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Calculation of the parameters of the extended Hubbard Hamiltonian for superconducting copper oxides

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Abstract. All kinds of parameters U_d , U_p , U_{dp} , E_d , E_p , t_{dp} , t_{pp} and t_{dd} in the extended Hubbard Hamiltonian which describe superconducting copper oxides are calculated directly by an *ab initio* method. The results show that a simple model such as the band structure or extreme (large U , single-band) Hubbard model gives an inadequate description of high T_c compounds. A more complex picture, the extended Hubbard model, may be appropriate. The values of U and t presented by us are in good agreement with the experimental data and comparable with those used by other theorists. The values of the charge transfer energy, however, are very dependent on the hole distribution. Our calculation method provides a way for approaching the relationship between the carrier distribution and the charge transfer energy.

In determining the mechanism of superconductivity in copper oxide compounds, the crucial step would be to understand the electronic properties of these materials. There are many indications pointing to strong electronic correlations in $\text{La}_{2-x}\text{M}_x\text{CuO}_4$ ($\text{M} \equiv \text{Sr}$ or Ba) and $\text{RBa}_2\text{Cu}_3\text{O}_{7-y}$ ($\text{R} \equiv \text{Y}$ or most of the rare earths). This follows from discrepancies between observed photoemission or inverse photoemission data and computed density-of-states curves [1], from the absence of a recognizable core hole x-ray photoemission spectroscopy (XPS) signal due to the $\text{Cu } 3d^8$ configuration in the XPS spectra [2], from satellites in valence band photoemission [3], from antiferromagnetism measurements [4], from direct evidence for holes on oxygen sites [5] and from two hole energies from $\text{Cu } L3VV$ Auger spectra [6].

From an analysis of the experimental data, however, the values of the correlation parameters U and hopping integrals t are very close, but the values for the copper-oxide charge transfer energy parameter Δ vary widely depending on the models used by different authors [7].

However, the numerous theories so far proposed are only valid in a limited range of parameters [7] with different limited ranges of parameters giving an effective Hamiltonian which works well on different areas of the phase diagram (see figure 1 and table 1).

To obtain an effective Hamiltonian that can represent the high T_c superconducting system, we need the correct values for the various parameters. This certainly is a very important problem.

As is well known for a long time it has proved to be very difficult to treat both

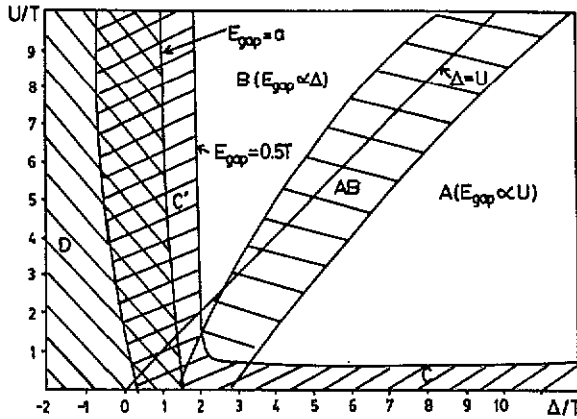


Figure 1. Phase diagram for transition elements: Δ , charge transfer energy $\epsilon_p - \epsilon_d$; U , d-d Coulomb interaction including exchange; T , hybridization interaction; and W , anion valence bandwidth, determined mainly by ligand-ligand hybridization.

correlations and hybridization simultaneously in solid-state physics. The first goal of this article is to calculate the parameters directly using an *ab initio* method, in the spirit of Hubbard's original work [8]. This is only the first simple step towards treating the HTSC as a model for ionic crystals. In this model, ionic wavefunctions are taken as zero-order wavefunctions of every compositive element of the HTSC oxides. As a natural extension of this work modifying this model to include the contribution of hybridization (or covalence, screening, etc) would seem to be the next logical step and this is now in progress.

The relevant physics of HTSC superconductors is believed to be contained in a simple Hamiltonian, the so-called extended Hubbard Hamiltonian, which can be expressed as

$$H_{\text{hole}} = H_{\text{hole}}^{\text{ion}} + H_{\text{hole}}^{\text{hop}} + H_{\text{hole}}^{\text{corr}} \tag{1}$$

Here $H_{\text{hole}}^{\text{ion}}$ includes the hole-on-site energies as

$$H_{\text{hole}}^{\text{ion}} = \sum_l \left[\sum_{p\sigma} E_p p^+ \sigma(l) p \sigma(l) + \sum_{d\sigma} E_d d^+ \sigma(l) d \sigma(l) \right]$$

where l is the unit cell index. $H_{\text{hole}}^{\text{hop}}$ describes the hybridization between the various orbitals and is given by

$$H_{\text{hole}}^{\text{hop}} = \sum_{pp'\sigma} [t_{pp'} p^+ \sigma p' \sigma + \text{HC}] + \sum_{dd'\sigma} [t_{dd'} d^+ \sigma d' \sigma + \text{HC}] + \sum_{pd\sigma} [t_{pd} d^+ \sigma p \sigma + \text{HC}]$$

where the t are hopping integrals. $H_{\text{hole}}^{\text{corr}}$ describes the Coulomb repulsion between the orbitals. *A priori* it only includes the largest terms, so it can be expressed as

$$H_{\text{hole}}^{\text{corr}} = \sum_d U_d n_{d\sigma} n_{d-\sigma} + \sum_p U_p n_{p\sigma} n_{p-\sigma} + \sum_{\substack{\sigma\sigma' \\ (pd)}} U_{pd} n_{d\sigma} n_{p\sigma'}$$

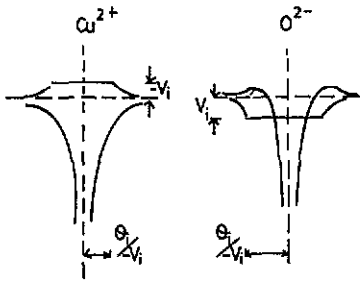


Figure 2. Madelung potentials for Cu^{2+} and O^{2-} : θ_i , net charges of ions; V_i , potential well depth.

where (pd) means that the orbitals are referred to nearest neighbours.

It is then possible to eliminate the oxygen orbitals, thus obtaining an effective single-band Hubbard Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} d_{i\sigma}^{\dagger} d_{j\sigma}^{\dagger} + U \sum_{i\sigma} n_{i\sigma} n_{j-\sigma} \quad (2)$$

i.e. the starting point of RVB theories. This becomes questionable if large values for the oxygen-related integrals become realistic. We believe that the extended Hubbard Hamiltonian (equation (1)) should be a good starting point for these systems.

First of all, let us briefly review the approximations made in the single narrow-band Hubbard model. In the Wannier representations, the $U_{ii} (= \langle ii | r^{-1} | ii \rangle)$ are assumed to be much greater in magnitude than any of the other integrals $U_{ij} (= \langle ik | r^{-1} | jl \rangle)$ suggesting the famous approximation which neglects all the integrals U_{ij} apart from U_{ii} . Next, Hubbard assessed the validity of this approximation when applied to transition-metal 3d electrons. For the sake of comparison Hubbard crudely estimated U to be 20 eV for 3d electrons in transition metals. The largest of the neglected terms are those of the type $\langle ij | r^{-1} | ij \rangle$ where i and j are nearest neighbours. These integrals were estimated to be 6 eV. Then Hubbard assumed that the screening effect may be approximated by multiplying the earlier estimate by a factor $\exp(-KR)$ where K is an appropriate screening constant and, in the case of 3d transition metals, $\exp(-KR) \simeq \frac{1}{2} - \frac{1}{3}$ (see figure 3).

A different type of approximation is the assumption that the interactions between the 3d electrons are important whereas those with electrons from other bands are only represented by the Hartree-Fock field.

It might be thought that U could be reduced by the screening of the interactions of the d electrons by the core electrons and by the d electrons themselves.

Hence, Hubbard effectively estimated U_{ii} to be approximately 10 eV and $U_{ij} \simeq 3$ eV. As a first approximation all the integrals $\langle ij | r^{-1} | k1 \rangle$ apart from $\langle ii | r^{-1} | ii \rangle$ were neglected by Hubbard.

For high T_c superconductors, however, we believe that equation (1) describing the effective extended Hubbard Hamiltonian is a better starting point than equation (2). To calculate the interaction parameters $U_{ii}, U_{ij}, T_{ij}, E_p, E_d$, etc, we have made the following approximations:

(i) We take the high T_c superconductors to be ionic solids, which can be described by models that assign charges ($\text{La}^{3+}, \text{Cu}^{2+}, \text{O}^{2-}$ etc) to point entities between which

short-range interactions are specified (involving screening by conduction electrons, etc), if needed.

(ii) The orbital wavefunctions $A_{n,l}(r - R_i)$ are used for the ions Cu^{2+} , O^{2-} instead of the Wannier functions ϕ . Ionic wavefunctions can be obtained from a self-consistent calculation of the ion potentials, adding the potential due to charged environments—the Madelung potential in high T_c compounds. In other words the orbital wavefunctions of ions in a crystal field are used but not those of the free ions.

(iii) We assume that the screening effect may be approximately estimated by a factor $\exp(-kr)$ and the interactions with electrons from other bands are only represented by the Hartree-Fock field which adds a correlation correction.

Let us interpret (ii) in detail. The charge density of an anion in a crystal is more localized about the nucleus than it is in a vacuum. No-one has experimentally observed free O^{2-} ions. Crystalline O^{2-} ions are stabilized by their environment. This is because the electrostatic potential in the region of an anion site lowers the potential energy of the electrons in this region and hence draws those electrons closer to the nucleus. In contrast, the electrostatic potential in the region of a cation site raises the potential energy of the electron in this region and therefore pushes those electrons far away from the nucleus. This effect can be approximated in an atomic calculation by imposing an external potential

$$V_i(r) = \begin{cases} -V_i & r < \theta_i / -V_i \\ \theta_i / r & r > \theta_i / -V_i \end{cases}$$

where $-V_i$ is the electrostatic interaction for the electrons at the site of the i th ion due to the rest of the ions in the crystal, and θ_i is the net charge of the i th ion (see figure 2). This is equivalent to placing a charged spherical shell which has a radius of $\theta_i / -V_i$ at every ionic site instead of the rest of the ions in the crystal. The many calculations on ionic crystals using this model by R E Watson, R G Gordon and L L Boyer *et al* [9] have shown good results.

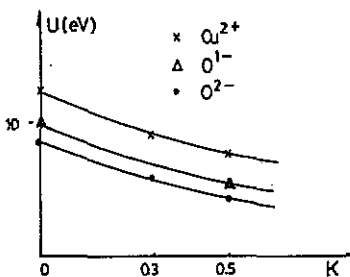


Figure 3. The dependence of on-site Coulomb repulsion U on the screening parameter K .

A value for V_i can be readily obtained by applying the Ewald method with the assumption that the rest of the ions are point charges. For the '214' high T_c structure (see table 1)

$$-V_i = 1.0465 \quad \text{for } \text{Cu}^{+2} \text{ sites and } \theta_i = 2$$

$$-V_i = -0.7716 \quad \text{for } \text{O}^{2-} \text{ sites and } \theta_i = -2.$$

Table 1. Calculated values of the Madelung potential for different charge distributions of (a) $\text{YBa}_2\text{Cu}_3\text{O}_7$, (b) $\text{La}_{2-x}\text{S}_{yx}\text{CuO}_4$.

(a)	$\text{YBa}_2\text{Cu}_3\text{O}_7$	Cu(2)	O(2)	O(3)	O(4)	Cu(1)
	$\text{Y}^{3+} + 2\text{Ba}^{2+} + \text{Cu}(1)^{3+} + 2\text{Cu}(2)^{2+} + 7\text{O}^{2-}$	1.056	-0.711	-0.707	-0.855	1.114
	$\text{Y}^{3+} + 2\text{Ba}^{2+} + \text{Cu}(1)^{2+} + 2\text{Cu}(2)^{2.5+} + 7\text{O}^{2-}$	0.994	-0.986	-0.978	-0.646	1.167
	$\text{Y}^{3+} + 2\text{Ba}^{2+} + \text{Cu}(1)^{2+} + 2\text{Cu}(2)^{2+} + 3\text{O}^{2-} + 4\text{O}^{1.75-}$	0.797	-0.888	-0.885	-0.624	1.181
	$\text{Y}^{3+} + 2\text{Ba}^{2+} + 2\text{Cu}(1)^{2+} + 2\text{Cu}(2)^{2+} + 5\text{O}^{2-} + 2\text{O}^{1.5-}$	0.795	-0.813	-0.960	-0.624	1.181
	$\text{Y}^{3+} + 2\text{Ba}^{2+} + \text{Cu}(1)^{2+} + 2\text{Cu}(2)^{1.75+} + 3\text{O}^{2-} + 4\text{O}^{1.875-}$	0.894	-0.739	-0.738	-0.626	1.111
(b)	$\text{La}_{2-x}\text{S}_{yx}\text{CuO}_4$	Cu	O(1)	O(2)		
	$2\text{La}^{3+} + \text{Cu}^{2+} + 2\text{O}(1)^{2-} + 2\text{O}(2)^{2-}$	1.047	-0.772	-0.741		
	$(2 - 0.15)\text{La}^{3+} + 0.15\text{S}_y^{2+} + \text{Cu}^{2+} + 2\text{O}(1)^{1.925-} + 2\text{O}(2)^{2-}$	0.801	-0.775	-0.774		

V_i is sensitive to the hole distribution which will be discussed later. When such a set of potential wells is used, realistic orbital functions and charge densities for Cu^{2+} and O^{2-} were obtained by solving the Schrödinger equation (or Dirac equation) self-consistently.

The density-functional theories lead to the following one-electron equation

$$\begin{aligned} \left(-\frac{1}{2}\nabla^2 + V_{\text{eff}}\right) A_i &= E_i A_i \\ V_{\text{eff}} &= V_{\text{Coulomb}} + V_{\text{ex}} + V_{\text{corr}} \end{aligned}$$

where V_{Coulomb} includes the nuclear attraction and the Coulomb repulsion potential due to the electrons. The local exchange potential is given in terms of the charge density ρ :

$$V_{\text{ex}} = -\left(\frac{3\rho(r)}{\pi}\right)^{1/3}$$

and the correlation potential is given by the Hedin-Lundquist formula

$$V_{\text{corr}} = -0.0225 \ln[1 + 33.85\rho^{1/3}].$$

Adding the Madelung contribution equation (2) becomes

$$\left(-\frac{1}{2}\nabla^2 + V_{\text{eff}} + V_i(r)\right) A_i = \epsilon_i A_i$$

which can be solved self-consistently.

We can use the method described earlier to calculate the interaction parameters expressed by the following equations:

$$U_{ij} = \int \frac{A_{ni}^2(\mathbf{r} - \mathbf{R}_i) A_{nj}^2(\mathbf{r} - \mathbf{R}_j)}{|\mathbf{r} - \mathbf{r}'|} \exp(-K|\mathbf{r} - \mathbf{R}'|) d\mathbf{r} d\mathbf{r}'$$

$$i_{ij} = \int A_{ni}(\mathbf{r} - \mathbf{R}_i) H(\mathbf{r}) A_{nj}(\mathbf{r} - \mathbf{R}_j) d\mathbf{r}$$

$$\epsilon_i = -E_i.$$

Table 2. Calculated results for (U_{ij}/t_{ij}) for (a) La_2CuO_4 (prime denotes the nearest neighbour of the same kind of ion); and (b) $\text{YBa}_2\text{Cu}_3\text{O}_7$ (prime denotes an ion in another CuO_2 layer). Data in parentheses are for the screening constant $K = 0.5$.

(a)	Cu^{2+}	$\text{O}^{2-}(1)$	$\text{O}^{1-}(1)$	$\text{O}^{2-}(2)$	$\text{O}^{2-}(1)'$	$\text{Cu}^{2+'}$		
Cu^{2+}	12.00 (7.27)	3.61 (0.58) 2.07	4.43 1.307	3.54 0.871	—	3.36 (0.098) 0.005		
$\text{O}^{2-}(1)$	—	8.69 (4.05)	3.59	2.97	2.99 (0.237)	—		
$\text{O}^{1-}(1)$	—	—	0.544	0.091	0.238	—		
			10.48	—	—	—		
(b)	Cu^{2+}	$\text{O}^{2-}(2)$	$\text{O}^{2-}(3)$	$\text{O}^{1-}(2)$	$\text{O}^{1-}(3)$	$\text{O}^{2-}(2)'$	$\text{Cu}^{2+(2)'$	$\text{O}^{2-}(4)$
$\text{Cu}^{2+(2)}$	11.99 (7.26)	3.43 2.27	3.42 2.28	4.14 1.64	4.14 1.51	—	3.63 0.090	4.41 0.357
$\text{O}^{2-}(2)$	—	8.83	2.55 0.268	—	3.21 0.302	2.56 0.129	—	—
$\text{O}^{2-}(3)$	—	—	8.32	3.21 0.308	—	—	—	—
$\text{O}^{1-}(2)$	—	—	—	10.11 (5.07)	—	—	—	—
$\text{O}^{1-}(3)$	—	—	—	—	10.10	—	—	—
$\text{O}^{1-}(2)'$	—	3.21 0.181	—	3.89 0.123	—	—	—	—

We have calculated the parameters for La_2CuO_4 and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (work on '2223' etc is in progress and the results will be published elsewhere). Only the results for the Cu-O_2 planes are listed in table 2.

For La_2CuO_4 , $\text{O}(1)$ denotes the oxygen in the basic plane, $\text{O}(2)$ the oxygen in the BaO plane, O^{-1} denotes one hole on an oxygen site. O-O and Cu-Cu are the near neighbours in the basic plane. From table 2(a) it can be seen that the $U_d \approx 12$ eV, $U_p \approx 8-10$ eV and $U_{dp} \approx 3$ eV. These values are about the same as those for $\text{YBa}_2\text{Cu}_3\text{O}_7$, and agree with those determined from experimental data (6-9 eV). Some of the data-fitting models take an exchange correction or a 0.7 factor into account, so these values are somewhat lower. If we take the screening effect by conduction carrier into account by setting $k \approx 0.5$, U_d and U_p decrease to 7 and 4.5 eV, respectively, and U_{dp} decreases more sharply to 0.1-0.6 eV where the value $k \approx 0.5$ may be an overestimate for the screening effect. The charge transfer energy $\Delta = E_p - E_d = 6.11 - 4.49 = 1.62$ eV. The hopping integral $t_{\text{Cu-O}} \approx 0.8-2$ eV, $t_{\text{O-O}} \approx 0.2-0.5$ eV. However, $t_{\text{Cu-Cu}} \approx 0.005$ eV may be too small. This suggests that we have to take the existence of the oxygen sublattice into account.

For $\text{YBa}_2\text{Cu}_3\text{O}_7$, $\text{Cu}^{2+(2)}$, $\text{Cu}^{2+(2)'}$ denote Cu^{2+} ions in the Cu-O plane on different sides of the Y plane respectively. $\text{O}(2)$ and $\text{O}(3)$ denote an oxygen on the a or b direction in the CuO_2 plane, $\text{O}(4)$ in the BaO plane. The values of U_d , U_p and U_{dp} and the effects of screening are about the same as those for La_2CuO_4 . The hopping integrals $t_{\text{Cu-O}} \approx 1.5-2.3$ eV and $t_{\text{O-O}} \approx 0.3$ eV are not very different from those of La_2CuO_4 . The charge transfer energy $E_p - E_d = 2$ eV is obtained by simple extrapolation, assuming on the average there is a quarter hole on every oxygen site. To be more

precise, a self-consistent solution should be recalculated by setting an appropriate hole distribution. In table 1 we show the Madelung potential constants for different hole distributions which can be expected to have no great effects on the values of U and t , but are sensitively dependent on Δ . The method presented in this article provides a way for approaching the relationship between the carrier distribution and the charge transfer energy (this work is in progress and the results will be published elsewhere).

In table 3 we give the values of the parameters which have been used or obtained so far by various authors, for experimental data-fitting or analytic calculations. From table 3 we can see that there is not much variation between the values for U and t , but there is for Δ . A different set of parameters, especially a different ratio for U and Δ , enables the effective Hamiltonian to work well for many areas of the phase diagram as shown in figure 1 and table 3. For example, the RVB Hamiltonian works well on the A range whereas the Emery-Hirsch Hamiltonian works on DC', Mila's on B etc. Our set of parameters works well on the C'-DC'-B range. The precise position depends on the value of Δ .

Table 3. List of the data which have been used or obtained so far by various authors.

		U_d	U_p	U_{dp}	U_{pp}	Δ	t_{dp}	t_{pp}
Shen	La ₂ CuO ₄	5-6	0	0	0	0.3	2.3-2.4	2.3-2.4
	YBa ₂ Cu ₃ O ₇	6	0	0	0	0.5	2.5	2.5
Fujimori	La ₂ CuO ₄	5	0	0	0	0.4	1.9	1.9
	YBa ₂ Cu ₃ O ₇	5	0	0	0	0.5	2.3	2.3
Mila	La ₂ CuO ₄	10	0	0-1	0	4	-1.3	0.3
Hubbard	3d	20(10)	6(3)	6(3)	6(3)	—	—	—
Schluter	—	9	6	2.5	—	1.5	1.5	—
Emery-Hirsch	—	5-6	2-3	1-2	—	1	1.3-1.5	1.3-1.5
Ours	La ₂ CuO ₄	12(7)	8.7(4.1)	3.6(0.58)	3.0	1.6	1.3	0.5
	YBaCu ₃ O ₇	12(7)	8.3	3.4(0.55)	3.2	2.0	1.6	0.3

To test these parameters let us see whether the magnetic properties of the undoped materials can be taken into account. La₂CuO₄ has been reported to be antiferromagnetic with a coupling constant $J = 0.1$ eV within the CuO₂ layers. For magnetic insulators, antiferromagnetism is explained by the superexchange theory which predicts the following expression

$$J = 4 \frac{t_0^4}{\Delta^2} \left(\frac{1}{\Delta} - \frac{1}{U_d + U_p/2} \right)$$

when U_p is non-vanishing. The formula yields values for the coupling constants. Our parameters yield $J \approx 0.18$.

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