Abstract

In the weak regime, we suggest a model where superconductivity types I and II bind assuming an adiabatic hypothesis where the frequency of oscillation of free electrons is much smaller than that of polarons coupled to phonons, and an itinerant antiferromagnetism appears. At the end of the article we derive an state’s equation which is tested according to generic experimental data.

The discovery of new classes of superconductors has been a constant in recent years[1]. However, the type I and type II superconductors keep the same basic characteristic of its description in BCS model: almost perfect diamagnetic behavior. Under controlled conditions, keeping the temperature mostly below the transition, worth the London equations that are accurate for Type I superconductors but not realize some properties of type II superconductors, especially the penetration of the magnetic field in the high transition temperature of some (especially of cupric oxides and recently the Iron arsenides) [2]. Therefore, it is desirable that any theory that allows for the critical temperature of superconductors of type II, in some limit, reduces to the usual BCS state $\acute{s}$. There have been developments in this direction for a perturbation theory in weak coupling, Eliashberg et al [3], but was abandoned due to the idea that superconductivity of type II have separate origin of type I. Series of recent experiments, especially EPR [4], try to prove set of theories that assume strong coupling and strongly localized nature where the most used techniques consist of Green’s functions in appropriate bases (For example helicity) whose solutions are exact [5] by deviating from the perturbative techniques. These approaches are derived from the great success of quantum field theory when applied to low-dimensional systems and in particular Strong Couplings for Heavy Fermions called where there is also large local magnetic influences. The Hubbard Hamiltonian applies very well to this kind of problems especially for Cold Atoms and Phases ferromagnetic and antiferromagnetic.

But the same experiments in EPR [4] in compounds of type YBCO also remind us of features which would fit a perturbative approach: possibility of itinerant antiferromagnetism, coexistence of holes, electron and polarons on the same phenomenon. More recently, we observed a type II superconductor where the spatial symmetry was not broken, there was no privileged plane for the superconducting conduction [2].

In this paper we propose a simple model as another of the many mechanisms that compose the type superconductivity II, where the wave $S$ of Cooper’s pairs receives boost with tunneling Josephson of free electrons in barriers produced by polarons phenomenologically[6]. Such barriers produce a state of Itinerant Antiferromagnetism in a dynamic electrons$\times$holes. In the case of cupric oxide, holes are produced by oxygen which reduces the copper. Once reduced ion Cu$^{+2}$ suffers an effect: the proximity of the orbitals 3p$^6$ and 3d$^9$ possibly produces hybridization. The ion Cu$^{+2}$ have one of the greatest potential third ionization of the known elements. This hybridization would increase the overall energy of the orbital p and d away from the atom’s nucleus, approaching the orbitals of the ions Cu$^{+2}$ neighbors, but with a hole produced by oxygen. And producing the following effects: The inner orbital hybridized form a potential barrier to the free electrons since it would be quite filled, the hole produced simultaneously by oxygen would form a well and a few free electrons would be released. This structure would vibrate
with frequency close to that of Phonons network and be coupled to the same, very close to a polaron. This state would be frozen (adiabatic hypothesis) relative to the free electrons because the oscillation frequency of the polaron would be much smaller than the free electrons ($\omega_P \ll \omega_e$).

Selective doping elements donors increase the number of barriers to a certain limit where excess barriers and reducing electrons available diminish the effect of Josephson tunneling in the state IAF (Itinerant AntiFerromagnetism). Therefore, the polaron electron-hole generates new ‘gap’ that can be additive to ‘gap’ BCS, sometimes competing and other reinforcing and increasing its critical temperature.

1 Frozen Phonon x Polaron State - Adiabatic Hipotesis.

How we work in perturbation hypothesis we keep the original BCS Hamiltonian and assuming a structure of barriers is generated by the dynamics electrons×hole where the coupling phonon×polaron produces a structure barriers. The validity of this hypothesis derives from the fact that the oscillation frequency of polarons be much smaller than the free electrons involved: $\omega_P \ll \omega_e$. Soon, though dynamic, the proposed structure is frozen in relation to frequency of free electrons, ie, our model arises from an adiabatic hypothesis. Follows the figure:

The latest models for cupric oxides adopt the strategy of making the odd dispersion of free electrons of the crystal as a function in momentum space[7], we will adopt the same strategy: $\epsilon_{-k} = -\epsilon_k$. This consideration derives from the fact that the wave function be symmetric BCS for long-range interactions. But locally, the short range of each individual electron wave must be antisymmetric whereas the order parameter that generates the ‘gap superconductor: $\langle c_{1k}^\dagger c_{-k} \rangle \neq 0$, and invariably, $\langle c_{1k}^\dagger c_{-k}^\dagger \rangle = 0$. Following similar reasoning any dispersion relation derived from global interactions, long-range, will be considered even function in momentum space: $F_{-k} = F_k$.

2 Hamiltonian

With great success Srieffer & Wolff [8] used a canonical transformation to include second order effects of an exchange. Kondo [9] e Appenbaum [10] treated perturbative form of the scattering of electrons by magnetic impurities. The dynamic nature of superconductivity does not seem limited by the low dimensionality of the system, then consider that the superconducting phase is not limited sites as suggested by models developed in recent years [11]. In particular, we will not use a local model sites (Hubbard) and define a Hamiltonian in momentum space.

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \varepsilon T c_{kT}^\dagger c_{kT} + U \sum_k c_k^\dagger c_k c_{-k}^\dagger c_{-k} +$$
$$+ \sum_k \left[ V_{k,T} c_k^\dagger c_{kT} + V_{k,T}^* c_{kT}^\dagger c_k \right]$$  (1)
In this Hamiltonian in particular see how the bound state produced by electron tunneling \( \epsilon_T c_k^{\dagger} c_{-k} \) the structure of the frozen barrier polaron (figure 1) affects the BCS interaction and how the mixing of populations via 'exchange' affects the critical temperature of the superconducting state. The terms mixture \( V_{k,T} c_k^{\dagger} c_{-k} \) are the first order \( V \sim V_{k,T} \sim V_{k,T}^* \) we consider very near and we will make canonical transformation in the second order [8] whereas that \( \Gamma = \pi N(\epsilon_T) AV E \) see how the set of quasi-bound states via tunneling affects the BCS term \( U \sum_k c_k^{\dagger} c_{-k} c_k^{\dagger} c_{-k} \), just only interested in the \( V^2 \) terms.

### 3 The Canonical transformation

We use the Baker-Hausdorff lemma so that only the terms proportional to \( V^2 \) 'mix' the terms of sector \( U \) of the Hamiltonian. We will eliminate the terms proportional to \( V^2 \):

\[
\overline{H} = H_0 + \frac{1}{2} \left[ \hat{S}, V \right] + \frac{1}{3!} \left[ \hat{S}, [\hat{S}, V] \right] + \ldots
\]  

We have a simple way for the operator \( \hat{S} \) [8]:

\[
\hat{S} = \sum_{k'} V_{k,n,-k'} c_{k'}^{\dagger} c_k
\]

Considering \( n_m = c_m^{\dagger} c_m \) and the usual relations \( \{ c_m^{\dagger}, c_l \} = \delta_{ml} \); \( \{ c_m^{\dagger}, c_l \} = \{ c_m, c_l \} = 0 \). We will only use the term \( \overline{H} = H_0 + \frac{1}{2} \left[ \hat{S}, V \right] \) the perturbative series, easily found;

\[
\overline{H} = \left[ \epsilon_T + \frac{1}{2} \sum_k \frac{V^2_{k,n-k}}{\epsilon_T - (\epsilon_k + U)} \right] n_T +
\]

\[
+ \sum_k \epsilon_k n_k + \left[ U + \frac{1}{2} \sum_k \frac{V^2_{k,n-k}}{\epsilon_T - (\epsilon_k + U)} \right] n_k n_{-k}
\]

(4)

In the case, \( n_T \ll N_k = \sum_k n_k \) incorporated \( E_T + \frac{1}{2} \sum_k \frac{V^2_{k,n-k}}{\epsilon_T - (\epsilon_k + U)} \sim E_T \) in \( \sum_k \epsilon_k n_k \). We got to the effective Hamiltonian, which reversed \( \epsilon_T \) with \( \epsilon_k \).

\[
H_{EFF} = \sum_k \left[ \epsilon_k n_k + \left( U + \frac{1}{2} \sum_k \frac{V^2_{k,n-k}}{\epsilon_k + (U - \epsilon_T)} \right) n_k n_{-k} \right]
\]

(5)

According to our previous considerations on two distinct populations: influence of fermionic about 'odd' dispersion \( \epsilon_k \) 'local, short-range' and Bosonic (Copper’s pairs) about the effects of Coulomb and tunneling of the quasi-bound states of the potential of the polaron binding.

### 4 Successive tunneling and the order parameter particle × hole.

We define an order parameter \( \Delta = \langle c_k^{\dagger} c_{-k} \rangle \), Hole × particle, consistent with our model, we will introduce later phonons in the 'gap' equation with Debye energy's cut-offs.

We can consider that \( \Delta \neq 0 \). We rewrite (5) in terms of this parameter. Plus, as we consider the energy \( \epsilon_T \ll U \). Locally, the denominator of the term \( \frac{1}{2} \sum_k \frac{V^2_{k,n-k}}{\epsilon_k + (U - \epsilon_T)} \) slightly affects the interaction BCS \( U \). Thus we can group the term \( U + \frac{1}{2} \sum_k \frac{V^2_{k,n-k}}{\epsilon_k + (U - \epsilon_T)} = \Delta_{NL} \), (return later to term), almost constant for times very close around the time of Fermi \( k \sim k_F \) using the BCS weak coupling hypothesis. Manipulating (5) and considering the order parameter:

\[
H_{EFF} = \sum_k \left[ \epsilon_k c_k^{\dagger} c_k + \Delta_{NL} c_k^{\dagger} c_k (1 - c_{-k} c_{-k}^{\dagger}) \right] =
\]

\[
= \sum_k \left[ (\Delta_{NL} + \epsilon_k) c_k^{\dagger} c_k + \Delta_{NL} c_k^{\dagger} c_{-k} c_{-k}^{\dagger} c_k \right]
\]

(6)
In our model we adopt the order parameter electron × hole $\langle c_k^+ c_{-k} \rangle \neq 0$, of (6) we find:

$$H_{EFP} = \sum_k \left[ (\Delta_{NL} + \epsilon_k) c_k^+ c_k + \Delta_{NL} \Delta_k^+ c_k \right]$$  \hspace{1cm} (7)

Now we use the assumption of the 'quasi bound states' QBS to manipulate summations and use the parity of the dispersions around $k_{Fermi}$. We impose $k_{Fermi} = 0$:

$$\sum_k = \sum_{-k} + \sum_{+k}$$  \hspace{1cm} (8)

The first summation on the right is opposite to the second sum to the right times. This is possible only with the hypothesis of QBS state, which transforms the equation (7), as follows:

$$H_{EFP} = \sum_k \left[ (\Delta_{NL} + \epsilon_k) c_k^+ c_k + \Delta_{NL} \Delta_k^+ c_k \right] +$$

$$+ \sum_{-k} \left[ (\Delta_{NL} + \epsilon_{-k}) c_{-k}^+ c_{-k} + \Delta_{NL} \Delta_{-k}^+ c_{-k} \right]$$  \hspace{1cm} (9)

To use our approach parity of dispersions local and non-local we unified de summation (8) around the Fermi energy. Taking the conversion $k \rightarrow -k$ in the sector $\sum_{-k}$ of equation (9) simultaneously embracing $\Delta \sim \Delta^*$, found:

$$H_{EFP} = \sum_k \left[ (\Delta_{NL} + \epsilon_k) c_k^+ c_k + \Delta_{NL} \Delta_k^+ c_k \right] +$$

$$+ \sum_{-k} \left[ (\Delta_{NL} + \epsilon_{-k}) c_{-k}^+ c_{-k} + \Delta_{NL} \Delta_{-k}^+ c_{-k} \right]$$

Around the Fermi energy, assuming $k_{Fermi} = 0$, with $\epsilon_{-k} = -\epsilon_k$ for dispersions of free electrons (local influences) and $F_{-k} = F_k$ for Non local and global influences, we arrive at the same Hamiltonian of ITINERANT ANTIFERROMAGNETISM [12]:

$$H_{EFP} = \sum_k \left[ (\Delta_{NL} + \epsilon_k) c_k^+ c_k + (\Delta_{NL} - \epsilon_k) c_{-k}^+ c_{-k} + \right.$$  

$$+ \Delta_{NL} \Delta \left( c_k^+ c_k + c_{-k}^+ c_{-k} \right)$$  \hspace{1cm} (10)

5 Itinerant Antiferromagnetism, Bogoluibov Transform and Gap equation.

The goal of our model is to link the particle × hole dynamics, with phonon × polaron and itinerant antiferromagnetism. Let’s perform a transformation Bogoluibov and then retrieve $\Delta_{NL}$ with $\theta = \theta_k$:

$$\begin{cases}
  c_k^+ = A_k^+ \sin \theta - A_{-k}^+ \cos \theta \\
  c_k = A_k \sin \theta - A_{-k} \cos \theta \\
  c_{-k}^+ = A_{-k}^+ \sin \theta + A_k^+ \cos \theta \\
  c_{-k} = A_{-k} \sin \theta + A_k \cos \theta
\end{cases}$$  \hspace{1cm} (11)
The rotation allows us to diagonalize (10), defining new base: \( u_k = \text{sen} \theta \) e \( v_k = \cos \theta \), manipulating the sums as in (8) using the hypothesis QBS:

\[
H_{EFF}^0 = \sum_k (\Delta_{NL} - \epsilon_k \cos 2\theta - \Delta_{NL} \Delta \sin 2\theta) A_k^* A_k \tag{12}
\]

Using the free energy HelmHoltz \( F = \langle H_{EFF}^0 \rangle - TS \), taking its minimum at the new base \( \frac{\partial F}{\partial \theta_k} = \frac{\partial \langle H_{EFF}^0 \rangle}{\partial \theta_k} = 2 \epsilon_k \text{sen}2\theta_k - 2\Delta \text{sen}2\theta_k \), and subjecting (12) to a thermal bath \((1 - 2f_k)\) being \( f_k = \frac{1}{e^{\epsilon_k / T} + 1} \), we get the equation of 'Gap' to our system:

\[
\epsilon_k t g 2\theta_k = \Delta_{NL} \Delta \tag{13}
\]

Fixing the free part and taking the thermal average \( \Delta_{NL} = U + \frac{1}{2} \sum_k \frac{V^2}{\epsilon_k + (U - cT)} \): setting usually via hypothesis BCS: \( t g 2\theta_k = \frac{\Delta_k}{\epsilon_k} \). Here we assume, analogous to the BCS model, which \( U \) and \( V_k \) are smooth functions on the closed Fermi energy range. So we can solve (14) an explicit form is required for the order parameter \( \Delta \). The physical sense of the parameter defines its shape as a function of \( k \), using as a reference text De Gennes [13] as a solution to the Josephson tunneling: \( E(k) = E_0 + J \cos k = E_0 + J \cos 2\theta_k \) in our model. Adapting our basic and simple form of a function \( \theta_k = k \). The wave packet in momentum space is obtained directly from \( \frac{\partial E(\theta_k)}{\partial \theta_k} = -2J \text{sen}2\theta_k \), i.e, the antiferromagnetic order parameter has its origin bound states formed by tunneling:

\[
\Delta = \langle c_{-k}^\dagger c_{-k} \rangle = \frac{\partial E(\theta_k)}{\partial \theta_k} = -2J \text{sen}2\theta_k \tag{15}
\]

Thus we can rewrite the equation of 'Gap':

\[
\Delta_k = -2J \sum_k \left( U + \frac{1}{2} \epsilon_k + (U - cT) \right) . \text{sen}2\theta_k \Delta(1 - 2f_k) \tag{16}
\]

But according to BCS hypothesis: \( \text{sen}2\theta_k = \frac{\Delta_k}{\sqrt{\epsilon_k + \Delta_k}} \):

\[
\Delta_k = -2J \sum_k \left( U + \frac{1}{2} \epsilon_k + (U - cT) \right) \cdot \frac{\Delta_k}{\sqrt{\epsilon_k + \Delta_k}} (1 - 2f_k) \tag{17}
\]

Note that with \( V \to 0 \), equation (17) returns to the 'Gap' original BCS equation. At this point we use \((1 - 2f_k) \to t g h \left( \frac{\epsilon}{cT} \right) \). In this model without the introduction of phonons there is no physical sense. Originally BCS theory introduces phonons with a 'cut-off' in the continuous limit in the energy space is the 'Debye temperature': \( \theta_D \). We adopt the ansatz that the Debye temperature assumes ~ \( 4 \times T_c \), i.e., the factor \( t g h \left( \frac{\epsilon}{cT} \right) \to 1 \), for \( k \theta_D > kT \), as an asymptotic limit. Therefore, for \( cT \sim cte \), and \( \Delta_k \sim cte \), turning to energy space in continuous limit, (17) is in the form:

\[
1 = -2J N \left[ U \int_{kT_c}^{k \theta_D} \frac{d \epsilon}{\epsilon} + \frac{V^2}{2} \int_{kT_c}^{k \theta_D} \frac{d \epsilon}{\epsilon^2} \right] . t g h \left( \frac{\epsilon}{kT_c} \right) \tag{18}
\]

In the asymptotic limit we propose, and \( N \) being the density of states:

\[
1 = -2J \left[ U \int_{kT_c}^{k \theta_D} \frac{d \epsilon}{\epsilon} + \frac{V^2}{2} \int_{kT_c}^{k \theta_D} \frac{d \epsilon}{\epsilon^2} \right] \tag{19}
\]

Using \( J_0 = 2J \), we find:

\[
1 = J_0 \left[ NU \ln \left( \frac{T_c}{\theta_D} \right) + NV^2 \frac{1}{2k} \left( \frac{1}{\theta_D} - \frac{1}{T_c} \right) \right] \tag{20}
\]

Assuming \( U < 0 \).
6 Conclusions and future developments.

The equation of state (20) in the limit \( V \to 0 \) and with \( J \to 1 \) recovers the original BCS equation considering \( U < 0 \). We determined an equation of state which returns the type I superconductivity when the second-order effects due to the polaron disappear. The effect is very similar to the Jahn-Teller effect. Relationship is established between the itinerant antiferromagnetism and superconductivity of type II.

To test the equation we calculate some experimental values [14]. In particular the YBCuO family. The values we used were: \( T_c \sim 100 \, K \); Debye Temperature \( \theta_D \sim 410 \, K \) (watching the most massive and abundant ion Cu); \( NU \sim -0.66 \); \( J_0 \sim 1.14 \); \( K_B = 8.617 \times 10^{-5} \, eV/K \) with \( \frac{1}{12} \sim 5802 \). And we find \( NV^2 \sim 0.00123 \).

In our little test, the ratio between the BCS interaction and second-order effect due to tunneling of electrons through structure of polarons is \( \frac{U}{V^2} \sim 550 \), i.e., an order of magnitude \( 10^3 \).

For future developments, we can study \( U(\omega) e V(\omega) \) like unique spatial configurations functions of ions and polarons, respectively.

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