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# On the nature of the superconducting gap in the cuprates

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## Abstract

Recent experiments indicate that the excitation spectrum of the cuprates is characterized, in the superconducting state, by two energy scales: the ‘coherence energy’  $\Delta_c$  and the ‘pseudogap’  $\Delta_p$ . Here we consider a simple generalization of the BCS model that yields exotic pairing and can describe, phenomenologically, the generic trends in the critical temperature  $T_c$  of cuprate superconductors. We use the model to predict the gap in the single-particle spectrum arising from the superconductivity and we find evidence that it corresponds to the lower of the two energy scales,  $\Delta_c$ , seen in the experiments. This provides further support to the view that the origin of the pseudogap is not superconducting fluctuations.

## 1. Introduction

In this paper we comment on the nature of the superconducting gap in the cuprates. Recently, Deutscher has identified two distinct energy scales at low temperatures (in the superconducting state), which he calls the coherence energy  $\Delta_c$  and the single-particle excitation energy  $\Delta_p$  [1]. The former corresponds to the superconducting gap seen in phase-sensitive experiments (Andreev reflection, penetration depth and Raman scattering), while the latter is the ‘pseudogap’ seen in experiments that probe the one-particle spectrum (photoemission and tunnelling). In fact some experiments belonging to the latter class seem to be able to detect both ‘gaps’ simultaneously: specifically,  $\Delta_c$  and  $\Delta_p$  appear to have been resolved, as two distinct features in the single-particle excitation spectrum, in angle-integrated photoemission experiments on LSCO by Sato *et al* [2] and in intrinsic *c*-axis tunnelling spectroscopy experiments on BSCCO by Krasnov *et al* [3]. Here we address the following question: ‘which, if any, of these two energies is the “superconducting gap”, in the BCS sense?’.

Since the issue that we wish to explore is fairly general, we use a minimal model which might be expected to contain the relevant physics. The basic idea is to exploit the fact that certain properties of cuprate superconductors seem to be approximately material independent.

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In particular, the critical temperature  $T_c$  [4] as well as the two energy scales  $\Delta_c$  and  $\Delta_p$  [1], when normalized to the critical temperature at optimal doping,  $T_{c,max}$ , appear to be fairly universal functions of the number of holes per  $\text{CuO}_2$  unit,  $n_h$ . Thus one could expect that a very simple model which captures the essential physics in these systems can describe this behaviour. More realistic models would only be required to calculate material-specific properties, such as  $T_c$  (as opposed to  $T_c/T_{c,max}$ ) accurately. In a sense the rationale behind our approach is the same as in the BCS model which, with a very simplified description of the electronic structure and the electron–electron interaction, can nevertheless predict the isotope effect and the constant value of the ‘BCS ratio’  $\Delta_0/k_B T_c$  very accurately, for most of the conventional superconductors. Unfortunately our model of the electron–electron interaction in the cuprates is only phenomenological, and hence we shall have little to say about the nature of the physical mechanism giving rise to pairing. Nevertheless, as we shall show presently the model has a number of physical features which if confirmed, by comparison with experiments, will shed some light on the central problem of the high- $T_c$  phenomena. In particular, the model that we shall use has been shown to describe quantitatively the rise and fall of  $T_c/T_{c,max}$  [5]. Moreover, it facilitates the investigations of superconductivity in both the BCS and Bose–Einstein (BE) limits [6]. The central new result, presented here, is that the prediction of the model for the superconducting gap in the single-particle excitation spectrum,  $\Delta_0$ , coincides, quite accurately, with the *lower* of the two energy scales identified by Deutscher, namely the ‘coherence energy’  $\Delta_c$ . On the basis of this we argue that, although the model is too simple to describe the superconducting state of the cuprates in detail, some of its properties may generically characterize these materials. In short, it provides evidence that  $\Delta_c$  can be understood as a BCS-like  $d_{x^2-y^2}$ -wave gap, while the other energy scale,  $\Delta_p$ , seems to be quite unrelated to superconductivity. Interestingly similar conclusions were reached in [7] on the basis of experimental investigations. Moreover, our approach, based on the universal properties of cuprate superconductors, complements the one recently adopted by Szotek, BLG and Temmerman [8], who used a detailed eight-band model of the electronic structure of a specific material (YBCO) to study the same question, reaching similar conclusions.

## 2. The model

Our model consists of free electrons (holes) of effective mass  $m^*$  interacting via the attractive ‘delta-shell’ potential (between opposite spins)

$$V(|\mathbf{r}|) = -g\delta(|\mathbf{r}| - r_0). \quad (1)$$

This is, arguably, the simplest generalization of the BCS model that can describe exotic pairing [5, 6]. The four parameters of the delta-shell model are the ‘coupling constant’  $g$  (which has dimensions of energy  $\times$  length), the distance at which the attraction takes place  $r_0$ , the effective mass  $m^*$  and the density of charge carriers per unit volume,  $n$ .

Although formally similar to the ‘contact potential’ of BCS theory, the physics described by the delta-shell potential are very different: it corresponds to non-retarded attraction at a finite distance  $r_0$ . In that sense, it is more similar to the Hubbard-like models with nearest-neighbour attraction [9]. But note that in the delta-shell model the distance  $r_0$  at which the electrons attract each other is a free parameter that can be varied continuously, and the non-interacting dispersion relation is that of free electrons with an effective mass  $m^*$ .

A preliminary analysis of this model has been carried out using a standard functional integral technique. The details of these calculations are to be found in [6]; however, some of the results will be summarized in what follows as the need arises and, for convenience, the relevant formulae have been reproduced in the appendix.

### 3. On the microscopic origin of the universality of the $T_c$ versus doping law

A remarkable feature of the experimental data on the superconducting cuprates is the dependence of  $T_c/T_{c,max}$  on the number of holes,  $n_h$ , per  $\text{CuO}_2$  unit [4, 10]. Namely,  $T_c/T_{c,max}$  rises and falls as  $n_h$  increases from below optimal doping,  $n_{h,max}$ , to above, and the functional form of this relation is the same for the different materials [4]. Explicitly, it is given by

$$T_c/T_{c,max} = [1 - 82.6(n_h - 0.16)^2]. \quad (2)$$

Remarkably, in the delta-shell model, the ratio  $T_c/T_{c,max}$  does not depend on  $g$ ,  $r_0$ ,  $m^*$  and  $n$  independently, but only on the two dimensionless quantities  $\tilde{n} \equiv n \frac{4\pi}{3} r_0^3$  and  $\tilde{g} \equiv \frac{g}{r_0} / \frac{\hbar^2}{2m^* r_0^2}$ . The dimensionless density  $\tilde{n}$  can be related to  $n_h$  through the value of the ratio  $r_0/r_{\text{Cu-Cu}}$ , where the effective Cu–Cu distance,  $r_{\text{Cu-Cu}}$ , is defined in terms of the proportionality between the number of holes per  $\text{CuO}_2$  unit and their density per unit volume:  $n_h = n r_{\text{Cu-Cu}}^3$ . Thus the values of the dimensionless coupling constant  $\tilde{g}$  and the rescaled range of the attraction,  $r_0/r_{\text{Cu-Cu}}$ , completely determine, for our model, the dependence of  $T_c/T_{c,max}$  on  $n_h$ . We find that, as in the cuprates,  $T_c/T_{c,max}$  rises and falls as a function of  $n_h$ , for fixed  $\tilde{g}$  and  $r_0/r_{\text{Cu-Cu}}$ . Moreover, as we have pointed out earlier [5], we can choose these two parameters so that this rise-and-fall reproduces the shape of the experimental curve, an inverted parabola defined by the position of its maximum and its width. The condition that  $\tilde{g}$  and  $r_0/r_{\text{Cu-Cu}}$  are fixed to the values that produce the best fit, in the d channel (Cooper pairs with angular momentum quantum number  $l = 2$ ), is equivalent to the following two relations between the four parameters  $g$ ,  $r_0$ ,  $m^*$  and  $r_{\text{Cu-Cu}}$ :

$$r_0 = 2.2 r_{\text{Cu-Cu}} \quad (3)$$

and

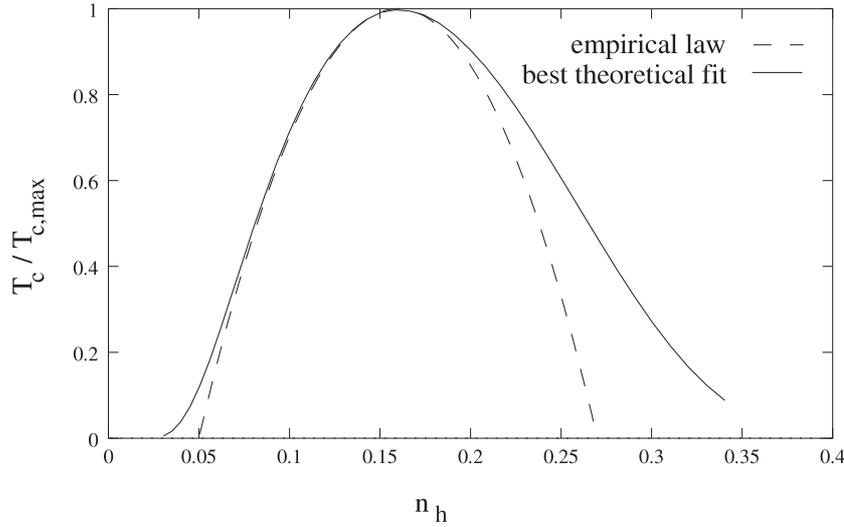
$$g/r_0 = 0.6 \hbar^2 / 2m^* r_{\text{Cu-Cu}}^2. \quad (4)$$

Note that  $m^*$  and  $r_{\text{Cu-Cu}}$  are normal state properties independent of the attractive interaction in equation (1). For clarity, the corresponding fit is recorded in figure 1. Evidently, the above relations determine  $g$  and  $r_0$  for each system, YBCO, LSCO etc, characterized by the frankly phenomenological, but nevertheless clearly material-specific, parameters  $m^*$  and  $r_{\text{Cu-Cu}}$ . Thus although the four parameters are independent of doping, their fixed values are different for different systems. The universal character of the empirical law of equation (2), on the other hand, is embodied in the fact that the relations (3), (4) between the four quantities are the same for all systems. By fitting relative quantities like  $T_c/T_{c,max}$  and universal trends with doping we can hope to have obtained results dependent more on the overall properties of our model than on its material-specific, no doubt inadequate, details.

We would also like to stress that other,  $l \neq 2$ , singlet pairing channels could not fit the observed dependence of  $T_c/T_{c,max}$  on the doping level. In particular, for pairs with angular momentum quantum number  $l = 0$  (s wave), the critical temperature is finite for arbitrarily small values of the density, in contradiction with the observed behaviour, while other pairing channels are negligible in the range of densities of interest [6]. Thus the interpretation of the observed rise-and-fall of  $T_c$  with doping in terms of the delta-shell model implies d-wave symmetry in agreement with the current consensus [12].

### 4. Pressure dependence of $T_c$

As a further validation of our model we shall consider, briefly, the dependence of  $T_c$  on pressure. Experimentally, there are two contributions to the variation of  $T_c$  with applied hydrostatic



**Figure 1.** The best fit of the rise and fall of the d-wave value of  $T_c/T_{c,max}$  to the empirical law.

pressure [16]. The extrinsic contribution is caused by a pressure-induced change of the doping level, combined with the universal  $T_c$  versus doping law (2). On the other hand, there is also an *intrinsic* enhancement of  $T_c$ , i.e. an increase of the value of  $T_{c,max}$ . For the values of the parameters given in equations (3), (4),  $T_{c,max}$  scales with  $\hbar^2/2m^*r_{\text{Cu-Cu}}^2$  and is given by

$$k_B T_{c,max} \approx 0.1 \hbar^2 / 2m^* r_{\text{Cu-Cu}}^2. \quad (5)$$

Thus although  $T_c/T_{c,max}$  is universal, in the sense that it only depends on  $n_h$ , the absolute value of  $T_c$  is material specific, as one would expect in view of the experimental data [14], because it depends also on  $m^*$  and  $r_{\text{Cu-Cu}}$ . Although, along the lines set in the introduction, we do not expect this simple model to reproduce the absolute values of  $T_{c,max}$  accurately, if it contains any of the relevant physics equation (5) must be compatible with the values of  $T_{c,max}$  observed experimentally. Notably, in the cuprates,  $T_{c,max}$  can go from  $\sim 30$  to  $\sim 150$  K, which is consistent with our prediction if  $r_{\text{Cu-Cu}} \sim 5 \text{ \AA}$  and the effective masses are of the order of a few times the bare electron mass. Moreover equation (5) provides a simple interpretation for the origin of the *intrinsic* enhancement of the critical temperature: it is due to the increase of the ‘localization energy’  $\hbar^2/2m^*r_{\text{Cu-Cu}}^2$  associated with the reduction in size of  $r_{\text{Cu-Cu}}$ . By taking the derivative of  $T_{c,max}$  with respect to the volume of the unit cell  $abc$  (which is proportional to  $r_{\text{Cu-Cu}}^3$ ) we can obtain an estimate of such enhancement:

$$\left. \frac{\partial \ln T_{c,max}}{\partial P} \right|_{P=0} \approx \left[ \frac{2}{3} + \frac{\partial \ln m^*}{\partial \ln(abc)} \right] k_V. \quad (6)$$

Here  $k_V \equiv -\partial \ln(abc)/\partial P$  is the compressibility of the material. Note that in writing (6) we have assumed that the relations (3), (4) do not depend on applied pressure. This would be consistent with the universality of (3), (4) if that universality were exact, but note that such universality is probably only approximate. Even so, we can easily use (6) to obtain a specific value as follows. We can employ the usual way of estimating the volume dependence of the electronic effective mass, which is of interest in many fields of solid state physics, by an appeal to the relationship between  $\hbar^2/2m^*$  and an appropriate hopping integral,  $t$ , in the tight-binding description of the relevant band. In the simplest case of a cubic lattice with constant  $r_{\text{Cu-Cu}}$  this is  $m^* \sim 1/tr_{\text{Cu-Cu}}^2$ . Then we use the dependence of  $t$  on the nearest-neighbour distance to

estimate the changes in  $m^*$  with changes in the lattice parameters. Thus we may use  $t \sim r_{\text{Cu-Cu}}^{-\gamma}$  and, assuming that we are dealing with d orbitals, take  $\gamma = 5$  [15]. This yields

$$\frac{\partial \ln T_{c,max}}{\partial P} \approx \frac{5}{3} k_V. \quad (7)$$

Unfortunately, we are not aware of many measurements of the variation of the *maximum* value of the critical temperature under applied hydrostatic pressure. However Wijngaarden *et al* [16] have studied the single-layer compound  $\text{Ti}_{0.5}\text{Pb}_{0.5}\text{Sr}_2\text{Ca}_{1-x}\text{Y}_x\text{Cu}_2\text{O}_7$  and from their data we deduce  $(\partial \ln T_{c,max}/\partial P)_{P=0} \approx 12.3 \times 10^{-3} \text{ GPa}^{-1}$ . Using the value of the compressibility calculated by Cornelius *et al* [17],  $k_V = 8.4 \times 10^{-3} \text{ GPa}^{-1}$ , and our formula in equation (7), we predict  $(\partial \ln T_{c,max}/\partial P)_{P=0} \approx 14.0 \times 10^{-3} \text{ GPa}^{-1}$ , in reasonable agreement with the experiment. Similarly, Schlachter *et al* [18] have obtained  $(\partial T_{c,max}/\partial P)_{P=0} \approx 0.8 \text{ K GPa}^{-1}$  for  $\text{YBa}_2\text{Cu}_3\text{O}_x$  which, using  $T_{c,max} \approx 92 \text{ K}$ , yields  $(\partial \ln T_{c,max}/\partial P)_{P=0} \approx 8.7 \times 10^{-3} \text{ GPa}^{-1}$ . The theoretical prediction in this case, using the value  $k_V = 8.1 \times 10^{-3} \text{ GPa}^{-1}$  quoted in [17], is  $(\partial \ln T_{c,max}/\partial P)_{P=0} \approx 13.5 \times 10^{-3} \text{ GPa}^{-1}$ . Thus the *intrinsic* enhancement of the critical temperature with applied hydrostatic pressure can be understood essentially, at the qualitative level, as the result of the change of the length  $r_{\text{Cu-Cu}}$ , and therefore of the corresponding localization energy  $\hbar^2/2m^*r_{\text{Cu-Cu}}^2$ , under pressure<sup>2</sup>.

We end by stressing that the results presented in this section (unlike those in the previous and following ones) refer to material-specific properties of the cuprates and therefore, in accordance with the philosophy outlined in the introduction, one must not expect our simple model to provide a detailed description of them. For example, it cannot describe the observed effect of the number of adjacent  $\text{CuO}_2$  planes per unit cell, nor of applied uniaxial stress [30], on  $T_c$ , since obviously the parameters  $r_{\text{Cu-Cu}}$  and  $m^*$  do not describe the varying degrees of anisotropy of the normal states.

## 5. The superconducting gap

We shall now return to the main topic of this paper. On the basis of the discussion in the previous sections, we can expect that the delta-shell model, together with the relations (3), (4), can describe quantitatively other material-independent properties of the superconducting state of the cuprates. In fact it *predicts*, with no adjustable parameters, the value of any such quantities. The most interesting one is the ratio between the energy gap to one-particle excitations, at zero temperature, and the critical temperature at optimal doping:  $2\Delta_0/k_B T_{c,max}$ . In the model, this quantity is universal, in the same sense as  $T_c/T_{c,max}$ , because  $\Delta_0$  also scales with  $\hbar^2/2m^*r_{\text{Cu-Cu}}^2$ .

In a very general context, there are two distinct scenarios, which we shall now briefly recall (see [19], and references therein). In the BCS regime ( $\mu > 0$ ) the fermionic quasiparticles with minimum excitation energy lie on a surface in  $k$ -space that is defined by  $\hbar^2 \mathbf{k}_{min}^2/2m^* = \mu$  and the corresponding gap is  $2\Delta_0 = 2|\Delta(\mathbf{k}_{min})|$ , where  $\Delta(\mathbf{k})$  is the usual BCS ‘gap function’. The extreme case of this is the BCS *limit*, defined by  $\mu \gg |\Delta(\mathbf{k})|$  for all  $\mathbf{k}$ , in which the chemical potential is approximately equal to the Fermi energy,  $\mu \approx \varepsilon_F$ , and so the fermionic quasiparticles with minimum energy have wavevector  $\mathbf{k}_{min} \approx \mathbf{k}_F$ , i.e. they lie in the Fermi surface. In the opposite, BE regime ( $\mu < 0$ ), quasiparticles with minimum excitation energy have  $\mathbf{k} = 0$  and the energy gap to single-particle (fermionic) excitations is  $2\Delta_0 = 2\sqrt{\mu^2 + |\Delta(0)|^2}$ , which, in the BE *limit* ( $\mu \ll -|\Delta(\mathbf{k})|$ ), becomes the binding energy

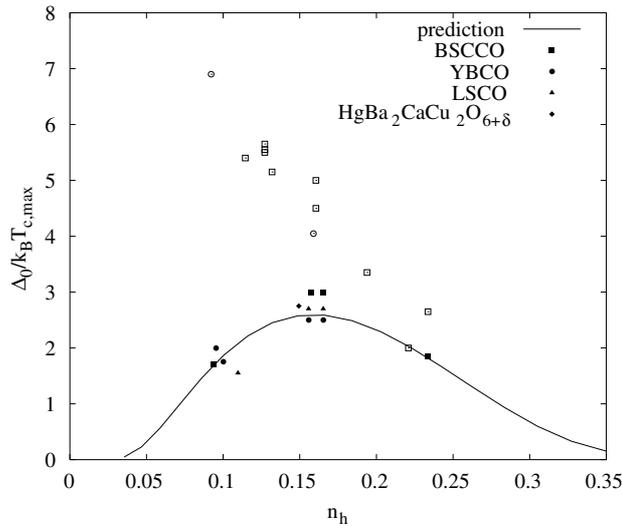
<sup>2</sup> Note that in deriving this result we have used that  $k_B T_{c,max} \propto \hbar^2/2m^*r_{\text{Cu-Cu}}^2$ , which is more general than (5) and, in fact, would hold for any model for which  $\hbar^2/2m^*r_{\text{Cu-Cu}}^2$  is the relevant energy setting the scale of  $T_{c,max}$ .

$\varepsilon_b$  of a pair:  $2\Delta_0 \approx 2\mu \approx \varepsilon_b$ . However in the BE regime the lowest-lying excitations are not fermionic, but bosonic, and therefore there is a second, smaller energy scale, which is associated with the break-up of coherence in the condensate without the dissociation of any pairs, whose value could be related to  $\Delta(\mathbf{k})$ .

The delta-shell model can display both BCS-like and BE-like behaviour, depending on the values of the dimensionless parameters  $\tilde{g}$  and  $\tilde{n}$  introduced above. Specifically, for the values that correspond to equations (3), (4), the model is close to the BCS limit [6]. In fact the rise-and-fall of  $T_c$  with the doping level that we have found in the delta-shell model is only present at low values of  $\tilde{g}$ . At higher values of the dimensionless coupling constant  $\tilde{g}$ , the critical temperature becomes a monotonic function of the density, which furthermore has a finite value for any finite value of  $n$ , as it tends towards the BE condensation temperature  $T_c^{BE} \propto n^{2/3}$ . Moreover the rotational symmetry of the model is restored in this limit due to the fragmentation of the condensate. Thus on the basis of the discussion presented in the previous section we conclude the first of the above scenarios to be operating in the cuprates. Namely, we expect there to be a single energy scale  $\Delta_c$  coming from the superconductivity, which would manifest itself both as the characteristic energy seen in phase-sensitive experiments and as a gap in the single-particle excitation spectrum. In this picture, the origin of the larger ‘pseudogap’ energy  $\Delta_p$  would be quite independent from superconductivity.

Figure 2 shows the experimental data from [1] for the two energy scales  $\Delta_c$  and  $\Delta_p$ , together with our theoretical prediction for the maximum value of the superconducting energy gap in the single-particle spectrum across the Fermi surface,  $\Delta_0$ , for the purported  $d_{x^2-y^2}$  symmetry of the order parameter [12]. All quantities are normalized to  $k_B T_{c,max}$ , which is the way in which, both in the model and, approximately, in the experiments, their values become material independent. Remarkably, the agreement between  $\Delta_0$  and  $\Delta_c$  is rather good. In particular the ratio of  $\Delta_0$  to  $k_B T_{c,max}$  is  $\sim 5$  at optimal doping, both in the theory and the experiments. Obviously, because of the simplicity of our model it is not easy to decide what to make of the above very good agreement. Nevertheless, at the minimum we conclude that it provides evidence in favour of the BCS-like scenario. Moreover the model seems again to confirm the current consensus on the symmetry of the order parameter: for pairs with  $d_{3z^2-r^2}$  symmetry,  $2\Delta_0/k_B T_{c,max} \approx 6.4$  at optimal doping, which is too high to fit the experiments (note that, unlike at  $T_c$ , at  $T = 0$  the different d-wave channels are non-degenerate). Presumably, it is the presence of the crystal field that makes one of the d-wave symmetries preferred over the others. Since this is absent from our model all we can do is examine each of the possible symmetries independently and compare them with the experiments.

Of course, our interpretation of the data presented in [1] differs from that of the author. In effect, it was assumed at the time that there was only one energy gap in the single-particle excitation spectrum, corresponding to the ‘pseudogap’ energy  $\Delta_p$ . This was legitimate back then because only experiments that probed the phase coherence of the condensate (Andreev, Raman, penetration depth) had been able to measure  $\Delta_c$ . However, as we mentioned in the introduction, it has recently been shown experimentally [2, 3] that there are actually two gaps in the spectrum of single-particle excitations: one of them corresponds to  $\Delta_p$ , while the other, smaller one closes in at  $T = T_c$ , very much like a BCS gap. It is this second gap that we have obtained in our calculations, and in our picture it should coincide with the coherence energy  $\Delta_c$ . As regards the other energy scale,  $\Delta_p$ , we have no sign of it in our theory and hence we are inclined to conclude that its origin is not superconductivity. In particular, it cannot be due to ‘preformed pair’ fluctuations of the superconducting order parameter which, as we have discussed, are ruled out on the basis of the empirically determined values of the parameters, equations (3), (4), and their interpretation in terms of the calculations presented in [6].



**Figure 2.** The theoretical prediction for the superconducting gap in the single-particle spectrum  $\Delta_0$  compared with the experimental data for the ‘coherence energy’  $\Delta_c$  (filled symbols) and the ‘pseudogap’ energy  $\Delta_p$  (open symbols) from [1]. All quantities are normalized to the critical temperature at optimal doping,  $T_{c,max}$ .

## 6. Conclusion

We have addressed the question of whether the coherence energy range  $\Delta_c$ , identified by Deutscher, at low temperatures, in cuprate superconductors, as distinct from the ‘pseudogap’ energy  $\Delta_p$ , can be understood as a superconducting gap in the sense of BCS theory. Capitalizing on the fact that certain properties of cuprate superconductors are approximately material independent, we have studied a simple model, obtained as the simplest generalization of the BCS model compatible with exotic pairing. It features free electrons with a non-retarded, effective interaction potential which is attractive at a well defined finite distance  $r_0$  and is zero for all other separations. This ‘delta-shell’ model provides a mechanism for the rise and fall of  $T_c$  with doping, as a consequence of the interplay between the carrier-carrier distance or, in other words, the Fermi wavelength  $|k_F|^{-1}$  and the new microscopic length scale  $r_0$ . Moreover, it can correlate this behaviour with the d-wave symmetry of the order parameter and it provides an interpretation of its approximate universality in terms of certain relations between the parameters of the model. On this basis, the model can be used to predict, with no fitting parameters, the corresponding universal behaviour of the gap in the quasiparticle spectrum due to the superconductivity. For the empirically determined values of the parameters the model is in the BCS regime, as opposed to that of BE condensation of ‘preformed pairs’, which leads to the prediction that the gap to single-particle excitations arising from the superconductivity is equal to  $\Delta_c$ . In fact the prediction for that gap agrees quite satisfactorily with the behaviour of  $\Delta_c$ , suggesting a different origin for the pseudogap  $\Delta_p$ .

The above conclusion is compatible with general arguments based on the available experimental data which indicate that the description of the charge carriers in the BE limit is inappropriate [20]. Although a model that accommodates this fact while still describing the pseudogap in terms of pairing fluctuations has been devised [21], it has also been

suggested [22, 23] that the pseudogap may follow from the spectral properties of stripe phases [24, 25]. More generally, a pseudogap may be a generic feature of systems that are intrinsically inhomogeneous due to the competition between ordered states separated by a first-order phase transition [26, 27]. Such a picture becomes especially appealing in the light of recent scanning tunnelling microscope studies of BSCCO [28, 29]. It could be investigated in our model by evaluating the density fluctuations induced by the attractive interaction, in addition to the pairing fluctuations considered in the present work.

Our analysis complements the one carried out by Szotek *et al* [8], who also modelled  $\Delta_c$  as a BCS superconducting gap, reaching similar conclusions. The main difference between our approach and theirs is that, instead of focusing on a specific material using a detailed description of the electronic structure, we have used a very simple model to capture those features that are approximately material independent. Specifically, our calculations are not based on a fit to the value of  $T_{c,max}$  (which cannot be predicted accurately by such a simple model), but rather to the width of the  $T_c/T_{c,max}$  versus  $n_h$  curve, and the position of its maximum, which are determined by the values of the range of the interaction  $r_0$  and its strength  $g/r_0$ , rescaled to the effective Cu–Cu distance  $r_{Cu-Cu}$  and the corresponding ‘localization energy’  $\hbar^2/2m^*r_{Cu-Cu}^2$ , respectively. Our result that the model is in the BCS limit for the empirically determined values of these parameters speaks in support of the methodology employed in [8], where this was assumed *a priori* by using a BCS-like mean-field theory to calculate  $T_c$ .

Finally we stress that the rise and fall of the critical temperature  $T_c$  and the superconducting gap  $\Delta_0$ , in the BCS limit, is probably a generic behaviour for attractive potentials with a minimum at some finite separation. Essentially, the gap function depends, in this case, on the *magnitude* of  $\mathbf{k}$  as well as on its direction:  $\Delta(\mathbf{k}) = \Delta(|\mathbf{k}|, \hat{\mathbf{k}})$ , and thus its value on the Fermi surface  $\mathbf{k} = \mathbf{k}_F$  depends strongly on the size of the Fermi surface, given by  $|\mathbf{k}_F|$ . This situation is quite different from the BCS model, and its usual d-wave generalizations (see, for example [13]) for which the gap function is independent of  $|\mathbf{k}|$ . Note that the present scenario for the rise and fall of  $T_c$  is quite different from previous proposals. In particular, in our picture this rise and fall is not due to the competition of superconductivity with other kinds of order or the suppression of  $T_c$  by fluctuations away from optimal doping. Moreover, the value of  $T_c$  does not necessarily correlate with the DOS on the Fermi surface<sup>3</sup>. It could be tested if an experimental method to measure directly the variation of the gap function  $\Delta(\mathbf{k})$  with  $\mathbf{k}$  in the radial direction of increasing  $|\mathbf{k}|$ , rather than along the Fermi surface, for example one that would give the value of  $(\partial \Delta_{\mathbf{k}}/\partial |\mathbf{k}|)_{|\mathbf{k}|=|\mathbf{k}_F|}$ , were available.

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<sup>3</sup> In the context of conventional, BCS superconductivity, this has usually been thought to be the primary mechanism by which  $T_c$  can have a non-monotonic dependence on doping. Interestingly, a rise and fall of the critical temperature with doping, which does not seem to correlate to the DOS, has been observed in experiments on gate voltage-doped  $C_{60}$  films [31].

## Appendix

In [6] the ground state of the delta-shell model was studied in the mean-field approximation in which the gap function  $\Delta_{\mathbf{k}}$  and the chemical potential  $\mu$  are determined by two coupled equations [11]. The theory is particularly transparent in terms of their dimensionless counterparts  $\tilde{\Delta}_{\tilde{\mathbf{k}}} \equiv (\frac{\hbar^2}{2m^*r_0^2})^{-1} \Delta(\mathbf{k})$  and  $\tilde{\mu} \equiv (\frac{\hbar^2}{2m^*r_0^2})^{-1} \mu$  (where  $\tilde{\mathbf{k}} \equiv \mathbf{k}r_0$  is the dimensionless wavevector). If  $\tilde{\Delta}_{\tilde{\mathbf{k}}}$  is expanded in spherical harmonics  $Y_{lm}(\hat{\mathbf{k}})$ , it is found to have the form

$$\tilde{\Delta}_{\tilde{\mathbf{k}}} = \sum_{lm} \tilde{\Delta}_{lm} j_l(|\tilde{\mathbf{k}}|) Y_{lm}(\hat{\mathbf{k}})$$

i.e. the radial part is given by the spherical Bessel functions  $j_l(|\tilde{\mathbf{k}}|)$ , and the two equations are, for singlet pairing ( $\tilde{\Delta}_{lm} = 0$  for  $l$  odd),

$$\tilde{\Delta}_{lm} = \tilde{g} \sum_{l'm'} \left\{ \int \frac{d^3\tilde{\mathbf{k}}}{(2\pi)^3} \frac{\tilde{\Lambda}_{lm,l'm'}(\tilde{\mathbf{k}})}{2\sqrt{(\tilde{\mathbf{k}}^2 - \tilde{\mu})^2 + \tilde{\Delta}_{\tilde{\mathbf{k}}}^2}} \right\} \tilde{\Delta}_{l'm'} \quad (8)$$

$$\tilde{n} = \int \frac{d^3\tilde{\mathbf{k}}}{6\pi^2} \left( 1 - \frac{\tilde{\varepsilon}_{\tilde{\mathbf{k}}}}{\sqrt{(\tilde{\mathbf{k}}^2 - \tilde{\mu})^2 + \tilde{\Delta}_{\tilde{\mathbf{k}}}^2}} \right) \quad (9)$$

where  $\tilde{g}$  and  $\tilde{n}$  are the dimensionless coupling constant and density defined in the text, and

$$\tilde{\Lambda}_{lm,l'm'}(\tilde{\mathbf{k}}) \equiv (4\pi)^2 j_l(|\tilde{\mathbf{k}}|) j_{l'}(|\tilde{\mathbf{k}}|) Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}). \quad (10)$$

All the ground-state properties that we discuss in the text were obtained by solving the above two equations self-consistently, for ‘trial ground states’ in which specific constraints were imposed on the  $\tilde{\Delta}_{lm}$ . Note that these equations are valid approximations not only in the BCS limit, encountered for large  $\tilde{n}$  or when  $\tilde{g}$  is below the threshold to bind an isolated pair, but also in the opposite, BE condensation limit [32, 33].

To find the condensation temperature  $T_c$  we went a small step beyond the mean-field theory, including quadratic fluctuations about it. In a manner similar to that reviewed in [19] we found that  $\tilde{\beta}_c = \frac{\hbar^2}{2m^*r_0^2} / k_B T_c$  is determined by

$$\frac{1}{\tilde{g}} = \frac{2}{\pi} \int_0^\infty d|\tilde{\mathbf{k}}| |\tilde{\mathbf{k}}|^2 j_l(|\tilde{\mathbf{k}}|)^2 \frac{1 - 2f[\tilde{\beta}_c(|\tilde{\mathbf{k}}|^2 - \tilde{\mu}_c)]}{2(|\tilde{\mathbf{k}}|^2 - \tilde{\mu}_c)} \quad (11)$$

$$\tilde{n} = \frac{4}{3\pi} \int_0^\infty d|\tilde{\mathbf{k}}| |\tilde{\mathbf{k}}|^2 \left\{ f[\tilde{\beta}_c(|\tilde{\mathbf{k}}|^2 - \tilde{\mu}_c)] + g \left( \tilde{\beta}_c \frac{|\tilde{\mathbf{k}}|^2}{2} \right) \tilde{w}_{l,|\tilde{\mathbf{k}}|}^{\tilde{\beta}_c, \tilde{\mu}_c} \right\} \quad (12)$$

where  $\tilde{\mu}_c$  is the value of  $\tilde{\mu}$  at the transition and  $f(z)$  and  $g(z)$  denote the usual Fermi and Bose distribution functions. The term containing the Bose function, times the ‘weight’  $\tilde{w}_{l,|\tilde{\mathbf{k}}|}^{\tilde{\beta}_c, \tilde{\mu}_c}$ , is the contribution from the above mentioned fluctuations, described here to the lowest non-trivial order in their frequency and momentum, and it signals the presence of preformed pairs, with the same internal angular momentum quantum number  $l$  as the condensate, above  $T_c$  (in these expressions, the contribution from other pairs has been neglected). This contribution dominates in the BE limit (where its ‘weight’ takes the form  $\tilde{w}_{l,|\tilde{\mathbf{k}}|}^{\tilde{\beta}_c, \tilde{\mu}_c} \approx 2l + 1$ , and thus it simply accounts for the degeneracy of the internal state of the pairs) while being negligible in the BCS limit. Note that the critical temperature is degenerate in the magnetic quantum number  $m$ , although it still depends on  $l$ .

From the point of view of the present paper it is particularly relevant that both  $\tilde{\Delta}_{lm} / k_B T_{c,max}$  and  $T_c / T_{c,max}$  depend only on the dimensionless parameters  $\tilde{g}$  and  $\tilde{n}$ , as direct consequences of equations (8), (9) and (11), (12), respectively.

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