

# D-wave Bose-Einstein condensation and the London penetration depth in superconducting cuprates.

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We show that bipolaron formation leads to a d-wave Bose-Einstein condensate in cuprates. It is the bipolaron energy dispersion rather than a particular pairing interaction which is responsible for the *d*-wave symmetry. The unusual low-temperature dependence of the magnetic field penetration depth  $\lambda(T)$  in cuprates is explained by the localisation of bosons in the random potential. Both linear positive and negative slopes of  $\lambda(T)$  are occur depending on the random field profile.

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The evidence for a *d*-like order parameter (changing sign when the *CuO*<sub>2</sub> plane is rotated by  $\pi/2$ ) has been reviewed by Annett, Goldenfeld and Legget [1] and more recently by Brandow [2] and by several other authors. A number of phase-sensitive experiments [3] provide unambiguous evidence in this direction; furthermore, the low temperature magnetic penetration depth [4,5] has been found to be linear in many cuprates as expected for a d-wave BCS superconductor. However, *SIN* tunnelling studies [6,7] and some high-precision magnetic measurements [8] show the more usual *s*-like shape of the gap function or even reveal an upturn in the temperature dependence of the penetration depth below some characteristic temperature [9]. One can reach a compromise between conflicting experimental results by mixing *s* and *d* order parameters or invoking ‘anomalous Meissner currents’ due to surface-induced bound states (often violating time reversal symmetry). However, the observation of the normal state pseudogap in tunnelling (STM) and photoemission spectra (ARPES), non Fermi-liquid normal state kinetics and thermodynamics, and unusual critical phenomena tell us that many high- $T_c$  cuprates are not *BCS* superconductors [10]. In particular, both ARPES [11] and STM [7] experiments have shown that the maximum energy gap is more than three times larger than that expected from the d-wave BCS theory and persists into the normal state irrespective of doping. The gap as well as other major features of STM and ARPES have been recently explained with bipolarons [12]. Comparison of tunnelling and Andreev gap determinations on yttrium, lanthanum and bismuth-based cuprates [6] at various doping levels have unambiguously revealed the existence of two energy scales as expected for the bipolaronic superconductors [13]. Hence an explanation for the *d*-like order parameter and the anomalous penetra-

tion depth should be found independent of the *BCS* gap equation.

While in a BCS superconductor all energy scales and symmetries are strictly identical, the symmetry of the Bose-Einstein condensate in the bipolaronic superconductor should be distinguished from that of the ‘internal’ wave function of a single bipolaron. In this letter we show that the Bose-Einstein condensate in cuprates is *d*-wave owing to the bipolaron energy band structure rather than to a particular pairing interaction (see also [12]), while the low temperature dependence of the penetration depth,  $\lambda(T)$  is determined by the localisation of bipolarons. Both linear positive and negative slopes of  $\lambda(T)$  occur depending on the random field profile.

Consideration of perovskite lattice structures shows that small inter-site bipolarons are perfectly mobile even if the electron-phonon coupling is strong and the bipolaron binding energy is large [14]. Different bipolaron configurations can be found with computer simulation techniques based on the minimization of the ground state energy of an ionic lattice with two holes. The intersite pairing of the in-plane oxygen hole with the *apex* one is energetically favorable in the layered perovskite structures as established by Catlow *et al* [15]. This apex or peroxy-like bipolaron can tunnel from one cell to another via a direct *single polaron* tunnelling from one apex oxygen to its apex neighbor. The bipolaron band structure has been derived by one of us [16] as

$$E_{\mathbf{k}}^{x,y} = t \cos(k_{x,y}) - t' \cos(k_{y,x}). \quad (1)$$

Here the in-plane lattice constant is taken as  $a = 1$ ,  $t$  is twice the bipolaron hopping integral between *p* orbitals of the same symmetry elongated in the direction of the hopping (*ppσ*) and  $-t'$  is twice the hopping integral in the perpendicular direction (*ppπ*). The bipolaron energy spectrum in the tight binding approximation consists of two bands  $E^{x,y}$  formed by the overlap of  $p_x$  and  $p_y$  *apex polaron* orbitals, respectively. The energy band minima are found at the Brillouin zone boundary,  $\mathbf{k} = (\pm\pi, 0)$  and  $\mathbf{k} = (0, \pm\pi)$  rather than at the  $\Gamma$  point owing to the opposite sign of the *ppσ* and *ppπ* hopping integrals. Only their relative sign is important, and we choose  $t, t' > 0$ . Neither band is invariant under crystal symmetry but the degenerate doublet is an irreducible representation; under a  $\pi/2$  rotation the *x* band transforms into *y* and vice versa.

If the bipolaron density is low, the bipolaron Hamiltonian can be mapped onto the charged Bose-gas [10].

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Charged bosons are condensed below  $T_c$  into the states of the Brillouin zone with the lowest energy, which are  $\mathbf{k} = (\pm\pi, 0)$  and  $\mathbf{k} = (0, \pm\pi)$  for the  $x$  and  $y$  bipolarons, respectively. These four states are degenerate, so the order parameter  $\Psi(\mathbf{m})$  (the condensate wave function) in the real (site) space  $\mathbf{m} = (m_x, m_y)$  is given by

$$\begin{aligned}\Psi_{\pm}(\mathbf{m}) &= N^{-1/2} \sum_{\mathbf{k}=(\pm\pi,0),(0,\pm\pi)} b_{\mathbf{k}} \exp(-i\mathbf{k} \cdot \mathbf{m}) \\ &= n_c^{1/2} [\cos(\pi m_x) \pm \cos(\pi m_y)],\end{aligned}\quad (2)$$

where  $N$  is the number of cells in the crystal,  $b_{\mathbf{k}}$  is the bipolaron (boson) annihilation operator in  $\mathbf{k}$  space (which is a  $c$ -number for the condensate), and  $n_c$  is the number of bosons per cell in the condensate. Other combinations of the four degenerate states do not respect time-reversal and (or) parity symmetry. The two solutions, Eq.(2), are physically identical being related by:  $\Psi_+(m_x, m_y) = \Psi_-(m_x, m_y + 1)$ . They have  $d$ -wave symmetry changing sign when the  $CuO_2$  plane is rotated by  $\pi/2$  around  $(0, 0)$  for  $\Psi_-$  or around  $(0, 1)$  for  $\Psi_+$  (Fig.1). The  $d$ -wave symmetry is entirely due to the bipolaron energy dispersion with four minima at  $\mathbf{k} \neq \mathbf{0}$ . With the energy minimum located at the  $\Gamma$  point of the Brillouin zone the condensate is  $s$ -like.

If the total number of bipolarons in one unit cell is  $n$  of which  $n_L$  are in localised states and  $n_D$  are in delocalised states then the number in the condensate  $n_c$  is

$$n_c = n - n_L - n_D \quad (3)$$

and the London penetration depth  $\lambda \propto 1/\sqrt{n_c}$ . Taking the delocalised bipolarons to be a free three-dimensional gas we have  $n_D \propto T^{3/2}$ . Here we use a simple model we have presented previously [17] to calculate the temperature dependence of  $n_L$  and find that at low temperature  $n_L$  varies linearly with temperature. Thus in the limit of low temperature we can neglect  $n_D$  and make the approximation

$$n_c \approx n - n_L \quad (4)$$

In this limit  $\lambda(T) - \lambda(0)$  is small and so

$$\lambda(T) - \lambda(0) \propto n_L(T) - n_L(0) \quad (5)$$

i.e.  $\lambda$  has the same temperature dependence as  $n_L$ .

The picture of interacting bosons filling up all the localised single-particle states in a random potential and Bose-condensing into the first extended state is known in the literature [18–21]. The comprehensive scaling analysis of neutral [20] and charged bosons [21] allows us to describe the quantum Bose glass-superfluid transition while the thermodynamics of each phase away from the transition can be studied with the physically plausible models of neutral [22] and charged bosons [17] in a random potential. These models are based on a separation

of localised single-particle states from delocalised states. The renormalisation of the single-particle energies by the collective mode does not affect the temperature dependence of any of the thermodynamic functions at low temperatures [17]. Hence, one assumes that at some temperature  $T_c$  bosons are condensed at the mobility edge  $E_c$  so that the chemical potential  $\mu = E_c$ , and some of the bosons are in localised states below the mobility edge.

For convenience we choose  $E_c = 0$ . When two or more charged bosons are in a single localised state of energy  $E$  there may be significant Coulomb energy and we take this into account as follows. The localisation length  $\xi$  is thought to depend on  $E$  via

$$\xi \propto \frac{1}{(-E)^\nu} \quad (6)$$

where  $\nu > 0$ . The Coulomb potential energy of  $p$  charged bosons confined within a radius  $\xi$  can be expected to be

$$\text{potential energy} \sim \frac{p(p-1)e^2}{\epsilon_0 \xi} \quad (7)$$

where  $\epsilon_0$  is the dielectric constant. Thus the total energy of  $p$  bosons in a localised state of energy  $E$  is taken to be

$$w(E) = pE + p(p-1)\kappa(-E)^\nu \quad (8)$$

where  $\kappa > 0$ . We can thus define an energy scale  $-E_1$ :

$$-E_1 = \kappa^{1/\nu} \quad (9)$$

From here on we choose our units of energy such that  $E_1 = -1$ . We take the total energy of charged bosons in localised states to be the sum of the energies of the bosons in the individual potential wells. The partition function  $Z$  for such a system is then the product of the partition functions  $z(E)$  for each of the wells,

$$z(E) = e^{\alpha p_0^2} \sum_{p=0}^{\infty} e^{-\alpha(p-p_0)^2} \quad (10)$$

where

$$p_0 = \frac{1}{2} \{1 + (-E)^{1-\nu}\} \quad (11)$$

$$\alpha = \frac{(-E)^\nu}{\theta} \quad (12)$$

and

$$\theta = \frac{k_B T}{(-E_1)} \quad (13)$$

The average number  $n_L$  of bosons in localised states is

$$n_L = \int_{-\infty}^0 dE \langle p \rangle \rho_L(E) \quad (14)$$

where the mean occupancy  $\langle p \rangle$  of a single localised state is taken to be

$$\langle p \rangle = \frac{\sum_{p=0}^{\infty} p e^{-\alpha(p-p_0)^2}}{\sum_{p=0}^{\infty} e^{-\alpha(p-p_0)^2}} \quad (15)$$

and  $\rho_L(E)$  is the one-particle density of localised states per unit cell below the mobility edge, which is taken to be

$$\rho_L(E) = \frac{N_L}{\gamma} e^{\frac{E}{\gamma}}. \quad (16)$$

We now focus on the temperature dependence of  $n_L$  at low temperature ( $\theta \ll 1$ ) for the case where the width of the impurity tail  $\gamma$  is large ( $\gamma > 1$ ). In the following we consider first the case  $\nu > 1$  and then  $\nu < 1$ .

If  $\nu > 1$  we can approximate  $n_L$  as

$$\frac{n_L}{N_L} \approx 1 + \frac{\nu - 1}{2(2 - \nu)\gamma} + \frac{2\theta}{(2 - \nu)\gamma} \ln 2 \quad (17)$$

So we expect  $n_L$  to be close to the total number of wells  $N_L$  and to increase linearly with temperature. Fig 2a compares this analytical formula with accurate numerical calculation for the case  $\nu = 1.5$ ,  $\gamma = 20$ . We also note that even when  $\gamma < 1$ ,  $n_L(\theta)$  will still be linear with the same slope provided that  $\theta \ll \gamma$ .

If  $\nu < 1$  we obtain, keeping only the lowest power of  $\theta$  (valid provided  $\theta^{\frac{1}{\nu}} \ll \theta$ )

$$\frac{n_L}{N_L} = \frac{1}{2} + \frac{\Gamma(2 - \nu)\gamma^{1-\nu}}{2} + \frac{1 - \nu}{2(2 - \nu)\gamma} - \frac{\theta}{\gamma} \ln 2 \quad (18)$$

Hence in this case  $n_L$  decreases linearly with increasing temperature (in the low temperature limit). Fig 2b compares this analytical formula with the numerical calculation for the case  $\nu = 0.65$ ,  $\gamma = 20$ .

Fig 3 shows that the low temperature experimental data [9] on the London penetration depth  $\lambda$  of *YBCO* films can be fitted very well by this theory with  $\nu < 1$ . It is more usual to see  $\lambda$  increase linearly with temperature [4,5] and this would correspond to  $\nu > 1$ .

The exponent  $\nu$  depends on the random field profile. We believe that  $\nu < 1$  is more probable for a rapidly varying random potential while  $\nu > 1$  is more likely for a slowly varying one. Both  $\nu < 1$  and  $\nu > 1$  are observed in doped semiconductors. Hence, it is not surprising that drastically different low-temperature dependence of the London penetration depth is observed in different samples of doped cuprates. In the framework of our approach  $\lambda(T)$  is related to the localisation of carriers at low temperatures rather than to any energy scale characteristic of the condensate. The excitation spectrum of the charged Bose-liquid determines, however, the temperature dependence of  $\lambda(T)$  at higher temperatures including an unusual critical behaviour near  $T_c$  [10].

Many thermodynamic, magnetic and kinetic properties of cuprates have been understood in the framework of the bipolaron scenario [10]. We admit, however, that one experimental fact is enough to destroy any theory. In particular, the single-particle spectral function seen by ARPES [11] was interpreted by several authors as a Fermi liquid feature of the normal state incompatible with bipolarons. Most (but not all) of these measurements indicated a large Fermi surface which one would think should evolve with doping as  $(1 - x)$  (where  $x$  is the number of holes introduced by doping) but such an evolution is in clear contradiction with kinetic and thermodynamic measurements which show an evolution proportional to  $x$ . Only recently it has been established that there is a normal state gap in ARPES and SIN tunnelling, existing well above  $T_c$  irrespective of the doping level [11,7,23]. The ‘Fermi surface’ shows missing segments just near the  $M$  points [23] where we expect the Bose-Einstein condensation. A plausible explanation is that there are two liquids in cuprates, the normal Fermi liquid and the charged Bose-liquid (this mixture has been theoretically discussed a long time ago [24]). However, it is difficult to see how this scenario could explain the doping dependence of  $dc$  and  $ac$  conductivity or of the magnetic susceptibility and carrier specific heat. On the other hand, the single-particle spectral function of a pure bipolaronic system has been recently derived by one of us [12]. It describes the spectral features of tunnelling and photoemission in cuprates, in particular, the temperature independent gap and the anomalous  $gap/T_c$  ratio, injection/emission asymmetry both in magnitude and shape, zero-bias conductance at zero temperature, the spectral shape inside and outside the gap region, temperature/doping dependence and dip-hump structure of the tunnelling conductance and ARPES. The zero-bias conductance and any spectral weight at the chemical potential appear only due to single polaronic states localised by the random field. The model is thus compatible with the doping evolution of thermodynamic and kinetic properties.

In conclusion we suggest, within the framework of the bipolaron theory of cuprates [10], explanations of the  $d$  wave symmetry of the ground state and the anomalous temperature dependence of the London penetration depth, compatible with the non Fermi-liquid normal state, anomalous critical behaviour, and the ARPES and tunnelling data

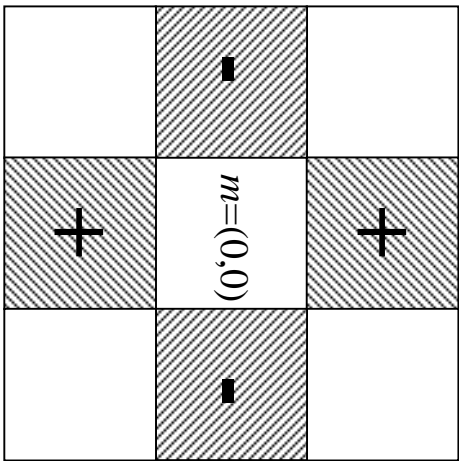
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FIG. 1. D-wave condensate wave function,  $\Psi_-(\mathbf{m}) = n_c^{1/2} [\cos(\pi m_x) - \cos(\pi m_y)]$  in the real (Wannier) space. The order parameter has different signs in the shaded cells and is zero in the blank cells.

FIG. 2. Dependence of the density of localised bosons  $n_L$  on temperature  $\theta$  for  $\gamma = 20$ . (a)  $\nu = 1.5$ , (b)  $\nu = 0.65$ . The solid lines correspond to the low temperature predictions from equations 17 and 18, while the dashed lines are derived from an accurate numerical calculation.

FIG. 3. Fit to the London penetration depth obtained by Walter *et al* [8] for a non-irradiated YBCO film. The parameter values from the fit were  $E_1 = -74K$ ,  $\gamma = 20$  and  $\nu = 0.67$ .



$y$  ↑

←  $x$

