Bose-Einstein condensation in quasi-2D systems: applications to high $T_c$ superconductivity

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We describe high-$T_c$ superconductivity in layered materials within a BCS theory as a BEC of massless-like Cooper pairons satisfying a linear dispersion relation and propagating within quasi-2D layers of finite width $\delta$ defined by the charge distribution about the CuO$_2$ planes. We obtain a closed formula for the critical temperature $T_c \propto \sqrt{\delta |e_0|/\lambda_{ab}}$, where $e_0$ is the binding energy of Cooper’s pairs, and $\lambda_{ab}$ the average in-plane penetration depth. This formula reasonably reproduces empirical values of superconducting transition temperatures for several different cuprate materials near the optimal doping regime, as well as for YBCO films with different doping degrees.

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Recent experimental studies of the spectral intensity of photoelectron emission in high $T_c$ cuprate superconductors have provided evidence that bound electron Cooper pairs (pairons) already exist at temperatures higher than the critical transition temperature $T_c$ [1]. This finding is consistent with several theoretical proposals that suggest that high $T_c$ superconductivity (HTSC) originates from a 2D Bose-Einstein condensate (BEC) of pairons pre-existing above $T_c$, coupled through a BCS-like phonon mechanism [2, 3]. The 2D character of the phase transition is associated with the layered structure of cuprates, which in the case of YBa$_2$Cu$_3$O$_{7-y}$ (YBCO) consists of a succession of layers along the c-axis with a unit cell of length $c \approx 12\AA$, and the chemical composition CuO-BaO-CuO$_2$-Y-CuO$_2$-BaO-CuO. It is widely accepted that the CuO$_2$ planes, which in the case of YBCO are equidistant from the central Y atom by a distance $\approx 1.5\AA$, are mainly responsible for the superconductivity in cuprates. Contour plots of the charge distribution derived from energy-band-structure calculations for YBCO reveal [4] that the SC charge carriers are mainly concentrated within a shell of width $\delta \approx 2.15\AA$ about the CuO$_2$ plane. We may thus assume that the number of SC charges per unit area, $n^{2D}$, is approximately determined by $n^{2D} = \delta n^{3D}$, where $n^{3D}$ is the volume charge density.

Following closely the formalism developed by Cooper [3], let us consider a quasi-2D system of fermions with effective mass $m^*$, kinetic energies $\varepsilon_k = \hbar^2 k^2/2m^*$ and $\varepsilon_{k'} = \hbar^2 k'^2/2m^*$, relative wave number $k = \frac{1}{2}(k_1 - k_2)$, and center of mass (CM) wave vector $\mathbf{K} = k_1 + k_2$. The fermions interact pairwise via the Cooper model interaction

$$V_{kk'} = -V_0 \text{ if } k_F < |k + \frac{1}{2}\mathbf{K}|, |k' + \frac{1}{2}\mathbf{K}| < K_{max},$$

(1)

and $V_{k,k'} = 0$, otherwise, with $V_0 > 0$. Here, $K_{max} = 2\sqrt{k_F^2 + k_D^2}$, where $k_F$ and $k_D$ are defined, respectively, by the Fermi energy $E_F = \hbar^2 k_F^2/2m^*$, and by the Debye frequency $\omega_D$ of lattice phonons of maximum energy $\hbar \omega_D = \hbar^2 k_D^2/2m^*$. A simple geometric construction shows that bound pairs will form only if the tip of vector $\mathbf{k}$ lies within the overlap of the two rings defined by condition (1) in k-space [1]. Thus, fermions lying outside this overlapping region are unpairable.

The variation of the bound state energy with the CM momentum $\hbar \mathbf{K}$ was discussed by Schrieffer [4] by considering the Cooper condition for the energy eigenvalues of the fermion pair:

$$V_0 \sum_{k} \frac{1}{\hbar^2 k^2/m^* + \hbar^2 K^2/4m^* - 2E_F - \varepsilon_k} = 1$$

(2)

where the summation is restricted to values of $\mathbf{k}$ allowed by interaction (1). The summation may be approximated by an integration over the density of states, $N(\varepsilon)$, which in 2D is independent of the energy: $N(\varepsilon) \equiv N_0 = m/2\pi \hbar^2$. In the small $K$ limit, it is found that

$$\varepsilon_K = \varepsilon_0 + c_1 \hbar K + O(K^2)$$

(3)
where \( \varepsilon_0 \) is the pairon binding energy \( \text{[5]} \) at zero momentum, namely

\[
\varepsilon_0 = -\frac{2\hbar\omega_D}{e^{2/\beta_0}N_0 - 1} \tag{4}
\]

and \( c_1 = 2v_F/\pi \) with \( v_F \) the Fermi velocity. Thus, Eq. \( \text{[3]} \) provides an approximate dispersion relation, linear at leading order, rather than quadratic. As a consequence, all \textit{excited} pairons behave like free massless particles with a common group velocity \( c_1 = \hbar^{-1}d\varepsilon_k/dk \), but a variable energy determined by their CM momenta \( \hbar K \). As pointed out by Schrieffer \( \text{[6]} \), the linear dispersion relation implies that in order for a pairon to remain bound (\( \varepsilon_K < 0 \)) its maximum allowed CM wavenumber is \( K_0 = |\varepsilon_0|/c_1 \), since pairons with \( K > K_0 \) will break up.

These features are not exclusive of the Cooper model interaction \( \text{[1]} \). For example, an attractive inter-fermion delta potential in 2D, imagined regularized to support a single bound state of energy \( -B_2 \), leads \( \text{[2]} \) to the dispersion relation \( \varepsilon_K = \varepsilon_0 + c_1 \hbar K + [1 - (2 - 16/\pi^2)E_F/B_2] \hbar^2 K^2/4m + O(K^3) \), with a \textit{linear} leading term and \( c_1 = 2v_F/\pi \) as with the Cooper model interaction. It is noteworthy that only in the vacuum limit \( v_F \to 0 \Rightarrow E_F \to 0 \) does this latter dispersion relation lead to the expected \textit{quadratic} form \( \varepsilon_K = \varepsilon_0 + \hbar^2 K^2/4m \). Then, in either case, the linear term is a consequence of the presence of the Fermi sea. It has been reported that a linear dispersion relation leads to very good fits of the BEC condensate-fraction curves for quasi-2D cuprates \( \text{[4]} \) as well as for 3D and even 1D superconductors.

Accordingly, we describe the total amount of charge carriers by means of an ideal mixture of non-interacting unpairable fermions, and breakable pairons with a linear dispersion relation \( \text{[3, 10]} \). The fermion number per unit area is \( n_f = n_{f1} + n_{f2} \), where \( n_{f1} \) and \( n_{f2} \) denote the number densities of unpairable, and pairable fermions, respectively. Unpairable fermions obey a usual Fermi-Dirac distribution, while the pairable fermion density at an arbitrary temperature \( T \) can be calculated as:

\[
n_{f2}(T) = 2 \left[ n_{0}^{2D}(T) + n_{0}^{2D,K<K_0}(T) \right] + n_{f2}^{u}(T), \tag{5}
\]

where \( n_{0}^{2D} \) represents the bosonic density of Cooper pairs with CM wave vector \( K = 0 \), \( n_{0}^{2D,K<K_0} \) the equivalent quantity with \( 0 < K < K_0 \), and \( n_{f2}^{u} \), the number density of \textit{pairable but unpaired} fermions. By asserting that in thermal equilibrium this kind of fermions arises precisely from broken pairons \( \text{[3]} \), we identify \( n_{f2}^{u}(T) = 2n_{0}^{2D,K<K_0}(T) \).

On the other hand, at \( T = 0 \) all pairable fermions should belong to the condensate (although, according to \( \text{[10]} \), this is strictly valid only in the strong coupling limit), and then \( n_{f2}(0) = 2n_{0}^{2D}(0) = 2n^{2D} \), where \( n^{2D} \) is the total boson number per unit area. Summarizing, the number equation for pairable fermions may be re-expressed in terms of bosonic quantities only: \( n^{2D} = n_{0}^{2D}(T) + n_{0}^{2D,K<K_0}(T) + n_{0}^{2D,K<K_{max}}(T) \). The last two terms in this equation belong to adjacent momental regions, and so they may be merged into a single 2D integral of a Bose-Einstein distribution:

\[
n_{0}^{2D}(T) = \frac{1}{(2\pi)^{3/2}} \int_{0}^{K_{max}} \frac{d^2K}{z^{-1}e^{\beta\varepsilon_K} - 1}, \tag{6}
\]

where \( \beta \equiv 1/k_B T, \ z \equiv e^{\beta\mu} \) is the fugacity and \( \mu \) the chemical potential. When the energy-shifted dispersion relation \( \varepsilon_K = \hbar c_1 K \) is introduced in \( \text{[6]} \) the integral may be evaluated by changing to the variable \( x \equiv \beta\hbar c_1 K \). Taking into account that \( c_1 \approx v_F \) and \( K_{max} \approx 2K_F(1+K_F^2/2K^2) \) the upper integration limit in \( \text{[6]} \) must be very large, namely \( x_{max} = \beta\hbar c_1 K_F \approx E_F/k_B T \gg 1 \). The last inequality is consistent with the maximum empirical value for the ratio \( k_B T_c/E_F \leq 0.05 \) reported \( \text{[14]} \) in exotic SCs, including cuprate SCs. Given the rapid convergence of Bose integrals, the upper integration limit \( x_{max} \) may safely be taken as infinite in \( \text{[6]} \), and the integral can be evaluated exactly by expanding the integrand in powers of \( z e^{-x} \). This gives

\[
n_{0}^{2D}(T) = \frac{(k_B T)^2}{\pi \hbar^2 c_1^2} \sum_{n=1}^{\infty} z^n/n!^2. \tag{7}
\]

The critical BEC temperature \( T_c \) is now determined by solving \( \text{[7]} \) for \( n_{0}^{2D}(T_c) = 0 \) and \( z(T_c) = 1 \). We obtain

\[
T_c = \frac{\hbar c_1}{k_B} \left( \frac{2\pi n^{2D}}{\zeta(2)} \right)^{1/2}, \tag{8}
\]

where the Riemann Zeta function of order two \( \zeta(2) = \pi^2/6 \).

A crucial element in the evaluation of \( \text{[8]} \) is to reliably estimate the fraction of charge carriers that actually contribute to the supercurrent. The 3D charge carrier density \( n^{3D} \) is usually determined from measurements of London penetration depths \( \lambda \). This parameter gives an estimate of the current that causes partial rejection of an
FIG. 1: Comparison of experimental critical temperatures vs. theoretical predictions as given by Eq.(13) as a function of the zero-temperature (inverse) penetration length $\lambda_{ab}^{-1}$ for YBCO systems with different doping degrees.

applied external magnetic field in the superconductor. Within the framework of this model, the supercurrent $J_s$ is due to massless-like pairons with a charge $2e$, density $n^{3D} = n_s/2$ (with $n_s$ the superfluid density), and moving with a speed $c_1$. In that case, $J_s = (2e)n^{3D}c_1\hat{K}$, where $\hat{K} \equiv K/K_0$ [2]. In order to obtain the expression for the associated penetration depth, we follow similar steps as those discussed in (2) and consider the contour integral of the pairon wavefunction phase in a homogeneous medium, and in presence of an external magnetic field $B = \nabla \times A$. The integral along any closed path vanishes:

$$\oint (\hbar K + \frac{2e}{c} A) \cdot dr = 0.$$  \hspace{1cm} (9)

Here, $c$ is the speed of light in vacuum. By eliminating $K$ in terms of $J_s$, and using Stoke’s theorem to evaluate $\oint$, we get a modified version of the London equation: $J = -\Lambda_p A$, where $\Lambda_p = 4e^2c_1n^{3D}/\hbar cK$. By taking now the curl of the modified London equation and introducing Ampere law $\nabla \times B = (4\pi/c)J_s$, it follows that the magnetic field satisfies $\nabla^2 B = \lambda^{-2} B$, where

$$\frac{1}{\lambda^2} = \frac{(2e)^2}{c^2} \left( \frac{4\pi c_1 n^{3D}}{\hbar K} \right). \hspace{1cm} (10)$$

This implies that the magnetic field decays exponentially within a distance $\lambda$ measured from the superconductor-vacuum interface. This expression is equivalent to the standard London formula $\lambda^{-2} = 4\pi e^2 n_s / m^* c^2$ for massive superelectrons with momentum $\hbar K = m^* c_1$. Notice that, depending on the wave number $K$, $\lambda$ varies between its minimum value $\lambda = 0$ for $K = 0$, corresponding to perfect diamagnetism, and its maximum, say $\lambda_0$, for $K = K_0$, which corresponds to pairon breakup. It seems natural to assume that this latter condition determines the experimentally observed value of the in-plane penetration depth at zero temperature, namely $\lambda_0 = \lambda_{ab}(T = 0)$. Here, $\lambda_{ab}^{-1}(0) = \lambda_a^{-1}(0) + \lambda_b^{-1}(0)$ is the geometric mean of the values of this parameter measured along the crystallographic directions $a$ and $b$. We introduce now the relation $n^{2D} = \delta n^{3D}$ and employ the dispersion relation (3) to eliminate $K_0$ from $\lambda_0$. The final expression for the 2D density of superconducting charge carriers is

$$n^{2D} = \frac{e^2}{c^2} \left( \frac{\delta |\varepsilon_0|}{16\pi c_1} \right) \frac{1}{\lambda_{ab}^2}. \hspace{1cm} (11)$$
By substituting (11) into (8) the critical temperature $T_c$ takes the form

$$T_c = \left( \frac{\hbar c}{2\pi k_B} \right) \frac{(3\delta|\varepsilon_0|)^{1/2}}{\lambda_{ab}}. \tag{12}$$

Notice that $T_c$ does not depend on the pairon speed $c_1$. The physical parameters such as $\omega_D$, $\varepsilon_0$, and $\lambda_{ab}$ are suitable to be determined by a number of experimental techniques \cite{11, 15}, while the layer width $\delta$ may be estimated from band-structure calculations \cite{4}. The parameter $\varepsilon_0$ may be alternatively estimated from the BCS energy gap at zero temperature $\Delta_0 = \hbar \omega_D / \sinh[1/N_0 V_0]$, valid for arbitrary coupling. Combining this last expression with (11) shows that $\varepsilon_0 = \hbar \omega_D - [(\hbar \omega_D)^2 + \Delta_0^2]^{1/2}$ holds. Furthermore, in the weak-coupling limit, $\Delta_0 = \hbar \omega_D \exp[-1/N(0)V_0]$, and $|\varepsilon_0| = \Delta_0^2/2\hbar \omega_D$. In that case, formula (12) may be conveniently rewritten and leads to the simple formula for the critical condensation temperature

$$T_c = \left( \frac{\hbar c}{2\pi k_B} \right) \left( \frac{3\delta}{2\hbar \omega_D} \right)^{1/2} \frac{\Delta_0}{\lambda_{ab}}. \tag{13}$$

This equation yields an alternative expression applicable in HTSCs for the BCS ratio $2\Delta_0/k_B T_c \simeq 3.53$.

According to (13), for fixed values of $\omega_D$, $\Delta_0$, and $\delta$, the critical temperature should increase linearly with $\lambda_{ab}^{-1}$. This dependence has been indeed observed in experimental studies of the correlation between the superfluid density, $n_\text{s}$, with critical temperatures of severely underdoped YBCO crystals, with $T_s$'s ranging from 3 to 17 K. The doping $p$ is the number of holes of copper atoms per CuO$_2$ plane. Broun et al. \cite{11} found that their samples of high-purity single YBCO crystals followed the rule $T_c \propto \lambda_{ab}^{-1} \times n_\text{s}^{1/2} \times (p - p_c)^{1/2}$, where $p_c$ is the minimal doping for the onset of superconductivity. A similar behavior has been observed by Zuev et al. in YBCO films with $T_s$'s from 6 to 50 K \cite{12}. They reported that, within some noise, all their data fall on the same curve $n_\text{s} \propto \lambda_{ab}^{-2} \times T_c^{2.3 \pm 0.4}$, irrespective of annealing procedure, oxygen content, etc. Thus, by assuming that, except for $\lambda_{ab}$, the YBCO parameters are approximately independent of $p$, we introduce in (13) the values: $T_D = 410$ K \cite{15}, $\Delta_0 = 145.5$ meV \cite{15}, and $\delta = 2.15$ Å \cite{4}, to get the relation $T_c = 16.79/\lambda_{ab}$ (µm$^{-1}$K). In Figure 1, adapted from \cite{12}, we compare this latter relation with the experimental data obtained for underdoped YBCO films, as well as data pertaining to a higher doping regime. We observe that the theoretical curve provides an excellent fit to the experimental measurements. On the other hand, the measured value of the penetration length in underdoped YBCO crystals systems is an order of magnitude bigger than in thin films \cite{11}, so that the specific values of the critical temperatures derived from (13) are not in such a good agreement as in the YBCO films. It has been pointed out that YBCO films seem to behave more similarly to other cuprates, like BiSrCaCuO or LaSrCuO, than YBCO crystals \cite{12}.

The theoretical values of $T_c$ for cuprates with different compositions have been also calculated either using formula (12). Here we focus on the following cuprates: 2(La$_{0.95}$Sr$_{0.05}$)CuO$_4$, YBa$_2$Cu$_3$O$_{6.60}$, YBa$_2$Cu$_3$O$_{6.95}$, Tl$_2$Ba$_2$Ca$_2$Cu$_2$O$_{8}$, Tl$_2$Ba$_2$Ca$_2$Cu$_3$O$_{10}$, Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$, and Bi$_2$Sr$_2$Ca$_2$Cu$_2$O$_{8}$. The characteristic parameters for these materials have been taken from tables reported in Refs. \cite{15, 16, 17, 18}. Concerning the layer of width $\delta$, for which no direct experimental determinations are available, an upper bound for $\delta$ is found by considering that $\delta < d$, where $d$ is the separation between adjacent CuO$_2$ planes. \cite{17}. In fact, as mentioned before, band-structure calculations for YBCO systems yield $\delta \approx 2.15$ Å or, since $d = 3.25$ Å, then $\delta \approx 0.67 d$. We do not expect that this relation should be radically altered for other layered cuprates, so that in the evaluation of $T_c$ we have assumed that

| Material                  | $T_D$ (K) | $\Delta_0$ (meV) | $\lambda_{ab}$ (nm) | $\delta$ (Å) | $T_c^{exp}$ (K) | $T_c^{th}$ (K) |
|--------------------------|-----------|------------------|---------------------|-------------|----------------|-------------|
| (La$_{0.95}$Sr$_{0.05}$)$_2$CuO$_4$ | 360       | 6.5              | 250                 | 4.43        | 36             | 36.4        |
| YBa$_2$Cu$_3$O$_{6.60}$    | 410       | 15.0             | 240                 | 2.15        | 59             | 56.0        |
| YBa$_2$Cu$_3$O$_{6.95}$    | 410       | 15.0             | 145                 | 2.15        | 93.2           | 92.6        |
| Bi$_2$Sr$_2$Ca$_2$Cu$_2$O$_8$ | 250       | 16.0             | 250                 | 2.24        | 80             | 72.2        |
| Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ | 260     | 26.5             | 252                 | 2.24        | 108            | 109.2       |
| Tl$_2$Ba$_2$Ca$_2$Cu$_2$O$_8$ | 260       | 22.0             | 221                 | 2.14        | 110            | 104.1       |
| Tl$_2$Ba$_2$Ca$_2$Cu$_3$O$_{10}$ | 280       | 14.0             | 200                 | 4.30        | 125            | 105.5       |
it is approximately valid for other cuprates besides YBCO. In Table I we present the results obtained using the above assumptions, together with the physical parameters involved in the calculation. In most cases we find a rather satisfactory agreement between the predicted and measured values of $T_c$. We observe that, in general, the exact formula (12) leads to lower $T_c$’s than the approximate one (13), although the values differ at most by 10%. We have not attempted to provide an estimation of the uncertainties of our theoretical results, since the accumulated data of the physical parameters involved in the calculation show a wide scatter.

In conclusion, HTSC can investigated using a BCS-like theory for a quasi-2D BEC of Cooper pairs satisfying a linear dispersion relation in their total or CM momentum. Simple expressions ensue for the critical transition temperature $T_c$. The formulas derived provide a functional relation $T_c \propto 1/\lambda_{ab}$. Although this apparently disagrees with Uemura’s phenomenological relation $T_c \propto n_s$ [14, 15], Zuev et al. [12] have pointed out that most data in the Uemura plot refer to cuprate samples which are not severely underdoped.

We show elsewhere that all relevant 2D expressions derived in this work arise as the limit $k_B T \delta/hc_1 \to 0$ of a more general 3D BCS-BEC theory for layered materials, and that conventional 3D results are recovered in the limit $k_B T \delta/hc_1 \to \infty$.

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