A model for High Temperature Superconductors using the Extended Hubbard Hamiltonian

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Abstract

We derive a method to study the phase diagram for high temperature superconductors (HTCS). Our starting point is the Hubbard Hamiltonian with a weak attractive interaction to obtain the formation of bound pairs. We consider this attractive potential at different positions for different compounds accordingly to the experimental results of the coherence length. We then construct a wave function of the BCS type by a variational method using the Fourier transform of this extended Hubbard potential and then derive an energy gap equation. This approach allows us to obtain the critical temperature as function of the doping concentration which gives very good agreement with the experimental phase diagrams of YBaCuO and La(Sr,Ba)CuO compounds. PACS: 74.20.Fg, 71.28+d, 74.70.tx
Most of the HTSC are quasi-two-dimensional insulators which become a metallic conductor and a superconductor below some critical temperature \[1,2\]. Another property very different from the usual superconductors is the very short coherence length of an electron (or hole) pair, \(\xi \approx 10\,\text{Å}\). At present, there is no clear consensus about the origin of the mechanism of attraction but in several proposed models \[3 \text{–} 5\], the superconductor state is achieved from a hard core charged boson (formed by real space pairs) condensation in analogy with the \(^3\text{He}\) problem. On the other hand, LDA calculations \[\text{3}\] indicates that the main features of the \(\text{La}_2\text{CuO}_4\) band structure can be understood in terms of a two-dimensional tight-binding model. Another important point is that the properties of the normal metallic state are different than those of a common metal described by a free electron gas \[2\]. As it is well known from the study of the Hubbard Hamiltonian \[\text{4}\], the on-site Coulomb correlations may explain the antiferromagnetism at low doping regime, the large magnetic fluctuations and the semiconductor-like properties of the metallic phase. On the other hand, in order to derive the formation of pairs and their binding energy, a weak attractive interaction \(U_1\) may be added to the Coulomb on-site repulsion \(U_0\) \[\text{4}\]. The existence of bound states suggests that the normal ground state for many electrons in a tight-binding band may become unstable in the presence of these interactions \(U_0\) and \(U_1\).

In this letter, we shall use a BCS type wave function and a variational method to derive an energy gap or order parameter equation. We shall also use the intersite attractive potential \(U_1\) at different positions than the usual nearest-neighbor of the extended Hubbard model. These choices of intersite positions are directly determined from the experimental values of the coherence length and therefore, they depend on the specific compound to be studied. This procedure enable us to obtain the variation of \(T_c\) on the hole concentration which we compare with the experimental critical temperatures curves for the \(\text{YBaCuO}\) and the \(\text{La(Sr,Ba)CuO}\) compounds. Thus, let us start considering the two-dimensional extended Hubbard model on a square lattice

\[
H = - \sum_{\langle ij \rangle, \sigma} t(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U_0 \sum_i n_{i\uparrow} n_{i\downarrow} - U_1 \sum_{\langle ij \rangle} n_{i} n_{j} \quad (1)
\]
where \( t \) is the transfer integral (and the band width is 16\( t \)), \( U_0 \) is the on-site Coulomb interaction and \( U_1 \) is an intersite attraction and \(< ij >\) refers to nearest-neighbor pairs.

Let us now study the two-electrons (or two-holes) problem. In this low-density limit, for s-wave pairs, an exact solution of the Schrödinger equation can be worked out in terms of the lattice Green’s function. The binding energy \( \Delta \) for a pair just below the bottom of the band is given by [4,8]

\[
tG_{00}(8t + \Delta) = \frac{-U_1/2t - U_0U_1/16t^2 - 1}{-4U_1/t - U_0U_1/2t^2 + U_0/t},
\]

(2)

To obtain \( \Delta \) we make use of an expansion for \( G_{00} \) in terms of an elliptic integral. In the limit of \( \Delta \ll t \), it was shown that [9]

\[
tG_{00}(8t + \Delta) \approx \frac{1}{2\pi} \left( (1.38 + 0.2\sqrt{\Delta/t}) - (0.25 + 0.125\sqrt{\Delta/t}) \ln(4\Delta/t) \right).
\]

(3)

These equations allow us to study how \( \Delta \) varies with \( U_0/t \) and \( U_0/U_1 \). In fact, Eq. (2) is valid only in the low density limit and it suggests the formation of electron (hole) pairs at the bottom of the band. A derivation of Eq. (2), using real space methods [8], shows that these electron pairs have center of mass at rest and consequently, behave like Cooper pairs with momenta \( \vec{k} \) and \(-\vec{k}\). After these preliminary considerations, let us focus on the many-body problem. For this purpose, we construct a trial wave function of the BCS type describing pair of electrons (or holes)

\[
|\Phi\rangle = \prod_k \left( u_{\vec{k}\uparrow} + v_{\vec{k}\downarrow} a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow} \right) |\Phi_0\rangle,
\]

(4)

where \( |\Phi_0\rangle \) is the empty band state and \( u_k^2 + v_k^2 = 1 \).

Following the variational approach [10], we must minimize the expression

\[
\langle \Phi | H - \mu | \Phi \rangle - \mu \langle \Phi | N | \Phi \rangle,
\]

(5)

which yields

\[
\langle \Phi | H - \mu | \Phi \rangle = 2 \sum_k \xi_k v_k^2 + \sum_{k\ell} V_{k\ell} u_{\vec{k}\uparrow} v_{\vec{k}\downarrow} u_{\vec{l}\downarrow} v_{\vec{l}\uparrow},
\]

(6)
with $\xi_\vec{k} = -4t(cos(k_xa) + cos(k_ya)) - \mu$ and with $V_{\vec{k}\vec{l}}$ being the interaction part of the potential that describes the transition of a pair from the state $\vec{k}, -\vec{k}$ to $\vec{l}, -\vec{l}$. The minimization procedure follows exactly as the BCS theory for the free electron gas \[1\] and we obtain the same type of $T = 0$ energy gap equation

$$\Delta_\vec{k} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \frac{\Delta_{\vec{l}}}{2 (\xi_{\vec{l}}^2 + \Delta_{\vec{l}}^2)^{1/2}}.$$  \(7\)

As we already mentioned, $V_{\vec{k}\vec{l}}$ is the Fourier transform of the potential of Eq. (1), which is approximately given by

$$V_{\vec{k}\vec{l}} = [V_{0}^{1/2} - 2V_{1}^{1/2} \cos(k_x - l_x)a][V_{0}^{1/2} - 2V_{1}^{1/2} \cos(k_y - l_y)a], \quad (8)$$

or

$$V_{\vec{k}\vec{l}} \approx V_0 - 4(V_0V_1)^{1/2} (\cos(k_x - l_x)a + \cos(k_y - l_y)a). \quad (9)$$

Comparing with the Hamiltonian Eq. (1), we identify $U_1 = \sqrt{V_0V_1}$ and $U_0 = V_0$ and we use that $V_0 > V_1$. Likewise BCS theory, we assume the gap to have the same functional form of the potential, namely, $\Delta_\vec{k} = \Delta(0)(cos(k_xa) + cos(k_ya))/2$. This functional form was also previously deduced for the RVB particle-particle energy gap \[11\] using self-consistent field methods \[10\]. Although this potential-energy gap relation is the same used in the BCS theory, it is worth to stress that the above potential is very different than the constant and isotropic mean potential of the original BCS theory and it has the correlations built on. We take $\mu$ equal to the hole maximum energy and we will assume that it grows linearly with the concentration of holes. Although this dependence is an ansatz here, it has been previously derived by auxiliary-bosons mean field theory \[11\]^[12].

We calculate the probability of finding a hole pair, that is, the condensation amplitude $F_{\vec{k}} = u_\vec{k}v_{\vec{k}}$. It has a maximum at $k_M$ and drops very rapidly with $|k| > k_M$, that is, the pair formation instability occurs mostly at the Fermi surface. This is the same result of the free-electron BCS theory, despite the fact that our potential (Eq. (9)) acts on all the first Brillouin zone. This is mainly due to the small values of the Fermi surface and the
very short coherence length which indicates that all carriers can be involved in pairing [4].
According to these considerations and taking \( \vec{k} = 0 \) in Eq. (7), we obtain

\[
1 = -\frac{1}{2\pi^2} \int_{0}^{\alpha_\Delta} \int_{0}^{\beta_\Delta} \frac{\left(V_0 - 4(V_1V_0)^{1/2}f(\alpha, \beta)\right)f(\alpha, \beta)}{\left((4t(f(\alpha, \beta) - f(\alpha_M, \beta_M))^2 + (\Delta f(\alpha, \beta)/2)^2\right)^{1/2}} d\alpha d\beta,
\]

(10)

where \( f(\alpha, \beta) \equiv \cos \alpha + \cos \beta \) and \( \alpha = k_xa \) and \( \beta = k_ya \). \( \alpha_M \) and \( \beta_M \) are the maximum \( T = 0 \) occupied values (like a Fermi momentum) that depend on the density of holes or, as more currently used, on the number of holes per Cu atoms, \( x \). Then we can show that \( \alpha_M = \beta_M \approx \arccos(1-x) \). The integrations are performed up to \( \alpha_\Delta \) and \( \beta_\Delta \), which are chosen at values where the condensation amplitude becomes very small, namely, \( F_{\vec{k}} \approx 0.01 \). This is usually attained for \( \xi_{\vec{k}} > 6\Delta(0) \) and larger values of \( k \) do not modify the final results. The two-dimensional integrals are done by an elementary Simpson’s rule algorithm [13]. Thus, for given values of \( V_1/V_0 \) and \( V_0/t \), there are corresponding values of \( \Delta(0) \) and clearly the relation among them depends on \( x \). Furthermore, there may be only real solutions at a certain range of \( x \).

We have derived an expression for the \( T = 0 \) energy gap (Eq. (10)). For \( T \neq 0 \), the excitations with their respective probability must be taken into account. The derivation of a self-consistently temperature-dependent gap equation is analogous to that which leads to Eq. (10). At this point, we again follow the BCS approach [10] and assume that \( \Delta(T) \) vanishes at the critical temperature \( T_c \), which yields the following equation

\[
1 = -\frac{1}{2\pi^2} \int_{0}^{\alpha_\Delta} \int_{0}^{\beta_\Delta} \frac{\left(V_0 - 4(V_1V_0)^{1/2}f(\alpha, \beta)\right)f(\alpha, \beta) \tanh\left(\frac{2\alpha \beta}{2K_B T_c}\right)}{4t(f(\alpha, \beta) - f(\alpha_M, \beta_M))} d\alpha d\beta,
\]

(11)

where we again integrate up to \( \alpha_\Delta \) and \( \beta_\Delta \) which except for \( x \) close to one, is almost entirely within the lower Hubbard band. It is a well known result that the correlation \( V_0 \) can split the half-filled conduction band into two, with the upper band being empty and the lower band being filled [14]. Accordingly the properties of our equations are also dominated by the lower band. We should also point out that in the derivation of Eq.(11), we used the entropy form of a non-interacting fermion system which is an approximation which is justified in the low energy gap limit, that is, for \( \Delta(0) \ll 16t \).
Now we compare Eq. (10) and Eq. (11) in order to relate $V_1/V_0$, $V_0/t$, $\Delta(0)$ and $T_c$. The first important thing to notice is that the different coherence lengths for different compounds suggests that the intersite attractive pair potential should be placed at a different site than the original nearest neighbor site of the extended Hubbard Hamiltonian. In other words, the minimum of the real attractive potential depends on the type of HTCS. This can be easily included in our equations by a change in the lattice parameter only in the potential (Eq. (4) and $\Delta_\mathbf{k}$ expressions. Thus, for the lanthanum compounds, since the lattice parameter is approximately $4\, \text{Å}$ and $\xi \approx 35\, \text{Å}$ \cite{2}, we expect that the minimum of the attractive pair potential occurs at a distance of the order of $8 - 9$ lattice parameters. Similarly, with a coherent length $\xi \approx 15\, \text{Å}$ \cite{2}, we expect the attractive pair potential minimum to be at $3 - 4$ lattice parameters for the yttrium compounds. Thus, in order to obtain values pertinent to the experimental results for the $La_{2-x}Sr_xCuO_4$ compounds, we use the attractive potential at the 6th-neighbor position and with $V_0/V_1 = 8^2$. We find a real solution only for values of $x \in [0.04, 0.35]$ and with a maximum value for $T_c$ at $x = 0.16$. Thus, the position of the maximum is fixed and the absolute values of $T_c$ depend only on $\Delta(0)$. Therefore, to compare with the measurements, we use $16t = 2ev$ \cite{6} and we choose $\Delta(0) = 80K$ in order to obtain $T_c = 35K$ at $x = 0.16$. In Fig.1, we plotted our values for $T_c$ as function of $x$ and we see that they provide an excellent fit for the experimental data points which were taken from Refs. \cite{4,5}. Furthermore, we obtain values for $\frac{\Delta(0)}{K_BT_c}$ greater than 2.3 (around $x = 0.16$) which agrees with earlier measurements \cite{15} which yielded values larger than 2.5. These results are considerably larger than the BCS value of 1.75.

For $YBa_2Cu_3O_{6+x}$ we place the attractive potential at the next neighbor position. With $V_0/V_1 = 5^2$, we find that there are solutions only for $x > 0.4$ and the maximum $T_c$ occur at $x = 0.96$, which is close to the measured maximum $T_c$ at $x = 0.93$. Now we choose $\Delta(0) = 180K$ which gives $T_c = 95K$ at $x = 0.96$. Our results are plotted in Fig.2 with also some experimental data points taken from Ref. \cite{2}. We notice that the agreement in this case is only qualitative and fail to reproduce the change in concavity around $x = 0.7$. A possibility is that this structure is due to inter-plane effects in the compounds richer in
oxygen and, therefore, it should not be reproduced by our two-dimensional treatment. A difficulty with our calculations is the variation of the values of $V_0/t$ (and $V_1/t$) with $x$. For the lanthanum compounds, as a result of Eqs.(10) and (11), we obtain $V_0/t = 11$ for $x = 0.16$ and at the onset of superconductivity, we find $V_0/t \approx 11$ (at $x = 0.05$). Although they are in the same order of magnitude of the expected values of $V_0/t = 16$ [14], such variation of the coupling with the concentration is artificial. It is probably due to the linear approximation used for the chemical potential.

In summary, we demonstrated that a variational procedure with a BCS type wave function in connection with a two-dimensional Hubbard Hamiltonian and with an attractive interaction is suitable to determine the superconducting state for layered HTSC. This approach allows us to derive the energy gap equation in $\vec{k}$-space, which is used to relate $T_c$ with $x$. The results yield an excellent fitting for the curves of the critical temperature as function of doping when we take an effective position for the attractive potential at a distance consistent with the measured values for the coherence length. The different positions for the attractive potential are probably due to the coupling to a bosonic field (phonons, excitons, plasmons, etc....). Such field is polarized along the electronic motion and induces an effective short range attraction (renormalized from its bare value) which varies for different compounds. Other experimental values, like the ratio $\Delta/T_c$, are well reproduced by our method. Thus, we conclude that the method derived here can be successfully applied to the two most studied compounds, even though, they have transitions at very different ranges of $T$ and $x$.

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FIGURES

FIG. 1. The critical temperature for $La_{2-x}Sr_xCuO_4$ as function of the hole concentration $x$. The solid line is plotted from our calculations and the black dots are experimental results taken from Refs.4 and 5.

FIG. 2. The critical temperature for $YBa_2Cu_3O_{6+x}$ as function of the hole concentration $x$. The solid line is plotted from our calculations and the black dots are experimental results taken from a plot in Ref.2.
