The Derivation of the Fundamental Superconducting Interaction
and the Phase Diagram of Cuprates

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Abstract. - We show that an electronic phase separation (EPS) transition described by the
Cahn-Hilliard theory yields regions of low free energy forming grains of low and high charge
densities. These local differences in the potential energy are studied numerically and used here for
the first time as the origin of an attractive interaction that gives rise to local pair formation. The
resistivity transition \( T_c \) occurs due to Josephson coupling among these superconducting regions or
grains. Using this approach within the Bogoliubov-deGennes calculations we derive the Gaussian
shape of \( T_c \) against the entire doping level \( p \). We find that every pairing gap develops locally at a
temperature \( T_p \), following the relation \( 2\Delta/k_B T_p \approx 8.0 \) in close agreement recent measurements.

Introduction. – There are increasing evidences that
the charge distribution in the \( CuO_2 \) planes of the high
temperature superconductors (HTSC) is microscopically
inhomogeneous. Several different experiments like neu-
tron diffraction [1–3], muon spin relaxation (\( \mu SR \)) [4, 5],
NQR and NMR [6, 7] have detected a position dependent
electronic density. These experiments indicated that such
disorder is stronger on the underdoped side of the phase
diagram and it is possibly related with the non Fermi liq-
uid behavior of the normal phase. However, recent STM
studies on Bi2212 reveal spatial variations of the electronic
gap amplitude on a nanometer length scale even on over-
doped compounds [8–10]. These data on overdoped sam-
ples, which behave as normal Fermi liquids at high temper-
atures, indicates that a phase separation transition may
occur at temperatures not much larger than \( T_c \). A tran-
sition at such low temperatures (of the order of 100K) is
likely to be an intrinsic electronic phase separation and not
due to ionic mobility.

On the theoretical side there are many predictions that
hole carriers may segregate into hole-rich and hole-poor
regions at low doping due to strong carrier-carrier corre-
lation effect [11–13].

Here we deal with a completely different approach, namely, a phase separation transition driven by the mini-
imization of the free energy [14]. As the temperature goes
below the pseudogap temperature [15, 16] \( T^* \), the phase
separation (PS) process starts. Such second order phase
transition is a direct explanation to the NQR measure-
ments [6] of two different signals coming from two different
types of local doping domains as the temperature goes
down. The origin of this EPS transition is the proxim-
ity to the insulator AF phase, common to all cuprates, as
we derived from the principle of the competing minimum
free energy [14]. When the temperature decreases below
\( T_{PS}(p) \), the free energy of the homogeneous system with
an average doping level or charge density \( p \) becomes higher
than the disordered one, made mainly of two values of the
local charge concentration at each point \( \vec{r}_i \). According the
stripe phase measurements [1,2] and the NQR data [6], the
local values of the density \( p(\vec{r}_i) \approx p(i) \) follows a bimodal
distribution [17] formed of AF domains with \( p(i) \approx 0 \) and
high hole density domains with \( p(i) \approx 2p \). These domains,
clusters or grains in the Cu-O planes are of nanometer size
containing 10-100 sites.

The Electronic Phase Separation. – To trace the
EPS and the cluster formation we use the general theory of
Cahn-Hilliard (CH) [18]. It describes how a system evolves
from small fluctuations around the average charge concen-
tration \( p \) near the phase separation temperature \( T_{PS}(p) \)
to a complete separation into low and high density grains,
passing by intermediates configurations as the tempera-
ture decreases. The order parameter of such transition
is the difference between the temperature dependent local charge or doping concentration \( p(i, T) \) and the average doping level \( p \), i.e., \( u(i, T) = (p(i, T) - p)/p \). The Ginzburg-Landau (GL) free energy functional in terms of \( u(i, T) \) for a given compound \( p \) near the transition temperature is given by

\[
f(i, T) = \frac{1}{2} \varepsilon^2 |\nabla u(i, T)|^2 + V(u(i, T)) \equiv K + V_{GL}. \tag{1}
\]

Where the potential \( V_{GL}(p, i, T) = A^2(T) u^2/2 + B^2 u^3/4 + \ldots \), \( A^2(T) = \alpha(T_{PS}(p) - T) \), \( \alpha \) and \( B \) are temperature independent parameters. \( \varepsilon \) gives the size of the grain boundaries among two distinct phases [19,20]. \( V_{GL}(p, i, T) \) changes with the site position "i"; \( V(u = 0) = 0 \) at the grain boundaries where \( u = 0 \), and has two minima \( V_{GL}(u, t) = -A^4(T)/B \) in the lowest and highest density sites where the order parameter assumes the value \( u_{min}(T) = \pm \sqrt{\alpha(T)/B} \). These two \( V_{GL} \) minima regions work as attractors for the holes, giving rise to the clusters and to the main point here; it creates an effective two-body attractive potential.

The CH equation can be written [21] in the form of a continuity equation of the local free energy \( f(i, T) \), \( \partial_t u = -\nabla . J \), with the current \( J = MV(\delta f/\delta u) \), where \( M \) is the mobility or the charge transport coefficient. Therefore,

\[
\frac{\partial u}{\partial t} = -M \nabla^2 (\varepsilon^2 \nabla^2 u + A^2(T) u - B^2 u^3). \tag{2}
\]

We have already made a detailed study of the CH differential equation by finite difference methods [19] which yields the density profile \( u(p, i, T) \) in a 105 \( \times \) 105 array as function of the time steps, up to the stabilization of the local densities, using parameters in the CH simulation that yield stripe [22,23] and patchwork [20,24,25] patterns at intermediate time regimes.

**The Fundamental Interaction.** – Here we introduce a new approach in order to derive the attractive potential that segregates the holes into grains of low and high density and which will be used as an effective two-body attraction to calculate the superconducting properties. The justification to this procedure is because, given the mesoscopic size of a grain and the low doping values of the HTSC, there are very few holes in each confined region.

Consequently we follow numerically the "kinetic" and potential energy \( (V_{GL}) \) map, that are the first and second term in Eq.(1). These energy maps show that the grains, either the low and high density ones, are regions of free energy minimum, as shown in Fig.(1). This figure describes a common intermediate regime of disorder, between a homogeneous system with a Gaussian distribution of densities and a bimodal distribution for a complete phase separation, as it is shown in the inset by the histogram of local densities \( p(i) \).

Following the \( V_{GL} \) values, from low temperatures up to \( T_{PS}(p) \) when the grains disappear completely, we can obtain the qualitative behavior of this attractive potential. Here we use parameters to reproduced the Bi2212 low temperature data of McElroy et al [8]

\[
V_{GL}(p, i, T) = V(p) V(T) = (-0.9 + 2.8 p)|u(i, T)|^2, \tag{3}
\]

where the values are in eV, \( V(p) \) is linear and vanishes at \( p \approx 0.32 \) following the behavior \( T^*(p) \) or \( T_{PS}(p) \). \( V(T) \) vanishes at \( T_{PS}(p) \) and increases as \( T \) decreases. The \( u(i, T) \) is also parameterized in a similar way, \( |u(i, T)|^2 = u(i)(1 - T/T_{PS})^{(3-T/T_{PS})} \) showing how the system becomes homogeneous at \( T_{PS} \), and the other limit at \( T = 0 \) of largest phase separation with \( A = B = 1 \).

The energy minimum at the grains and the grain boundary energy barrier keep the holes confined forming metallic clusters with typical Fermi energies much smaller than the bulk Debye energy, the so called anti-adiabatic regime [26]. This condition with the effective hole attraction toward the cluster center is highly favorable to unipolaron formation [26]. Then the effective hole attraction, modelled by \( V_{GL} \), is taken as the origin of the superconducting interaction in the form of a local two-body attraction in the Bogoliubov-de Gennes (BdG) theory. This assumption is in agreement with the observation that a large electron mobility and a small Fermi energy produces a large Nernst Effect [27] as observed in many cuprates [28].

**BdG-CH Combined Calculations.** – To calculate the local superconductivity amplitude or gap function \( \Delta_d(i, T) \) in a plane, we use the BdG theory with the extended Hubbard Hamiltonian in a similar fashion as we did before for a phenomenological next neighbor
pounds, characterized by very large $T_c$ appreciably around the granular superconductors \cite{33} to the electronic grains, tally verified by temperature dependent tunneling \cite{31} and the sequence of the present granular theory has been experimentally the superconducting transition in cuprates occurs in two steps, similar to a superconducting material embedded in a non-superconducting matrix \cite{30}: First by the appearance of intragrain superconductivity and by Josephson coupling with phase locking at a lower temperature, what provides a clear interpretation to the presence of the superconducting amplitude $\Delta_d(i, T)$ above $T_c(p)$.

The Cuprates Phase Diagram. – In this approach $T_c(p)$ is not directly related with the intragrain superconductivity, and the amplitudes $\Delta_d(i, T)$ do not change appreciably around $T_c(p)$, specially for underdoped compounds, characterized by very large $T_{on}(p)$. This consequence of the present granular theory has been experimentally verified by temperature dependent tunneling \cite{31} and angle resolved photon emission \cite{32}. Using to the theory of granular superconductors \cite{33} to the electronic grains,

$$E_J(p, T) = \frac{\pi \hbar}{4e^2 R_n} \tanh(\frac{\Delta(T, p)}{2K_B T_c}),$$

(4)

Where $\Delta(T, p)$ is the average of the BdG superconducting gaps calculations $\Delta_d(i, T)$ on a $24 \times 24$ square taken from the $105 \times 105$ mesh after the CH simulations as that shown in Fig.(1). The $R_n$ is the normal resistance of a given compound, which we take as proportional to the $\rho_{ab}$ measurements \cite{34} on the complete series of $La_{2-x}Sr_xCuO_2$. These $R_n$ values are given in the legend of the Fig.(2) top panel. The average $\Delta(T, p)$ as function of $p$ are plotted in the low panel of Fig.(2) with the $T_c(p)$ results from Eq.4 are in the inset and yields the well known dome shape with excellent agreement with the Bi2212 values. This is one of the most important result of our CH-BdG calculations.

The STM Results and Interpretation. – According to the recent STM data \cite{9,10}, the low values of $T^*(p) \sim T_{PS}(p)$ for overdoped samples rules out any ionic mobility as the origin of the inhomogeneities in overdoped samples and probably at all dopings. Thus we want to show that these STM results can be interpreted by the granular behavior resulting from the EPS, calculating the symmetric local density of states (LDOS) at different local doping,

$$N_i(E) = \sum_{\phi} \left[ u_n(x_i)^2 + v_n(x_i)^2 \right] \times \left[ f_{\phi}'(E - E_n) + f_{\phi}'(E + E_n) \right],$$

(5)

where $f_{\phi}$ is the Fermi function, the prime is the derivative with respect to the argument, and $u_n, v_n$ and $E_n$ are respectively the eigenvectors and positive eigenvalues (quasi-particles exciting energy) of the BdG matrix equation \cite{14,20,22,23,25}.

Here we concentrate on a $p = 0.23$ compound that is close to the Bi2212 compounds used in recently STM ex-
In particular, for this case, we have a small oscillations far from the Fermi level, and with small oscillations near the Fermi level, they also have lower local conductivity, although the LDOS at points with high density. The calculations at points with high density yield the coherent peaks, which closes completely at $T_c = 50K$. This behavior is quite common to the sites with high density and the building up of spectral weight at the Fermi level. As the temperature increases and reaches $T = 50K$ we see that the LDOS at high density regions have much smaller LDOS around the Fermi level, while the LDOS at low density regions with high density have still a large dip that gives a $\Delta(i = 109, t = 50K) \sim 20meV$. This dip in the LDOS stays much above the resistivity transition $T_c = 60K$ in close agreement with the STM maps of Gomes et al [9].

Since the $V_{GL}$ potential (Eq.(3)) vanishes with the order parameter, the LDOS for both cases converge to the same value as the temperature approaches the "melting" temperature $T_{PS} = 140K$, as it is demonstrated in the Fig.(3) by the $T = 120K$ curve.

Another striking result of the CH-BdG calculations is that, despite the uncertainty on $T_c(i)$ (or $T_p$ in the notation of Gomes et al [9]) for very small gaps, mostly of our results follow close the measured relation $2\Delta d / K_B T_c(i) \approx 7.9$ [9]. For the case of $i=175$, $T_c(i) = 52K = 4.5meV$ and $2\Delta d(i,0) = 34meV$ which gives a ratio of 7.6. For $i=109$, taking the first peak in Fig.(3b) at $26meV$ which closes completely at $T \approx 74K$, we obtain again $2\Delta d / K_B T_c(i) \approx 8.1$ again in close agreement with the STM data [9] but larger than the value measured by tunneling of $2\Delta d / K_B T_c(i) \approx 6.0$ [29]. Since the lower density (insulator) grains have much smaller LDOS around the Fermi level, they also have lower local conductivity, although the gaps measured by the position of the LDOS peaks, as discussed above, are larger than high density sites with their coherent peaks. Consequently regions with larger gaps have lower conductivity as it was recently measured [10].

**Conclusion.** In summary we have made a detailed study of the EPS in HTSC using the CH theory that allows us to followed the local free energy minima that generate the high and low density grains in the Cu-O planes. The differences in these free energy local minima were calculated numerically and used in the BdG approach as the superconducting interaction in the electronic grains of cuprates in the non adiabatic limit. These calculations give rise to the intragrain superconductivity and they provide a scenario to the pseudogap phase, as composed of local regions with finite superconducting amplitude $\Delta(i, p, T)$ without phase locking. The Josephson coupling calculations in connection with the measured values of the resistivity yield an accurate $T_c(p)$ curve for the whole doping values of the Bi2212 series. The LDOS calculated in the high density grains yield the coherent peaks,
and those in the low density regions give larger gaps and ill
defined peaks in agreement with the STM data in Bi2212. As
far as we know, this present work is the only one to
give an interpretation to all the whole STM results.

All of these calculations in close agreement with current
data led us to conclude that the EPS is an important
ingredient above the superconducting phase and generates
mostly of all the intricate normal phase physics of the
HTSC.

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