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Abstract. — We use a total Hamiltonian containing both an electron-phonon induced attractive part of the interaction between electrons, and a Coulomb repulsive part formulated in the Hubbard model. By diagonalising it in the Bogoliubov and Valatin mean field approximation, we obtain equations for a two valued superconducting gap function, with a much more precise statement about the repulsive cut off energy than in the Morel and Anderson model. By applying these equations to our bidimensional electronic model for a CuO2 plane, we find that the calculated superconducting gap decreases very slowly with increasing doping $x$ in $La_{2-x}Sr_xCuO_4$, and we compare to the behaviour of the antiferromagnetic gap.

1. Introduction

In a previous paper [1] we explained why, in an itinerant electron model, the antiferromagnetic phase of $La_{2-x}Sr_xCuO_4$ was stable only for small values of the doping ratio $x$. In the present paper, we show that, on the contrary, in the same model, the superconducting phase exists for much larger values of $x$.

From the beginning, the true physical nature of the electronic structure of this type of compounds is highly controversial, one of the most important questions being to know whether the electrons are localised by the correlations, or not. But very recent experimental photoemission data [2-4] clearly show, not only the existence of a Fermi energy, but also the existence of a bidimensional saddle point in the energy spectrum, indicating the itinerant nature of the electron gas and its bidimensional character. Of course, various methods have been used to calculate the band structure of these materials [5-7]. However, since our purpose was to calculate the variation of the superconducting gap as the Fermi level continuously moves in the very neighbourhood of the Van Hove singularity of the electronic density of states, we preferred to use a completely analytical expression of the latter, and we used a simplified tight-binding model.
To explain the existence of an antiferromagnetic phase and of a superconducting phase in the same compound, according to the value of $x$, we start from a model Hamiltonian which is assumed to contain both the Hubbard intra-atomic repulsive term $Un_{i\uparrow}n_{i\downarrow}$, $n_{i\sigma}$ being the number operator of electrons on atomic site $i$ with spin $\sigma$ and $U$ the positive repulsive Coulomb parameter, and the usual B.C.S. attractive terms, with an effective coupling constant $V_{kk'}$ depending on the wave vector $k$ and $k'$. By introducing the creation (annihilation) operator $c^\dagger_{k\sigma}(c_{k\sigma})$ for non-interacting electrons with energies $E_k$, our total Hamiltonian is

$$H = H_0 + H_1 + H_2$$

with

$$H_0 = \sum_{k,\sigma} E_k c^\dagger_{k\sigma} c_{k\sigma},$$

$$H_1 = \frac{U}{N} \sum_{k_1k_2k_3k_4} c^\dagger_{k_4} c^\dagger_{k_2} c_{k_3} c_{k_1} \delta_{k_1+k_2+k_3+k_4},$$

$$H_2 = \sum_{k,k'} V_{k,k'} c^\dagger_{k_1} c_{-k_1} c^\dagger_{-k'1} c_{k'1},$$

where $N$ is the number of unit cells in a CuO$_2$ plane, and the symbol of Kronecker $\delta_{k,k'}$ ensures the wave vector conservation. Expression (3) was obtained by Fourier-transforming the Hubbard Hamiltonian. It can be noticed that $V_{kk'}$ is itself proportional to $1/N$.

As the ranges of the interactions contained in $H_1$ and $H_2$ are different, their respective constants $U$ and $V_{kk'}$ do not have the same dependence on the wave vector: the intra-atomic repulsive term $U$ gives rise to a coupling constant which extends to the entire band, whereas $V_{kk'}$ is drastically restricted to a narrow domain close to the Fermi energy.

In Section 2, we include the repulsive terms of $H_1$ when diagonalising $H$ in the mean-field approximation, in the superconducting state. This leads to a set of two equations when calculating the superconducting gap $\Delta_k$, which has two distinct values $\Delta_1$ and $\Delta_2$ whether the energy is smaller or larger than the cut off energy contained in $V_{kk'}$.

In Section 3, we numerically solve the previous equations for $\Delta_1$ and $\Delta_2$ as functions of the doping ratio $x$, at the absolute zero, for a CuO$_2$ plane, by using our previous tight-binding model [8]. Our important result is that $\Delta_1$ and $\Delta_2$ decrease only slowly as the Fermi energy moves away from the logarithmic singularity, when $x$ increases. In Section 4, we give an approximate version of our exact results, and discuss its validity.

### 2. Equations for the Superconducting Gap

To apply the mean-field approximation to the superconducting state, a well known procedure consists in expressing the B.C.S. part $H_0 + H_2$ of $H$ in terms of the Bogoliubov-Valatin (BV) fermion operators

$$\begin{align*}
\gamma^\dagger_{k1} &= u_k c^\dagger_{k1} - \nu_k c_{-k1}, \\
\gamma^\dagger_{k1} &= u_k c^\dagger_{-k1} + \nu_k c_{-k1},
\end{align*}$$

where the real coefficients $u_k$ and $\nu_k$ must be chosen so as to diagonalise $H_0 + H_2$ in the self-consistent mean-field approximation, with $u^2_k + \nu^2_k = 1$.

Our purpose is to diagonalise by the same procedure our total Hamiltonian $H$ including the repulsive part $H_1$. Thus we have to express $H_1$ itself in terms of the same BV operators,
CALCULATED SUPERCONDUCTING GAP

leading to

\[ H_1 = \frac{U}{N} \sum_{k_1 k_2 k_3 k_4} \left( u_{k_4} \gamma_{k_4}^\dagger + \nu_{k_4} \gamma_{-k_4}^\dagger \right) \left( u_{k_2} \gamma_{k_2} - \nu_{k_2} \gamma_{-k_2} \right) \times \left( u_{k_3} \gamma_{k_3}^\dagger - \nu_{k_3} \gamma_{-k_3}^\dagger \right) \left( u_{k_1} \gamma_{k_1} - \nu_{k_1} \gamma_{-k_1} \right) \delta_{k_1+k_2,k_3+k_4} \]  

(6)

In the mean-field approximation, the BV operators are assumed to describe independent quasi-particles. But the exact expression (6) of \( H_1 \) is a sum of terms which are products of four BV operator terms. Then it must be linearised by replacing, in each one of these terms, the product of two of the four BV operators by its averaged value. These two operators are chosen in all the possible ways among the four operators, the anticommutation rules for fermions being taken into account. The operators \( \gamma_{k\sigma} \) are looked for so as to diagonalise the total mean-field Hamiltonian. Thus the involved averaged values are:

\[ \langle \gamma_{k\sigma} \gamma_{k'\sigma'}^\dagger \rangle = f_k \delta_{kk'} \delta_{\sigma\sigma'}, \quad \langle \gamma_{k\sigma}^\dagger \gamma_{k'\sigma'} \rangle = (\gamma_{k\sigma} \gamma_{k'\sigma'}) = 0, \]

where \( f_k \) will appear at the end as the Fermi-Dirac occupation factor. The resulting simplified expression \( \tilde{H}_1 \) of \( H_1 \) is

\[ \tilde{H}_1 = \frac{U n}{2} \sum_k \left\{ u_k^2 \sum_{\sigma} \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + \nu_k^2 \left( 2 - \sum_{\sigma} \gamma_{k\sigma}^\dagger \gamma_{k\sigma} \right) \right. \\
+ 2u_k \nu_k \left( \gamma_{k\sigma}^\dagger \gamma_{-k\sigma} + \gamma_{-k\sigma}^\dagger \gamma_{k\sigma} \right) \} - NU \frac{n^2}{4} \\
+ \Delta C \sum_k \left\{ (u_k^2 - \nu_k^2) \left( \gamma_{k\sigma}^\dagger \gamma_{-k\sigma} + \gamma_{-k\sigma}^\dagger \gamma_{k\sigma} \right) \right. \\
+ 2u_k \nu_k \left( 1 - \sum_{\sigma} \gamma_{k\sigma}^\dagger \gamma_{k\sigma} \right) \} - N \frac{\Delta C^2}{U} \]

(7)

where

\[ \Delta C = \frac{U}{N} \sum_k u_k \nu_k (1 - 2f_k) \]

(8)

and where \( n = 1 - x \) is the averaged number of electrons per copper atoms, with

\[ nN = \sum_{k\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = 2 \sum_k \left\{ u_k^2 f_k + \nu_k^2 (1 - f_k) \right\}, \]

(9)

Adding expression (7) of \( \tilde{H}_1 \) to the well-known similarly linearised expression \( \tilde{H}_0 + \tilde{H}_2 \) of \( H_0 + H_2 \) [9], one gets the linearised expression \( \tilde{H} \) of \( H \). Then, introducing the chemical potential \( \mu \), and the total number operator \( \mathcal{N} \), one gets

\[ \tilde{H} - \mu \mathcal{N} = W_0 + \sum_{k\sigma} \varepsilon_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + \sum_k \Gamma_k \left( \gamma_{k\sigma}^\dagger \gamma_{-k\sigma} + \gamma_{-k\sigma}^\dagger \gamma_{k\sigma} \right) \]

(10)

with

\[ W_0 = \sum_k \left\{ 2 \left( \varepsilon_k + \frac{U n}{2} - \mu \right) \nu_k^2 - \left( \Delta_k^{(0)} - \Delta C \right) \left( 1 + 2f_k \right) u_k \nu_k \right\} - NU \frac{n^2}{4}, \]

(11)

\[ \varepsilon_k = \left( \varepsilon_k + \frac{U n}{2} - \mu \right) \left( u_k^2 - \nu_k^2 \right) + 2 \left( \Delta_k^{(0)} - \Delta C \right) u_k \nu_k, \]

(12)
\[ \Gamma_k = 2u_k \nu_k \left( E_k + \frac{U_n}{2} - \mu \right) - \left( \Delta_k^{(0)} - \Delta C \right) \left( u_k^2 - \nu_k^2 \right), \] \hspace{1cm} (13)

and

\[ \Delta_k^{(0)} = - \sum_{k'} V_{kk'} u_k \nu_{k'} \left( 1 - 2f_{k'} \right). \] \hspace{1cm} (14)

\( W_0 \) is the ground state energy, \( \varepsilon_k \) is the energy of an elementary excitation, and \( \Delta_k^{(0)} \) would be the superconducting gap if the Coulomb repulsion were not taken into account. We see from the above expressions (10-13) that the effect of adding the repulsive part \( H_1 \) to \( H_0 + H_2 \) is simply to replace \( \Delta_k^{(0)} \) by

\[ \Delta_k = \Delta_k^{(0)} - \Delta C \] \hspace{1cm} (15)

and \( E_k \) by \( E_k + U \frac{n}{2} \).

The diagonalisation of \( \tilde{H} - \mu \mathcal{N} \) is achieved by imposing the condition \( \Gamma_k = 0 \), leading to

\[ \varepsilon_k = \sqrt{\Delta_k^2 + \varepsilon_k^2}, \] \hspace{1cm} (16)

\[ \nu_k^2 = 1 - u_k^2 = \frac{1}{2} \left( 1 - \frac{\varepsilon_k}{\varepsilon_k} \right), \] \hspace{1cm} (17)

\[ f_k = \frac{1}{1 + e^{\varepsilon_k/2k_BT}}, \] \hspace{1cm} (18)

where we have introduced the self-consistent Hartree-Fock one-particle energy \( \varepsilon_k = E_k + U \frac{n}{2} - \mu \), referred to the chemical potential \( \mu \), which actually depends on the doping ratio \( x = 1 - n \).

Of course, the above results (16-18) have exactly the same form as if the Coulomb repulsion were not taken into account. But, from equations (8), (14) and (15) of \( \Delta_C \), \( \Delta_k^{(0)} \) and \( \Delta_k \) respectively, the implicit equation for the gap \( \Delta_k \) is modified and becomes

\[ \Delta_k = - \sum_{k'} \left( V_{kk'} + \frac{U}{N} \right) \frac{\Delta_{k'}}{2\varepsilon_{k'}} \text{ th} \left( \frac{\varepsilon_{k'}}{2k_BT} \right). \] \hspace{1cm} (19)

The following step is to assume, as usually, that the attractive coupling constant \( V_{kk'} \) has a non-vanishing value \( -V/N \), with \( V > 0 \), only if both \( |\varepsilon_k| \) and \( |\varepsilon_{k'}| \) are smaller than some cut off energy \( \hbar \omega_0 \). Then it results from equation (19) that the energy gap \( \Delta_k \) has two distinct constant values \( \Delta_1 \) and \( \Delta_2 \) according to the sign of \( |\varepsilon_k| - \hbar \omega_0 \):

\[ \Delta_k = \begin{cases} 
\Delta_1 = VC(T) - UD(T) & \text{if } |\varepsilon_k| \leq \hbar \omega_0 \\
\Delta_2 = -UD(T) & \text{if } |\varepsilon_k| > \hbar \omega_0,
\end{cases} \] \hspace{1cm} (20)

with

\[ \begin{aligned}
&\left\{ \begin{aligned}
C(T) &= \frac{1}{N} \sum_{|\varepsilon_k| \leq \hbar \omega_0} \frac{\Delta_k}{2\varepsilon_k^2} \text{ th} \left( \frac{\varepsilon_k}{2k_BT} \right) \\
D(T) &= \frac{1}{N} \sum_k \frac{\Delta_k}{2\varepsilon_k^2} \text{ th} \left( \frac{\varepsilon_k}{2k_BT} \right).
\end{aligned} \right.
\] \hspace{1cm} (21)

From their respective definitions (8) and (14), \( \Delta_C \) has a constant value on the entire electronic band, but \( \Delta_k^{(0)} \) has a non-vanishing constant value only for \( |\varepsilon_k| \leq \hbar \omega_0 \).

It clearly appears from the previous equations that the repulsive part of the interaction, as it results from the Hubbard model, extends to the entire electronic band, whatever the Fermi energy is. This statement is more precise than the Morel and Anderson prescription to introduce a phenomenological large cut off energy for this repulsive part [10].
3. Exact Solution in a CuO₂ Plane at \( T = 0 \) K

In this section, we apply the equations of Section 2 to a single CuO₂ plane, using the same model for the electronic density of states, per copper atom and per spin, as in our previous paper [1]:

\[
D(E) = \frac{1}{2\pi^2 t} \ln \frac{16t}{|E|},
\]

where \( E \) is the bare single particle energy, as it appears in equation (2), with \(|E| \leq 4t\). Thus, at \( T = 0 \) K, equation (21) becomes

\[
C(0) = \frac{\Delta_1}{4\pi^2 t} \int^{\hbar\omega_0}_{-\hbar\omega_0} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_1^2}} \ln \frac{16t}{|\varepsilon - U\frac{n}{2} + \mu|},
\]

\[
D(0) = C(0) + \frac{\Delta_2}{4\pi^2 t} \int^{\hbar\omega_0}_{-\hbar\omega_0} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_2^2}} \ln \frac{16t}{|\varepsilon - U\frac{n}{2} + \mu|}
\]

\[
+ \frac{\Delta_2}{4\pi^2 t} \int^{4t+U\frac{3}{2} - \mu}_{-4t+U\frac{3}{2} - \mu} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_2^2}} \ln \frac{16t}{|\varepsilon - U\frac{n}{2} + \mu|},
\]

where \( \varepsilon = E + U\frac{n}{2} - \mu \). The chemical potential \( \mu \) is related to the doping ratio \( x = 1 - n \) by equation (9), which, with equation (17), leads to:

\[
2\pi^2 t x = \int^{\hbar\omega_0}_{-\hbar\omega_0} \frac{\varepsilon}{\sqrt{\varepsilon^2 + \Delta_1^2}} \ln \frac{16t}{|\varepsilon - U\frac{n}{2} + \mu|} d\varepsilon
\]

\[
+ \int^{4t+U\frac{3}{2} - \mu}_{-4t+U\frac{3}{2} - \mu} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_2^2}} \ln \frac{16t}{|\varepsilon - U\frac{n}{2} + \mu|} d\varepsilon.
\]

The parameter \( \delta = U\frac{n}{2} - \mu \), which appears in the above equations, is the opposite of the Fermi level shift from the logarithmic singularity at the middle \( U\frac{n}{2} \) of the band. Our purpose is to calculate the variations of \( \Delta_1 \) and \( \Delta_2 \) as functions of the doping ratio \( x = 1 - n \). From equation (20) with \( T = 0 \), we have

\[
\begin{align*}
C(0) &= \frac{\Delta_1 - \Delta_2}{V}, \\
D(0) &= -\frac{\Delta_2}{U}.
\end{align*}
\]

For any given values of \( \delta \), we first calculate \( \Delta_1 \) and \( \Delta_2 \) from the implicit equations (23, 24) and (26), and then \( x \) from equation (25).

Actually, all the integrals in equations (23, 24) and (25) are easily performed by introducing new variables \( \xi \) or \( \eta \) such that \( \varepsilon = |\Delta_1| \) \( \text{sh} \) \( \xi \) or \( |\Delta_2| \) \( \text{sh} \) \( \eta \), leading to:

\[
C(0) = \frac{\Delta_1}{4\pi^2 t} \left\{ 2\xi_1 \ln \frac{32t}{|\Delta_1|} - \xi_1^2 - \xi_2^2 + \frac{\pi^2}{6} - \frac{1}{2} \left( \text{Li}_2 \left( e^{-2(\xi_1 - \xi_0)} \right) + \text{Li}_2 \left( e^{-2(\xi_1 + \xi_0)} \right) \right) \right\},
\]

\[
D(0) = C(0) + \frac{\Delta_2}{4\pi^2 t} \left\{ (\eta'' + \eta' - 2\eta_1) \ln \frac{32t}{|\Delta_2|} - \frac{1}{2} \left( \eta''^2 + \eta'^2 - \eta_1^2 \right) \right. \\
- \left. \left( \text{Li}_2 \left( e^{-(\eta'' - \eta_0)} \right) + \text{Li}_2 \left( e^{-(\eta'' + \eta_0)} \right) + \text{Li}_2 \left( e^{-(\eta' + \eta_0)} \right) + \text{Li}_2 \left( e^{-(\eta' - \eta_0)} \right) \right) \right\},
\]

\[
+ \frac{1}{2} \left( \text{Li}_2 \left( e^{-2(\eta_1 - \eta_0)} \right) + \text{Li}_2 \left( e^{-2(\eta_1 + \eta_0)} \right) \right).\]
Fig. 1. — Reduced superconducting energy gaps $\Delta_1/t$ and $\Delta_2/t$ versus doping $x$, exactly calculated (full line), by expanding $D(0) - C(0)$ (dashed line) and by the approximate formula (34) (dotted line), with $U = V = 2t$ and $\hbar\omega_0 = 0.2t$.

\[
2\pi^2tx = |\Delta_1| \left\{ 2\xi_1 \text{ sh}\ \xi_0 + \text{ ch}\ \xi_0 \ln \left| \frac{\text{ sh}(\xi_1 - \xi_0)}{\text{ sh}(\xi_1 + \xi_0)} \right| - \text{ ch}\ \xi_1 \ln \left| \frac{\text{ sh}\ \xi_1 - \text{ sh}\ \xi_0}{\text{ sh}\ \xi_1 + \text{ sh}\ \xi_0} \right| \right\} \\
+ |\Delta_2| \left\{ (1 + \ln 4)(\text{ ch }\eta'' - \text{ ch }\eta') + \text{ sh }\eta_0(\eta'' - \eta' - 2\eta_1) + \text{ ch }\eta_1 \ln \left| \frac{\text{ sh}\ \eta_1 - \text{ sh}\ \eta_0}{\text{ sh}\ \eta_1 + \text{ sh}\ \eta_0} \right| \right\}
\]

\[
+ \text{ ch }\eta_0 \left( \text{ Argsh} \left( \frac{1 + \text{ sh }\eta_1 \text{ sh }\eta_0}{\text{ sh }\eta_1 - \text{ sh }\eta_0} \right) - \text{ Argsh} \left( \frac{1 - \text{ sh }\eta_1 \text{ sh }\eta_0}{\text{ sh }\eta_1 + \text{ sh }\eta_0} \right) \right) \\
- \text{ Argsh} \left( \frac{1 + \text{ sh }\eta'' \text{ sh }\eta_0}{\text{ sh }\eta'' - \text{ sh }\eta_0} \right) + \text{ Argsh} \left( \frac{1 - \text{ sh }\eta'' \text{ sh }\eta_0}{\text{ sh }\eta'' + \text{ sh }\eta_0} \right) \right\},
\]

where the new parameters are defined by $\delta = U\frac{\eta}{2} - \mu = |\Delta_1| \text{ sh }\xi_0 = |\Delta_2| \text{ sh }\eta_0, 4t - \delta = |\Delta_2| \text{ sh }\eta', 4t + \delta = |\Delta_2| \text{ sh }\eta''$, and $h\omega_0 = |\Delta_1| \text{ sh }\xi_1 = |\Delta_2| \text{ sh }\eta_1$, and where we have introduced the dilogarithm function [11]:

\[
\text{Li}_2(z) = \int_0^z \frac{\ln(1 - \theta)}{\theta} d\theta = \sum_{p=1}^{\infty} \frac{z^p}{p^2}
\]

with the properties $\text{Li}_2(z) + \text{Li}_2(-z) = \frac{1}{2} \text{Li}_2(z^2)$ and $\text{Li}_2(1) = \frac{\pi^2}{6}$.

Of course, the results depend on the choice of the parameters. For instance, the calculated variation of $\Delta_1$ and $\Delta_2$ versus $x$, which are shown in Figure 1, have been obtained from $h\omega_0 = 0.2t$ and $U = V = 2t$. We see that $\Delta_1$ and $|\Delta_2|$ monotonously and only slowly decrease as the doping ratio $x$ increases. Their maximum values are obtained for $x = 0$. With the chosen values of the parameters, they are $\Delta_1m \approx 0.016t$ and $|\Delta_2m| \approx 0.018t$. For instance, with $t = 1$ eV, one finds $\Delta_1m/k_B \approx 160$ K and $|\Delta_2m|/k_B \approx 180$ K.

Obviously, these results do not take into account the fact that the antiferromagnetic phase is more stable for small values of $x$, forbidding the superconducting phase to exist, as we pointed
out before [1]. But it is precisely because the calculated gap decreases so slowly with $x$ that one can understand, in our model, that a high $T_c$ superconducting phase can exist once the antiferromagnetism has been destabilised by doping.

4. Approximate Version of our Results

The calculated gaps $\Delta_1$ and $\Delta_2$ are much smaller than $4t$ and $\hbar \omega_0$. The shift $-\delta$ of the Fermi level from the singularity is much smaller than $4t$, and also than $\hbar \omega_0$ as long as the doping ratio is not too large. Furthermore, it is clear from equation (23) that $C(0)$ is very sensitive to the value of the parameter $\delta = U \frac{\pi}{2} - \mu$, because the logarithmic singularity is contained inside the integration range. On the contrary, the two integrals appearing in equation (24) extend to the entire band except the narrow energy range from $-\hbar \omega_0$ to $\hbar \omega_0$ which contains the logarithmic singularity. Thus, $D(0) - C(0)$ has only a small dependence on $\delta$, at least as long as $\delta$ is reasonably smaller than $\hbar \omega_0$.

Then expanding $D(0) - C(0)$, one gets as a leading term:

$$D(0) - C(0) \simeq \frac{\Delta_2}{4\pi^2t} \ln \frac{4t}{\hbar \omega_0} \ln \frac{64t}{\hbar \omega_0}.$$  \hspace{1cm} (30)

By using the approximate expression (30) instead of the exact expression (28), but by keeping the exact expression (27) for $C(0)$, our numerical results are essentially not modified. Only a very small shift in the data appears for the largest values of the doping ratio, as shown in Figure 1.

The great advantage of the simplified version (30) is that, when associated with the exact equations (26) and (27), it leads to a very simple relation between $\Delta_1$ and $\Delta_2$, as can been seen by eliminating $C(0)$ and $D(0)$ between these equations, leading to:

$$\Delta_2 = -\frac{U^*}{V - U^*} \Delta_1,$$  \hspace{1cm} (31)

with

$$U^* = \frac{U}{1 + \frac{U}{4\pi^2t} \ln \frac{4t}{\hbar \omega_0} \ln \frac{64t}{\hbar \omega_0}}.$$  \hspace{1cm} (32)

and where $\Delta_1$ is the solution of the implicit equation

$$\frac{4\pi^2t}{V - U^*} = 2\xi_1 \ln \frac{32t}{|\Delta_1|} - \xi_1^2 - \xi_0^2 + \frac{\pi^2}{6} - \frac{1}{2} \left( \text{Li}_2 \left( e^{-2(\xi_1 - \xi_0)} \right) + \text{Li}_2 \left( e^{-2(\xi_1 + \xi_0)} \right) \right).$$  \hspace{1cm} (33)

From equation (33), the superconducting energy gap $\Delta_1$ is determined by a coupling constant $V - U^*$, where $V$ is the attractive part of the interaction, and $U^*$ the effective Coulomb repulsive part. Equation (32) shows how to calculate $U^*$ in our model, from the bare Coulomb repulsive parameter $U$, the band width $8t$ and the cut off energy $\hbar \omega_0$ for the attractive part, in a more explicit way than usual previous formulations [10, 12]. It leads to large reduction of the repulsive part, independent of the doping ratio. For instance, with our previous numerical values, one gets $U^* \simeq U/2$.

Another consequence of equation (32) is that, when calculating the isotopic effect, which in our case appears as the relation between $\Delta_1$ and $\omega_0$, one must take into account not only the existence of a logarithmic singularity in the electronic density of states [8, 13], but also the influence of $\omega_0$ on $U^*$, which can be large also.
In principle, the exact expression (27) of $C(0)$ can be expanded as we did for $D(0) - C(0)$. But, as we pointed out before, in the case of $C(0)$ this expansion is valid only in the limit of a very small doping ratio. Explicitly, the expansion of $C(0)$ contains a term in $(\delta/\Delta_1)^2$, which does not exist in $D(0) - C(0)$, and which is small only for very small values of $x$. As a consequence, the following approximate expression of the superconducting gap

$$\Delta_1 \simeq 32t \exp \left[ -\sqrt{\left( \ln \frac{16t}{\hbar \omega_0} \right)^2 + \frac{4\pi^2 t}{V - U^*} - \frac{\pi^2}{6} + \left( \frac{\delta}{\Delta_{1m}} \right)^2} \right], \quad (34)$$

obtained by expanding $C(0)$, is itself valid only for $|\delta|$ much smaller than $\Delta_{1m}$, and does not reproduce our exact results for larger $\delta$, as shown in Figure 1. Nevertheless, for $x = 0$ and thus $\delta = 0$, the analytical expression (34) of $\Delta_1$ is correct.

5. Conclusion

From our results contained in this paper and our previous one [1], we conclude that in our bidimensional itinerant electronic model for superconducting copper oxides, the calculated superconducting gap decreases with increasing doping much more slowly than the antiferromagnetic Slater gap does. This explains why a high $T_c$ superconducting phase can exist for a doping large enough to destabilise the antiferromagnetism.

References