a small system with different hole occupations. Let us consider, for example, a system of two Cu and one O sites. In the undoped configuration, this system contains two holes with respect to the closed shell state. By doping one generates more holes. The possibility of an

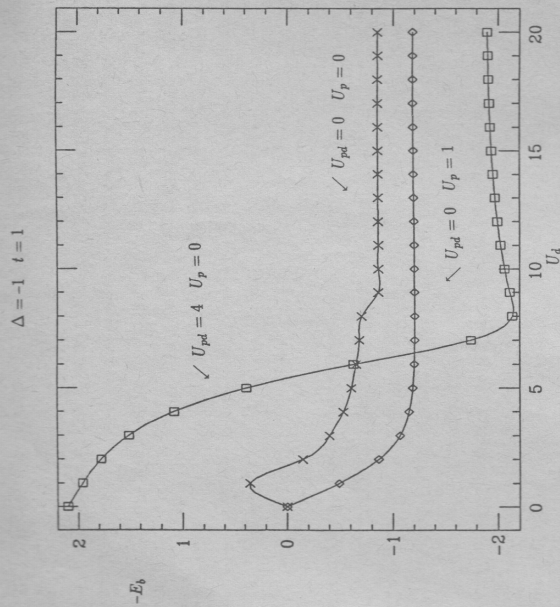


Figure 1: Study of possible attractions between holes by exact diagonalization of a small system. Note that this calculation refers to a fixed electron $\Delta_e = -\Delta + U_d - U_p - 2U_{pd}$.

attraction is studied by considering

$$E_b = E(2 \text{ holes}) + E(4 \text{ holes}) - 2E(3 \text{ holes}) \quad (2.1)$$

where $E(n \text{ holes})$ refers to the ground state energy (including all many-body effects) of the 3 sites system with n holes. In practice we have computed these energies by exact diagonalization. Some results are shown in Fig. 1.

One may notice that if $U_{pd} = 0$ the range of parameters that lead to attraction is very narrow. For $U_{pd} \neq 0$ one gets a broader range of attraction, in agreement with other authors,^(3,4) however a large value for U_{pd} appears to be rather unrealistic.

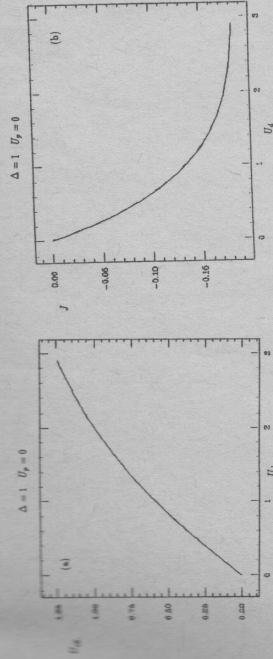


Figure 2: Dependence of U_{eff} (a) and J (b) on U_d for the case $\Delta = 1$, $U_p = 0$.

3.- Effective Hamiltonian Approach.

In view of the limitations of the previous approach we have devised a different strategy. The idea is to identify the various interactions in an effective Hamiltonian. In order to do this in a non perturbative way we compare features of the spectra arising from the exact diagonalization with the analogous features of the following effective Hamiltonian referring only to Cu sites.

$$H_{\text{eff}} = E_0 \sum_{i,\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} - t_{\text{eff}} \sum_{\langle i,j \rangle, \sigma} d_{i,\sigma}^\dagger d_{j,\sigma} + U_{\text{eff}} \sum_i n_{i,\uparrow} n_{i,\downarrow} - J \sum_{\langle i,j \rangle} \left(S_i \cdot S_j - \frac{1}{4} n_i n_j \right) \quad (3.1)$$

In this way the determination of each term is possible and one may have an attractive interaction for singlets (negative J) even if the total effect (E_b) is finally repulsive. It is enough to compare the states with zero, one and two holes. We will present here only some results; the details of this method will be reported elsewhere.⁽⁵⁾ In the limit $t \ll \Delta$ we recover the results of the perturbative approach. By considering instead cases in which the perturbative treatment would break down, like for example $t/\Delta = 1$, we obtain the results shown in Fig. 2 for U_{eff} and J respectively. One may note the appreciable reduction of U_{eff} and the fact that J is negative for any value of U_d and Δ . Of course the present method of elimination of the oxygens is only valid if $\Delta > 0$. If one instead has $\Delta < 0$ the same procedure could be employed for eliminating the Cu sites. It is worthwhile mentioning that $J = 0$ for $U_d = 0$ provides a consistency check of our approach.

We have then considered the effect of U_p as shown in Fig. 3. One can see that in this case J is negative only for large values of U_d .

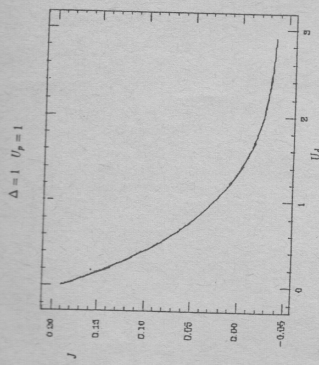


Figure 3: Same as Fig. 2(b) but with $U_p = 1$. The effect of $U_p > 0$ corresponds, approximately, to adding a positive constant term to J .

These results show the possibility of identifying an effective attraction in a non-perturbative scheme. However, whether the same procedure could be applied to the configurations with two, three and four holes (that would correspond to a more than a half filling of the hole band) remains at the moment an open question.

4.- Generalization to Extended Systems.

The approach discussed in the previous section can be generalized to one and two dimensional infinite systems. With respect to the small systems the infinite ones have the advantage of translational symmetry that allows for an analytical treatment.⁽⁶⁾ Here we only report the results for the energy dependent effective interactions of a pair of holes with $q_{cm} = 0$ in an empty lower band. For two dimensions they are:

$$t_{\text{eff.}} = -\frac{t^2}{\Delta - E} \quad (4.1)$$

$$E_0 = -\frac{4t^2}{\Delta - E} \quad (4.2)$$

$$U_{\text{eff.}} = U_d - \frac{2t_{\text{eff.}}}{\Delta - 2E} \left[\frac{U_p(U_d - 2E)}{2\Delta + U_p - 2E} \right] \quad (4.3)$$

$$J = -\frac{t_{\text{eff.}}(U_d - U_{\text{eff.}})}{E_0 + U_{\text{eff.}}/2 - E} \quad (4.4)$$

where E is the energy of each hole. In two dimensions J comes out to be dependent on symmetry. The expression given here is valid for s -waves. The main difference between the exact result for the extended system and the numerical calculation for the small

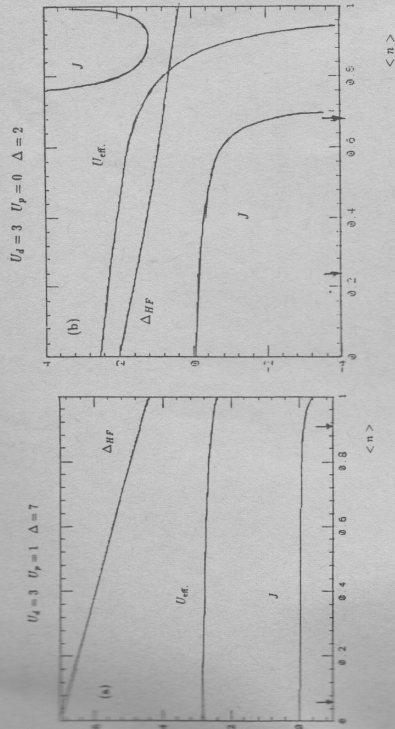


Figure 4: Δ_{HF} , U_{eff} and J vs. $\langle n \rangle$. (a) $\Delta = 7$, $U_p = 1$, $U_d, t = 1$. (b) $\Delta = 2$, $U_p = 0$, $U_d = 3$, $t = 1$. The arrows delimitate the region in which local magnetic moments develop.

system is due to the denominator $E_0 + U_{\text{eff}}/2 - E$ of Eq. (4.4). For particular values of the parameters this resonance can be inside the energy band. In Fig. 4 we show the values of the effective interactions at the Fermi energy for different band fillings calculated within the Hartree-Fock approximation.

For large values of Δ nothing very special happens, J and U_{eff} are more or less constant and the former is small and negative. Therefore the nearest neighbour attraction cannot overcome the on-site repulsion and no pairing is possible. A quite different situation is obtained for smaller values of Δ : The resonance moves inside the band and for proper occupations J becomes large, opening the possibility of s -wave pairing. Note that for $\langle n \rangle \simeq 1$, U_{eff} becomes negative which represents another situation that could lead to superconductivity.

5.- Discussion and Conclusions.

We have presented the first results of a new approach aimed at a non-perturbative determination of the attraction due to superexchange via oxygen in the metallic state. In the usual approach, instead, one obtains a superexchange interaction in the large U limit that is naturally associated to an insulating state. Our results show that such an attractive interaction is indeed present in the metallic state and that in some cases it can become very large and overcome the effective repulsion. The comparison of the analytical calculation for two holes in a band and the analogous numerical results for

a small system shows that this last one provides a good description for the bottom of the band. However, it misses the resonance effect derived in the extended approach that can be responsible for very large attractive interactions. This means that in trying to determine pairing from numerical analysis of finite systems, one should have a large number of energy states and the appropriate filling in order to recover this effect. The limit of the analytical approach is that it is strictly valid for only two holes in a band and that the effect of partial band-filling has been described only within Hartree-Fock approximation. It would be very important therefore to extend the analytical calculation beyond Hartree-Fock and to perform numerical analysis of finite systems with the precautions we have mentioned.

References.

- (1) H. Eskes and G. A. Sawatsky, in print. See also: G. A. Sawatsky, this proceedings.
- (2) S. Robaszkiewicz, R. Micnas and J. Ranninger, *Phys. Rev B* **36**, 180 (1987).
- (3) J. E. Hirsch, S. Tang, E. Loh Jr. and D. J. Scalapino, *Phys. Rev. Lett.* **60**, 1668 (1988).
- (4) C. Balseiro, A. G. Rojo, E. R. Gagliano and B. Alascio, *Solid State Comm.* **64**, 901 (1988).
- (5) R. Medina, U. Marini-Bettolo and S. J. Sciufto, to be published.