Single origin of the nodal and antinodal gaps in cuprates

Yves Noat$^{1(a)}$, Alain Mauger$^2$ and William Sacks$^2$

$^1$ Sorbonne Université, Institut des Nanosciences de Paris, CNRS, UMR 7588 - 4 Place Jussieu, 75005 Paris, France

$^2$ Sorbonne Université, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, CNRS, UMR 7590 4 Place Jussieu, 75005 Paris, France

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Abstract – Recent angle-resolved photoemission electron spectroscopy (ARPES) experiments demonstrate that the momentum dependence of the spectral gap in underdoped cuprates does not follow a pure $d$-wave form (Anzai H. et al., Nat. Commun., 4 (2013) 1815). This deviation is highly controversial. It has often been interpreted as a proof of the non-superconducting origin of the antinodal gap in the underdoped regime. In this paper, we show that the measured angular dependence of the spectral gap can be explained by the basic nature of pairs in high-$T_c$ cuprates. Hole pairs, or pairons, form as a result of the local antiferromagnetic environment on the scale $\xi_{\text{AF}}$, the magnetic coherence length. The spatial extension of the pairon wave function beyond first nearest neighbours gives rise to the anomalous angular dependence of the gap, in quantitative agreement with experiments. This simple interpretation strongly indicates the common origin of the nodal and antinodal gaps.

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Introduction: Are there two energy scales in superconducting cuprates? – One of the most challenging problems of high-$T_c$ cuprates is the interpretation of the spectral gap. Contrary to conventional superconductors where the spectral gap vanishes at the critical temperature, as described by the Bardeen-Cooper-Schrieffer (BCS) theory [1], in cuprates a gap persisting at the critical temperature $T_c$, the so-called pseudogap, is directly observed in angle-resolved photoemission spectroscopy (ARPES) [2,3] or scanning tunneling spectroscopy [4]. Whether or not the pseudogap is linked to superconductivity remains a fundamental question.

More recently, low-temperature experiments revealed a non-trivial angular dependence of the gap as a function of doping. While in overdoped samples the gap follows a strictly $d$-wave behavior, a clear deviation from $d$-wave is observed on the underdoped side of the phase diagram (see [5] and references therein). This so-called two-gap behavior was first revealed by electronic Raman scattering [6] and photoemission [7] and later confirmed by tunneling spectroscopy [8]. It is most often interpreted as the result of the competition between superconductivity and the phase responsible for the pseudogap [7,9–11]. As first noted by Kondo et al. [12] and Terashima et al. [13], the shape of $\Delta(\theta)$ can be properly described by including an additional harmonic term to the usual $d$-wave dependence:

$$\Delta(\theta) = \Delta_0 [B \cos(2\theta) + (1-B) \cos(6\theta)]. \quad (1)$$

An analogous formula was later used by Anzai et al. [14] who carefully studied the angular dependence of the gap as a function of doping. The fit of the ARPES data can be used to determine the doping dependence of the nodal and antinodal gaps. By this procedure, Anzai et al. found a dome shape for the nodal gap, which was then interpreted as the order parameter [14], suggesting that the superconducting (SC) state is restricted to the near nodal region in $k$-space (i.e., in the Fermi arc region, as in ref. [10]).

A separate analysis performed by Vishik et al. [11] led to a completely different conclusion, namely that the nodal gap is almost doping independent in the underdoped regime while it is almost equal to the antinodal value in the overdoped regime. The crossover between the two behaviors occurs for a doping value $p \sim 0.18$ (i.e., slightly

$^{(a)}$E-mail: yves.noat@insp.jussieu.fr (corresponding author)
higher than the optimum doping value $p \sim 0.16$). This discrepancy between the two analyses clearly indicates that a more careful attention should be paid to the method used to infer the nodal gap value. From an overview of the literature on this question [5], one concludes that the connection of the nodal and antinodal gaps to the SC state remains an important unsolved issue for understanding high-$T_c$ superconductivity.

In this paper, we reconcile the contradictory experimental analysis and give a simple explanation for the angular dependence of the gap in the whole doping range, from underdoped to overdoped regimes. Our analysis demonstrates that the latter is essentially governed by the doping dependence of the antiferromagnetic coherence length $\xi_{AF}$, which determines the size of pairs forming the SC condensate.

**Angular dependence of the gap.** – There is an overall agreement that, at least in the overdoped regime, the spectral gap as a function of angle has a simple $d$-wave form:

$$\Delta(\vec{k}) = \Delta_p [\cos(k_x a) - \cos(k_y a)].$$

At the Fermi surface ($k = k_F$), this formula can be well approximated by

$$\Delta(\theta) \simeq \Delta_p \cos(2\theta).$$

The angle in the above formula is taken from the $(\pi, \pi)$ corner of the first Brillouin zone. With these coordinates, the antinodal direction ($\pi, 0$) corresponds to $\theta = 0$ while the nodal direction ($k_x = k_y$) corresponds to $\theta = \pi/4$.

Deviations from this standard form have been observed in the underdoped regime by several groups [11–15]. Such deviations, as in figs. 1 and 2, occur if the doping is lower than some value, which varies from experiment to experiment (see [5] for a review). The latter is generally higher than the optimum doping value [5].

Although the angular dependence of $\Delta(\theta)$ includes new harmonics as mentioned above, in the underdoped regime the overall shape still has a $d$-wave character. We find it useful to reformulate eq. (1), in an alternate algebraic form:

$$\Delta(\theta) = \Delta_p \left[ 1 - \alpha \sin^2(2\theta) \right] \cos(2\theta)$$

(4)

In this form, the gap at the antinode is by definition $\Delta(0) = \Delta_p$, while the so-called nodal gap is defined by

$$\Delta_N = \left. \frac{1}{2} \frac{d\Delta(\theta)}{d\theta} \right|_{\theta = \pi/4} = \Delta_p (1 - \alpha).$$

(5)

Note that while the common name often given to $\Delta_N$ is the nodal “gap”, it is in fact the slope of $\Delta(\theta)$ at the node. Thus, $\alpha$ appears as the key parameter giving rise to the difference between the nodal and the antinodal gaps.

We have fit the experimental spectra from Anzai et al. [14] for different doping values. As shown in fig. 1 the agreement between eq. (4) and the experiment is remarkable. While in the overdoped regime, the shape of $\Delta(\theta)$ is perfectly $d$-wave, a clear deviation is observed in the underdoped side of the phase diagram. This deviation grows as the doping is lowered. We have also analysed data from Vishik et al. [11] as well as the one reported by Hashimoto et al. [15]. As shown in fig. 2, eq. (4) also perfectly reproduces the angular dependence of the gap they have observed in a wide doping range.

We now come to the determination of the slope of $\Delta(\theta)$, i.e., the nodal gap. In ref. [11], the latter was derived from
the linear fit of the gap value near the node. This method, however, is not correct, because the curvature of the experimental curve does not vanish at any value of $\theta$ in the underdoped regime, so that the slope found by assuming a priori a linear behavior near the node depends on both the number of experimental points and the extention in $\theta$ chosen to make such a fit.

Contrary to the procedure used in [11], where the slope was tentatively estimated from the experimental points near the node, we calculate the nodal gap from the fit of $\Delta(\theta)$ using eq. (5). This is a fundamental point in the analysis. Indeed, it should be stressed that in order to deduce precisely the slope of $\Delta(\theta)$ at the node, given by eq. (4), one needs to properly fit the whole curve from the node to the antinode. This difference explains the discrepancy in the determination of $\Delta_N$ reported in [11] and [14].

The nodal gap inferred from our analysis is plotted in fig. 3 which proves the consistency of the data of both refs. [14] and [11]. Although the nodal gap has a dome shape, it is nevertheless clear that it does not follow $T_c$. The maximum of $\Delta_N(p)$ is shifted with respect to that of $T_c(p)$. Moreover $\Delta_N(p)$ does not vanish for $p = p_{\text{min}}$ where the superconducting phase first appears. This finding seems to discard the hypothesis that the nodal gap is directly the order parameter, contrary to the conclusion raised in [14].

In addition, the doping dependence of the parameter $\alpha$ which characterizes the deviation from $d$-wave, closely follows the one deduced from the data of Anzai et al. [14], which gives good confidence in our analysis.

The present approach thus reconciles ARPES experiments where contradictory interpretations were given. We now turn to the physical origin of the anomalous angular dependence.

**Pairons: hole pairs in a short-range antiferromagnetic background.** – As demonstrated by pioneering works in the early nineties in the context of the Hubbard or $t$-$J$ Hamiltonians, two holes in an antiferromagnetic background can form a bound state for a sufficiently large $t/J$ ratio [16–19], with the expected $d$-wave symmetry [20]. These works strongly suggest the existence of hole pairs in an AF background, although the description in terms of strongly correlated electrons might fail in the overdoped side of the phase diagram [21].

We have extended this concept to realistic systems [22] where the key point is the small but finite antiferromagnetic coherence length. Indeed, in cuprates, the long-range antiferromagnetic state is broken by hole doping at $p = p_{\text{AF}}$, giving rise to a superconducting state with short-range AF correlations for $p > p_{\text{min}}$ [23]. The superconducting phase emerges from the metallic phase in the doping range $p_{\text{min}} < p < p_{\text{max}}$.

In recent papers, we have proposed that high-$T_c$ superconductivity can be explained in terms of the formation of hole pairs, or pairons, in their local antiferromagnetic environment [22], on the scale of $\xi_{\text{AF}}$. In [22] each pairon is associated with an AF cell of area $\xi_{\text{AF}}^2$ which naturally explains the linear behavior of the antinodal gap energy with doping.

Two different temperatures can be distinguished corresponding, respectively, to the formation of the pairs and their condensation, both being linked to a single energy scale, $J$, the exchange energy. Pairons form at a temperature $T^+$ higher than the critical temperature and undergo a Bose-like condensation at $T_c$ as a result of repulsive pair-pair interactions [24].

The pairon model is supported by several experimental facts, in particular by

i) the presence of a low-temperature energy gap within the vortex core where coherence is lost [25], which strongly suggests the presence of preformed pairs;

ii) the concomitant disappearance of superconductivity and antiferromagnetic correlations as a function of doping (for $p = p_{\text{max}}$) [26];

iii) the scaling of the critical temperature with the exchange energy $T_c \propto J$ [27], which is a direct consequence of the nature of pairons and of the corresponding phase diagram [22].

The nature of pairons is revealed in the excitation spectrum as a function of temperature. Indeed, two well-defined signatures are observed in ARPES measurements: a Fermi arc near the node at $T_c$ and below [28] and a gap without coherence peaks, the pseudogap, in the antinode above $T_c$ [2,3]. The latter display the characteristic Bogoliubov quasiparticle dispersion indicating preformed pairs [29,30]. In the pairon model, the Fermi arc is the result of fermion excitations, due to the composite fermion character of pairons, while the pseudogap is a
manifestation of an incoherent state of excited pairons, absent in a conventional BCS superconductor [31].

**Origin of the angular dependence of the gap.** – The pairon model also provides a physical explanation for the observed gap angular dependence. Indeed, to understand the shape of $\Delta(\theta)$, one needs to consider how the gap is modified at low doping as the size of antiferromagnetic correlations increases. For this purpose, we start from the expression of the hole pair wave function in relative coordinates. In our previous work [31], only first nearest neighbours were considered (red dots in fig. 4):

$$\psi_{\text{pair}}^{(1)}(\vec{r}) = \frac{1}{\sqrt{4}}[\varphi(\vec{r} - ax) + \varphi(\vec{r} + ax) - \varphi(\vec{r} - ay) - \varphi(\vec{r} + ay)],$$

where $a$ is the lattice parameter, and $\varphi(\vec{r}) = e^{-\frac{x^2}{a^2}}/\sqrt{2\pi a^2}$. The parameter $b$ fixes the spatial extension of the pair wave function in relative coordinates. The overlap between the various amplitudes in eq. (6) has been neglected. Note that the sign in the above formula originates from the antiferromagnetic symmetry which imposes that the wave function must vanish in the lattice diagonal (corresponding to the nodal direction in $k$-space).

It follows that the associated gap is expressed in the standard $d$-wave form (eq. (2)) [31]:

$$\Delta(k) = \tilde{\varphi}(k_F) A_1 g_1(k_x, k_y),$$

where $\tilde{\varphi}(k_F)$ is the Fourier transform of $\varphi(\vec{r})$ taken at $k = k_F$, $A_1$ is a constant and

$$g_1(k_x, k_y) = \cos(k_x a) - \cos(k_y a).$$

As the doping is lowered, the size of the pairons, of the order of $\xi_{AF}$, increases. The delocalized wave function must then include the contribution of next nearest neighbours (blue dots in fig. 4):

$$\psi_{\text{pair}}(\vec{r}) = \sum_i \psi_{\text{pair}}^{(i)}(\vec{r})$$

with $\psi_{\text{pair}}^{(i)}(\vec{r}) \propto \sum_{\vec{r}_j} c_i \varphi(\vec{r} - \vec{r}_j)$; the sum runs over all the $i$-th nearest neighbours and $c_i = \pm 1$ determines the sign of each term and is imposed by the AF symmetry, as explained below. The second-neighbour correction is expressed as

$$\psi_{\text{pair}}^{(2)}(\vec{r}) \propto -\varphi(\vec{r} - 2ax - 2ay) + \varphi(\vec{r} + ax + 2ay) + \varphi(\vec{r} + 2ax + ay) - \varphi(\vec{r} + ax + ay) + \varphi(\vec{r} + ax + ay) - \varphi(\vec{r} - ax + ay).$$

The Fourier transform of the wave function $\psi_{\text{pair}}(\vec{r})$ (eq. (9)) then gives rise to additional terms. As described in a previous paper [31], the pairon wave function can then be expressed as a superposition of Cooper pairs in $k$-space. Extending the calculation derived in [31], we obtain the gap function

$$\Delta(\vec{k}) = \tilde{\varphi}(k_F) \sum_i A_i g_i(k_x, k_y),$$

where $\tilde{\varphi}(k_F) A_i g_i(k_x, k_y)$ is the contribution to the gap amplitude of the $i$-th nearest neighbours. The first term has the standard $d$-wave form, while the second-nearest-neighbour contribution, deduced from eq. (10), is expressed as

$$g_2(\vec{k}) = [-\cos(2k_x a + k_y a) + \cos(k_x a + 2k_y a) + \cos(k_x a - 2k_y a) - \cos(2k_x a - k_y a)].$$

There are two possible signs for the second-neighbour correction to the wave function, $g_2(\vec{k})$. The positive sign in front of the bracket was chosen in order to properly describe the experimental results. It is compatible with the AF symmetry, introducing new nodal lines in the second-neighbour correction, in agreement with the higher angular harmonics of eq. (4). This effect reduces the nodal gap compared to the antinodal value (see fig. 4(b)).

**Discussion.** – The previous expression accounts quantitatively for the angular dependence of the gap. The reason is that, for any choice of $A_1$ and $A_2$, the above formula is strictly equivalent to formula 4 used for the fits (i.e., there is an equivalence between the parameter $\alpha$ used in eq. (4) and $A_2/A_1$). The correspondence between the parameter using formula (4) and (11) restricted to second neighbours can be found in table 1. It is relatively straightforward to express the coefficients $A_i$ reflecting the weight of the $i$-th neighbour in the hole pair wave function. We have numerically evaluated $A_i$ for $i = 3$ and 4 which turn out to be negligible so that only second neighbours contribute to the angular dependence of the gap at low doping.
Table 1: Experimental parameters \((T_c, \Delta_p, \Delta_N)\) from Anzai et al. [14] and parameters deduced from the fits (the nodal gap \(\Delta_N, \alpha, \eta, \frac{\xi}{\sqrt{\eta}}\)) as a function of the doping value \(p\). We also indicate the calculated value of \(\xi_{AF}(p)\) (a units) obtained using eq. (14) with \(p_{AF} = 0.02\) for each doping value.

| \(p\) | \(T_c\) (K) | \(\frac{2\Delta}{kT_c}\) | \(\Delta_p\) (meV) | \(\Delta_N\) (meV) | \(\alpha\) | \(\eta\) | \(\frac{A_2}{A_1}\) | \(\xi_{AF}\) (a units) |
|------|----------|-----------------|-----------------|-----------------|--------|-------|-------------|-----------------|
| 0.25 | 37.5     | 5.6             | 9               | 9               | 0      | 0     | 0           | 2.9             |
| 0.22 | 63       | 7               | 19              | 19              | 0.05   | 0.015 | 0.01       | 3.16            |
| 0.194| 80       | 7.8             | 26.9            | 23.6            | 0.12   | 0.051 | 0.036      | 3.4             |
| 0.164| 91       | 9.6             | 37.7            | 30.16           | 0.2    | 0.082 | 0.06       | 3.7             |
| 0.131| 73       | 15.6            | 49              | 30.87           | 0.37   | 0.185 | 0.13       | 4.2             |
| 0.117| 66       | 19.6            | 55.8            | 26.8            | 0.52   | 0.275 | 0.2        | 4.5             |
| 0.077| 42       | 36.8            | 66.6            | 21.9            | 0.7    | 0.364 | 0.295      | 5.9             |

The second-neighbour correction to the gap must be directly related to the extension of the pairon wave function, \(i.e.,\) to the size of the AF correlations. Let us rewrite eq. (11) in the equivalent form:

\[
\Delta(\vec{k}) = \tilde{\varphi}(k_F) A_1 \left[ g_1(k_x, k_y) + \frac{A_2}{A_1} g_2(k_x, k_y) \right]. \tag{13}
\]

Assuming that \(A_2 = \eta e^{-\frac{d_2-d_1}{\xi_{AF}}}\), with \(d_1 = a\) and \(d_2 = \sqrt{5}a\) being the distance between two holes when first and second neighbours sites are occupied (red and blue dots in fig. 4), for each doping value, the correction to pure \(d\)-wave symmetry can be found.

The doping dependence of the antiferromagnetic correlation length has been deduced from neutron experiments and is close to \(1/\sqrt{\eta}\) [32,33]. We take

\[
\xi_{AF}(p) \propto \frac{a}{\sqrt{p-p_{AF}}}, \tag{14}
\]

where \(a\) is the lattice parameter. The parameter \(p_{AF}\) has been introduced in order to describe more precisely the data of ref. [33] than with the \(1/\sqrt{p}\) dependence.

It accounts for the divergence due to the long-range order onset at the AF transition for \(p = p_{AF} \approx 0.02\). The values of \(\eta\) corresponding to each doping value is given in table 1.

As indicated in the table, \(\xi_{AF}(p)\) varies between \(\sim 3a\), and \(\sim 6a\) in the entire SC doping range. Since \(a \sim 3.8\,\text{Å}\), it explains why the third and fourth nearest neighbours do not have a significant contribution. This leaves only the second-neighbour contribution (with the coefficient \(A_2\)) to fit the experimental curves of \(\Delta(\theta)\). The precise fits to the experimental ARPES data can be done with either using the \(\alpha\) parameter, and eq. (4), or the ratio \(A_2/A_1\), using eq. (13).

Both the \(\alpha\) parameter and the ratio \(A_2/A_1\), representing the extension of the pairon wave function to the second neighbors, vary continuously and monotonically with doping which is a strong indication that \(\Delta_N\) and \(\Delta_{AF}\) have a single origin. The evolution of the shape of \(\Delta(\theta)\) as a function of doping can thus be coherently interpreted as a direct consequence of the spatial extension of pairons, which follows \(\xi_{AF}(p)\) as a function of hole concentration as predicted in [22]. However it should be stressed that another microscopic model, such as resonant valence bond theory [34], which would predict a wave function with a similar symmetry cannot be completely ruled out.

As shown in the phase diagram of fig. 3, the nodal gap has a dome shape but does not follow \(T_c\). As mentioned before, this behavior demonstrates that the nodal gap is not the order parameter. Examining its shape, it is tempting to extrapolate the behavior of \(\Delta_N\) for lower doping values. Its finite value at \(p = p_{min}\) would suggest that a non-zero nodal gap persists in the small doping range \(p_{AF} < p < p_{min}\) between the long-range AF order Mottn transition and the superconducting state where the sample is in an insulating state with short-range AF correlations [23].

This hypothesis is in agreement with the findings of Chatterjee et al. [35] who measured the ARPES spectra for a strongly underdoped non-superconducting sample of \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) \((p \approx 0.04)\), and found a gap with nodes, as in the SC state. While the absence of deviation from \(d\)-wave symmetry in this sample is not completely understood, the presence of a gap suggests the existence of non-condensed pairons in this system. Compatible with this discussion is the recent discovery of a gap with a similar angular dependence as in cuprates in electron-doped Mott insulator \(\text{Sr}_2\text{IrO}_4\) [36,37]. In both cases, it is remarkable that the presence of a gap without superconducting coherence may reveal an incoherent gas of pairons in the insulating phase.

**Conclusion.** – In this paper, we have shown that the deviation of the superconducting gap from pure
d-wave symmetry observed in cuprates by ARPES can be interpreted as the result of the existence of hole pairs, or pairons, in their local antiferromagnetic background. In the overdoped regime, the gap has a pure d-wave symmetry, due to the small extension of the pairon wave function, restricted to first nearest neighbours. In the underdoped regime, the pairon wave function extends beyond first nearest neighbours, on the scale of the antiferromagnetic coherence length, which reduces the gap amplitude near the nodal direction.

The model reproduces quantitatively the measured angular dependence of the gap and its doping dependence. Furthermore, it reconciles some divergences in the interpretation of ARPES data in the literature. One concludes that the nodal and antinodal gaps originate from the same phenomenon, both intimately linked to the superconducting phase transition.

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