TOPICAL REVIEW

Theory of extrinsic and intrinsic tunnelling in cuprate superconductors

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Abstract

There has been a huge theoretical and experimental push to try to illuminate the mechanism behind the high-temperature superconductivity of copper oxides. Cuprates are distinguishable from conventional metallic superconductors in originating from the doping of the parent charge-transfer insulators. The superconducting parts are weakly coupled two-dimensional doped layers held together by the parent lattice. Apart from their high-$T_c$ they have other characteristic features including the ‘superconducting’ gap (SG) which develops below the superconducting critical temperature and can be seen in extrinsic and intrinsic tunnelling experiments as well as using high-resolution angle-resolved photoemission (ARPES); there also exists another energy gap, the ‘pseudogap’ (PG), which is a large anomalous gap that exists well above $T_c$. We present a brief review of recent theories behind the pseudogap and discuss in detail one specific (polaronic) approach which explains the SG, PG and unusual tunnelling characteristics of cuprate superconductors.

(Some figures in this article are in colour only in the electronic version)

Contents

1. Introduction: pseudogap scenarios 1
2. Experimental results for PG and SG: tunnelling and some other probes 2
3. Bosonic (bipolaronic) superconductivity 4
4. Energy band structure of cuprates 5
5. NS tunnelling 6
6. SS tunnelling 7
7. Summary 10
Acknowledgments 10
References 10

1. Introduction: pseudogap scenarios

Since the discovery of high-$T_c$ superconductivity in 1986 by Bednorz and Müller [1], there has been a huge theoretical effort to understand the mechanism behind it. A lanthanum barium copper oxide was the first compound displaying this phenomenon [1], now we know there are many compounds displaying high-temperature superconductivity that contain copper and oxygen, these make the cuprate family. Cuprates have unique properties, as well as their high transition temperature, $T_c$, they also have two energy scales, or gaps. The smaller of the two is the BCS-like ‘superconducting’ gap (SG) which develops below the superconducting critical temperature and can be seen by extrinsic and intrinsic tunnelling experiments as well as high-resolution angle-resolved photoemission (ARPES) experiments. There also exists another energy gap, the ‘pseudogap’ (PG) which is a large anomalous gap that exists well above $T_c$. The PG phenomena was first observed in spin responses [2, 3] and with scanning tunnelling spectroscopy [4] in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. Shortly after, the same gap was observed through infrared measurements [5], many experiments have since exhibited this PG.

The first explanation of the pseudogap was offered in the form of real-space preformed hole pairs [6] called small bipolarons. These bipolarons are bound together by a strong electron–phonon interaction (EPI). Many theoretical explanations have since been proposed for the origin of the PG which can roughly be divided into two groups. The first of these groups argues that the PG originates from some order, either static or fluctuating. The second understands the PG is the precursor of the SG, and reflects pair fluctuations above $T_c$. 

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Some of the theories from the first group see the superconducting state of cuprates as being the result of a doped Mott insulator (for example [7], see [8] for a review). In his resonating valence bond (RVB) theory, Anderson focuses on the ground state and low lying excitations, the origin of the PG is seen as the spin gap associated with the breaking of RVB singlets [9]. It has been suggested that adding impurities to (or doping) cuprates could weaken the order parameter (for example this order parameter could be antiferromagnetic spin fluctuations [10]) and thus be the cause of the PG. Some believe the PG could be the result of $SU/2$ rotations (for example [11]) in the underdoped region which connect fluctuations of staggered flux states and d-wave superconductivity. Chakravarty et al [12] proposed a static orbital current state called a d-density wave was the origin of the PG based on phenomenological grounds. It has been argued that the PG is a consequence of a spin density wave (SDW) or charge density wave (CDW) state [13], or an interplay between the two [14]. It has also been suggested that the PG could be the result of inhomogeneous charge distributions containing hole-rich and hole-poor domains [15, 16], or the cause of the SG and PG could be the inter-band pairing of an itinerant band and defect states [17].

The second group bases the understanding of the PG and high-$T_c$ superconductivity on pairing interactions. Preformed Cooper pairs have been suggested [18], where the pairing is not in real-space but instead in momentum–space. It has however been implied that the short coherence length of cuprate superconductors suggests they lie somewhere between the BCS limit of very large momentum–space pairs and the opposite case of small real-space pairs undergoing a Bose–Einstein condensation (BEC) [19]. The BCS–BEC crossover has been studied in detail, for example in [20] a superfluid state is approached in a system of localized bosons (tightly bound electron pairs) in contact with a reservoir of itinerant fermions (electrons), it is assumed the spontaneous decay and recombination between the two species causes superconductivity and the PG is a consequence of this, opening up in the fermionic density of states (DOS). Another idea involving the BCS–BEC crossover utilizing the nearest-neighbour attractive Hubbard model suggests the cause of the PG is the existence of two different bosonic modes leading to an angle-dependent boson distribution function where two-particle states ‘eat’ the single-particle spectral weight in certain areas of momentum [21].

Attractive Hubbard models have been considered as the origin of superconductivity and the PG. For example, studies of the normal-state of the two-dimensional attractive Hubbard model have been carried out using quantum Monte Carlo (QMC) calculations [22], also the excited and ground state properties of the two-dimensional attractive Hubbard model have been studied using the conserving, self-consistent $T$-matrix formalism in the intermediate-coupling regime and at low electron concentration [23]. Other approaches emphasize the weak phase stiffness in underdoped cuprates which is a result of low superfluid density and it leads to a suppression of $T_c$ by phase fluctuations [18]. A diagrammatic theory of the one-band Hubbard model was proposed, where the temperature of the onset of the PG is related to the scattering rate [24]. The effects of classical phase transitions on the quasiparticle spectra were contemplated in underdoped cuprates in the PG regime above $T_c$ by taking into account mean-field d-wave quasiparticles that are semically coupled to supercurrents induced by fluctuating unbound vortex–antivortex pairs [25]. Another idea with incoherent d-wave quasiparticles suggests that when the phase-coherence length exceeds the Cooper pair size, a PG appears [26], the phase fluctuations of a $d_{x^2−y^2}$ pairing gap in a two-dimensional BCS-like Hamiltonian approach is thought to be the origin of the PG [27]. A phenomenological theory was produced that allowed the modelling of the effect of local superconducting correlations and long-range phase fluctuations on the spectral properties of high-temperature superconductors by reasoning that the PG is connected to the character of the excitations that are responsible for destroying superconductivity [28].

2. Experimental results for PG and SG: tunnelling and some other probes

Femtosecond spectroscopy is a tool for studying the temperature dependence of gaps, for example [29] investigates the temperature independence of the PG and dependence of the SG in Y$_{1-x}$CaBa$_2$Cu$_3$O$_{7−δ}$ and HgBa$_2$Ca$_2$Cu$_3$O$_{8+δ}$. Raman spectroscopies have also been able to find two energy scales [30]. ARPES has provided valuable information about cuprates, ARPES performed on Bi$_2$212 [31–34], Bi$_2$201 [35], LSCO [36], LBCO [37] and CaNaCuOCl [38] has verified the presence of two energy gaps in cuprates.

Scanning tunnelling microscopy (STM) offers a powerful technique to look at the doping, temperature and spatial dependence of the DOS with high resolution. It is sensitive to the DOS near the Fermi energy and to a gap in the quasiparticle excitation spectrum. Extrinsic tunnelling experiments have left us with many questions regarding the properties of cuprates. STM tunnelling spectra exhibit an SG and PG [39–41] whose origin currently remains unaccounted for, despite many ideas discussed above. STM results on single crystals of Bi$_2$212 (for example [42–44]) and LSCO [45, 46] have demonstrated the temperature, doping and spatial dependence of the SG and PG. In particular, in NS tunnelling, Kato et al [46] found that the PG is not uniform in real-space and its spatial average increases with decreasing hole concentration in spite of suppression of critical temperature. On the other hand a smaller gap (presumably SG) is uniform across the sample and is less doping dependent. See figures 1 and 2 for recent examples of STM with cuprates.

Intrinsic (superconductor–superconductor, SS) tunnelling experiments on small Bi$_2$212 [47–50] and LSCO [51] mesas have found sharp quasiparticle peaks at the SG and broad humps representing the PG [47]. The PG exists above and below $T_c$ and can persist up to room temperature [47]. The advantages of intrinsic tunnelling are that it is a direct spectroscopic technique that avoids problems like surface deterioration [49], it probes the bulk electronic properties of samples, it offers high resolution whilst being mechanically
Figure 1. STM results with Bi2212 samples, taken at 20 K, so the sample is in the superconducting state [42]. Both the SG and PG are evident, the SG indicated by the black vertical arrows, the PG by the horizontal arrows. Each colour indicates tunnelling spectra taken at a different doping concentration. The SG is unaffected by the doping unlike the PG. Reproduced with permission from [42]. ©American Physical Society.

Figure 2. STM results with La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [46]. These results are more difficult to obtain than STM with Bi2212 since LSCO cannot be cleaved so easily. Asymmetry is present in each spectra as is the SG and PG. At each doping level the spectra is taken at different spatial positions on the LSCO sample. Here, the SG is almost position and doping independent, the PG is dependent on both position and doping. Notice the similarity of these results with those of Bi2212, figure 1. Reproduced with permission from [46]. ©JPSJ.

In the tunnelling spectra of conventional semiconductors or Mott insulators, asymmetry is expected. Consider a semiconductor where the number of electrons is twice the number of ions as each ion can accommodate a spin up and spin down electron. Removing $X$ electrons from the sample leaves the number of electrons as $2N - X$. When positive bias is applied to the sample, the electrons tunnel from the tip to the sample, application of negative bias gives tunnelling in the opposite direction. The probability of an electron tunnelling is, for negative bias (sample to tip), proportional to the number of electrons available, this is $2N - X$. For positive bias (tip to sample) the probability of tunnelling is proportional to the number of holes available in the sample for the electrons in the tip to tunnel to, this is $X$. The ratio of the integrated negative and positive conductance is given by $R = (2 - x)/x$, where $x = X/N$. Similarly we can consider a Mott insulator where the Coulomb repulsion is so strong that the number of electrons is equal to the number of ions as each ion can accommodate just one electron. Removing $X$ electrons from the sample leaves the number of electrons as $N - X$. Following the same idea as for the semiconductor, we have $R = (1 - x)/2x$ [61]. This is a very basic formulation ignoring any electron hopping, it is used to give us an idea of the magnitude of the asymmetry we can expect to see in a semiconductor or Mott insulator. It can be seen in figure 4 that although...
both insulators exhibit asymmetry, they do not account for the magnitude of asymmetry seen in STM experiments with cuprate superconductors without the consideration of disorder and matrix elements [62].

Despite intensive research, a detailed microscopic theory capable of describing unusual ARPES and tunnelling data has remained elusive and so the relationship between the SG and PG has remained unknown. A detailed and consistent interpretation of SG and PG could shed light on the key pairing interaction in cuprate superconductors.

High values of $T_c$ and small isotope effect on $T_c$ in optimally doped YBa$_2$Cu$_3$O$_{6.9}$ led some authors to conclude that the pairing interaction between electrons cannot be mediated by phonons. However experiments [63, 64] showed that a partial substitution of yttrium by praseodymium, or of barium by lanthanum leads to the isotope effect simultaneously with the decrease of $T_c$: either these substituted compounds have a different mechanism of superconductivity, or the mechanism is always phonons and the absence of the isotope effect in YBCO is due to something else. In favour of this option is the tunnelling spectra at high voltages of NCCO [65] and BSCCO [66, 67]. Evidence from the doping dependent oxygen isotope effect (OIE) on the carrier mass suggests a strong EPI in cuprate superconductors, where lattice vibrations play a significant but unconventional role, see [68] and references therein.

In the remaining part of the paper we review a bipolaron theory of NS and SS tunnelling in the bosonic and cuprate superconductors [62, 69, 70]. The theory is based on the assumption that the EPI is strong enough in cuprates and similar ionic charge-transfer insulators to form small mobile bipolarons, which has been convincingly supported by a number of experimental observations [71]. To clarify the terminology we first introduce bosonic superconductivity (section 3). The results on the NS and SS tunnelling are presented in sections 5 and 6, respectively.

3. Bosonic (bipolaronic) superconductivity

The BCS theory [72] is capable of successfully describing the superconducting properties of elemental superconductors with a small EPI strength. The theory was modified in 1960 to give a strong-coupling theory [73] describing the properties of intermediate-coupling superconductors (the difference between a weak and strong-coupling superconductor is given by the electron–phonon coupling constant, $\lambda$ [74]). The mean-field BCS–Eliashberg theory is applied when the electron correlation length is large compared to the distance between them. The mechanism behind superconductivity is the momentum–space pairing of electrons through electron–phonon interactions. It was first realized by Fröhlich in 1950 that electrons could be attracted to one another through their interactions with phonons; he suggested superconductivity was instigated by EPI. The isotope effect observed experimentally verified Fröhlich’s proposition that EPI causes superconductivity.

When the coupling constant is increased above $\lambda \approx 1$, the kinetic energy of electrons becomes small compared with the potential energy from the local lattice deformation, thus all electrons in the Bloch band become dressed with phonons (for a recent review see [75]). The electron becomes a quasiparticle, a small polaron, which can propagate through the lattice in a narrow (polaronic) band together with the lattice deformation. For a further extension of the BCS theory towards a strong interaction between electrons and ion vibrations, $\lambda > 1$, it was predicted that instead of Cooper pairs, a charged Bose gas of tightly bound small bipolarons would be evident [76] with a polaronic BCS-like high-$T_c$ superconductivity in the crossover region [77]. These bipolarons are real-space pairs of two electrons with their phonon cloud.

Different from Cooper pairs in the momentum–space, the ground state of the strongly coupled electrons and phonons is the real-space pairing of these single polarons into bosonic bipolarons where they form a condensate which can be described as a charged Bose-liquid on a lattice if the carrier density is small enough to avoid their overlap [71]. In the superconducting state, if the temperature is finite, not all the polarons will condense and those that have not condensed interact with the condensate through the same potential that binds them together. The single-particle Hamiltonian is described as [62, 69]:

$$H_0 = \sum_\nu \left[ \xi_\nu p_\nu^\dagger p_\nu + \frac{\Delta_{c\nu}}{2} \left( p_\nu^\dagger p_{\nu+1}^\dagger + h.c. \right) \right].$$

where $\xi_\nu = E_\nu - \mu$, $E_\nu$ is the normal-state single polaron energy spectrum in the crystal field and disorder potentials renormalized by EPI and spin fluctuations and $\Delta_{c\nu} = -\Delta_{\nu\nu}^c$ is the coherent potential proportional to the square root of the condensate density, $\Delta_c \propto \sqrt{n_c(T)}$. The operators $p_\nu^\dagger$ and $p_\nu^\dagger$ create a polaron in the single-particle quantum state $\nu$ and in the time reversed state $\bar{\nu}$ respectively.
As in the BCS case, the single-particle energy spectrum $\epsilon_\nu$ is found by applying the Bogoliubov transformation to diagonalize the Hamiltonian, which is thus written:

$$H_0 = \sum_\nu \epsilon_\nu (\alpha_\nu^\dagger \alpha_\nu + \beta_\nu^\dagger \beta_\nu),$$

(2)

where $p_\nu = u_\nu \alpha_\nu + v_\nu \beta_\nu^\dagger$, $p_\nu = u_\nu \beta_\nu - v_\nu \alpha_\nu^\dagger$, $\epsilon_\nu = \sqrt{\xi_\nu^2 + \Delta_\nu^2}$ with $u_\nu^2, v_\nu^2 = \frac{1}{4} (1 \pm \frac{\Delta}{\mu})$. This spectrum is different to the BCS quasiparticles because the chemical potential ($\mu$), is negative with respect to the bottom of the single-particle band, $\mu = -\Delta_p$. A single-particle gap $\Delta$, is defined as the minimum of the single-quasiparticle energy spectrum. Without disorder, for a point-like pairing potential with the s-wave coherent gap, $\Delta_{ck} \approx \Delta_c$, one has [69]:

$$\Delta(T) = \sqrt{\Delta_p^2 + \Delta_c(T)^2}.$$  

(3)

The full gap varies with temperature from $\Delta(0) = \sqrt{\Delta_p^2 + \Delta_c(0)^2}$ at zero temperature to the temperature independent $\Delta = \Delta_p$ above $T_c$, which qualitatively describes some earlier and more recent [50] observations including Andreev reflection in cuprates ([69] and references therein).

### 4. Energy band structure of cuprates

In our theory we adopt the parent band structure based upon a Mott or any semiconductor insulator structure. The copper band is split into two; an upper and lower band which makes the Mott insulator, the gap between the two is approximately 5–8 eV. The semiconductor oxygen p-band lies within this gap and its charge-transfer gap is approximately 1–2 eV, so we consider a parent lattice that is half Mott insulator, half semiconductor. We have assumed the local density approximation and generalized tight binding (‘LDA + GTB’) band structure [78], see figure 5. Following [79] one can amend this structure with the impurity bandtails. When the cuprate is doped an impurity ion locally introduces a distinct energy level within the charge-transfer gap. The random spatial distribution of impurities when doping causes a bandtail effect of the DOS, similar to that of a heavily doped semiconductor. This band structure explains the charge-transfer gap, sharp quasiparticle peaks near $\frac{\pi}{2}$ of the Brillouin zone and a high energy waterfall observed by ARPES in underdoped cuprate superconductors [79]. Only the impurity states with binding energy below $\mu = 0$ contribute at $T = 0$ K. It has been suggested that the band structure should be metallic due to Fermi arcs seen by ARPES which could form part of a large Fermi surface; however this does not take into account strong correlations and the existence of the charge-transfer gap over a wide range of dopings [78, 80].

For tunnelling to be possible, a state must be occupied by a carrier and at the same energy level on the other material a state must be vacant. The probability of a single-particle state being occupied is given by the Fermi–Dirac distribution. We consider single-particle tunnelling only, this is in key with STM results as they measure one-particle tunnelling only (rather than Josephson tunnelling where the tunnelling of pairs can occur). The tunnelling process is described by the standard perturbation theory, where the tunnelling Hamiltonians are perturbations, then the Fermi–Dirac golden rule (FDGR) is applied.
5. NS tunnelling

To find the NS tunnelling Hamiltonian each different tunnelling scenario needs to be considered, figure 6. Suppose on the left we have the metallic tip with undressed carriers as opposed to the polaron and bipolarons on the right, superconducting side. This means for tunnelling left to right we have the annihilation of a free carrier on the left accompanied by the creation of a polaron on the right. Alternatively we might have the annihilation of a carrier on the left and the annihilation of a polaron on the right with the creation of a bipolaron on the right. This can be expressed in terms of the Hamiltonian [70]: (‘h.c.’ is the Hermitian conjugate, describing the tunnelling in opposing direction)

$$H_{NS} = P \sum_{v, v'} \rho_{v'} c_v + \frac{B}{\sqrt{N}} \sum_{v, v'} b_{v'} c_v + \text{h.c.}$$  

Here \(c_v\) and \(b_{v'}\) describe the annihilation of a carrier in the metallic tip in state \(v\) and the creation of a composed boson in the superconductor in state \(v'\) respectively, \(N\) is the number of lattice cells. \(P\) and \(B\) are tunnelling matrix elements respectively with and without the involvement of a bipolaron. Generally \(B \geq P\), because the presence of an additional hole lowers the tunnelling barrier for an injection of the electron [70]. Using the Bogoliubov coefficients

$$u_{v'}^2 = \frac{1}{2} \left( 1 + \frac{\xi_v}{\epsilon_{v'}} \right), \quad v_{v'}^2 = \frac{1}{2} \left( 1 - \frac{\xi_v}{\epsilon_{v'}} \right),$$

(5)

to replace the polaron operators with linear combinations of the quasiparticle operators yields:

$$H_{NS} = P \sum_{v, v'} \left( u_{v'} \alpha_{v'} + v_{v'} \beta_{v'} \right) c_v + \frac{B}{\sqrt{N}} \sum_{v, v'} b_{v'} \left( u_{v'} \beta_{v'} - v_{v'} \alpha_{v'} \right) c_v + \text{h.c.}$$  

(6)

Using the Fermi–Dirac golden rule

$$W = \frac{2\pi}{h} |(\langle n | H_{\text{tun}} | 0 \rangle)|^2 \delta(E_n - E_0),$$

(7)

where the initial state is 0 and the final state is \(n\), yields:

$$W^{\text{in}}_{NS} = \frac{2\pi P^2}{h} \sum_{v, v'} \left[ u_{v'}^2 (1 - f_{v'}) F_v \delta(\xi_v + eV - \epsilon_{v'}) \right. + v_{v'}^2 F_v \delta(\xi_v + eV + \epsilon_{v'}) + \frac{2\pi B^2}{N} \sum_{v, v'} (1 + n_{v'}) \times \left[ u_{v'}^2 f_v F_v \delta(E_{v'} - \xi_v - eV - \epsilon_{v'}) + v_{v'}^2 (1 - f_v) F_v \delta(E_{v'} - \xi_v - eV + \epsilon_{v'}) \right],$$

(8)

$$W^{\text{out}}_{NS} = \frac{2\pi P^2}{h} \sum_{v, v'} \left[ u_{v'}^2 f_v (1 - F_v) \delta(\xi_v + eV - \epsilon_{v'}) + v_{v'}^2 (1 - f_v) \delta(\xi_v + eV + \epsilon_{v'}) + \frac{2\pi B^2}{N} \sum_{v, v'} n_{v'} \times \left[ u_{v'}^2 (1 - f_v) (1 - F_v) \delta(\xi_v - \xi_v - eV - \epsilon_{v'}) + v_{v'}^2 f_v (1 - F_v) \delta(E_{v'} - \xi_v - eV - \epsilon_{v'}) \right. \right.$$

$$+ \left. v_{v'}^2 f_v (1 - F_v) \delta(E_{v'} - \xi_v - eV + \epsilon_{v'}) \right].$$

Here \(W^{\text{in}}\) and \(W^{\text{out}}\) are transition rates in and out of the superconductor, \(f_v = 1/(e^{\epsilon_{v'}/kT} + 1)\) is the single quasiparticle distribution function, \(n_{v'}\) is the bipolaron (Bose) distribution function, \(F_v = 1/(e^{\epsilon_{v'}/kT} + 1)\) describes the distribution of carriers in the normal-metal, \(V\) is the voltage drop across the junction and the bipolaron chemical potential in the superconductor differs from the normal-metal by 2 eV. To find the current we use the equation

$$I = e(W_{\text{in}} - W_{\text{out}}),$$

(10)

which gives [62]:

$$I_{NS}(V) = \frac{2\pi e P^2}{h} \sum_{v, v'} \left[ u_{v'}^2 (F_v - f_{v'}) \delta(\xi_v + eV - \epsilon_{v'}) + v_{v'}^2 (F_v + f_{v'} - 1) \delta(\xi_v + eV + \epsilon_{v'}) \right] + \frac{2\pi e B^2}{h} \sum_{v, v'} \left[ u_{v'}^2 (F_v f_v - (x/2)(1 - F_v - f_{v'})) \times \delta(\xi_v + eV - \epsilon_{v'}) + v_{v'}^2 (F_v (1 - f_v)) \delta(\xi_v + eV + \epsilon_{v'}) \right],$$

(11)

where \(x/2\) is the atomic density of composed bosons in the superconductor. The boson energy dispersion is neglected here for more transparency, assuming that they are sufficiently heavy for their bandwidth to be relatively small. Using \(\sum_{v'} \rightarrow \int_{-\infty}^{\infty} \rho_M(\xi) \, d\xi\), \(\sum_v \rightarrow \int_{-\infty}^{\infty} \rho_M(\xi) \, d\xi\), and neglecting the energy dependence of the metallic DOS \(\rho_M(\xi)\) since near the Fermi energy it is approximately a constant, we obtain:

$$I_{NS} = \frac{2\pi e P^2 \rho_M}{h} \int d\xi \int d\xi' \rho_N(\xi'),$$

(12)

where \(\rho_N(\xi)\) is the normal-state single-particle DOS in the doped charge-transfer insulator. At zero temperature, the Fermi–Dirac distribution becomes a step function, \(F(\xi - eV) \rightarrow 1\) and \(f(\xi) \rightarrow 0\). To find the conductance, the current is differentiated with respect to the voltage and we have:

$$\sigma_{NS} = \frac{2\pi e P^2 \rho_M}{h} \int d\xi \int d\xi' \rho_N(\xi') \times \left[ u_{v'}^2(\xi') \delta(\epsilon_V - \xi') \delta(\xi - \epsilon') \right.$$}

$$+ \left. v_{v'}^2(\xi') \delta(\epsilon_V - \xi') \delta(\xi + \epsilon') \right] + \frac{2\pi e B^2 \rho_M}{h} \int d\xi \int d\xi' \rho_N(\xi').$$

(13)
\[
\times \left[ a^2(\xi') \delta(\epsilon V - \xi') \delta(\xi - \epsilon') \left( 1 + \frac{x}{2} \right) \right]. \tag{13}
\]

Using the Bogoliubov coefficients defined earlier, equation (5), we find:

\[
\sigma_{NS} \propto \Theta(eV - \Delta_\nu) \left\{ \rho_S(eV) \left( 2 + \frac{x}{2} \right) \right. \times \left. \left\{ \rho_N \left( \sqrt{(eV)^2 - \Delta_\nu^2} \right) + \rho_N \left( - \sqrt{(eV)^2 - \Delta_\nu^2} \right) \right\} \right. \\
+ \left. \left( 1 - \frac{x}{2} \right) \rho_N \left( \sqrt{(eV)^2 - \Delta_\nu^2} \right) \right. \]

\[
- \rho_N \left( \sqrt{(eV)^2 - \Delta_\nu^2} \right) \right\} \right. \}
\tag{14}
\]

where \( \Theta(x) \) is the Heaviside step function, \( \rho_S(E) = E/\sqrt{E^2 - \Delta_\nu^2} \) for s-wave symmetry of the coherent gap which does not depend on the quantum number \( \nu \) and we assume here \( P = B \) for more transparency. Similarly, the conductance can be found for d-wave symmetry, where the coherent gap is now a function of \( \nu \), \( \Delta_{\nu\nu} = \Delta_0 \cos 2 \phi \), \( \phi \) is an angle along a constant energy contour. The DOS in the superconducting state is given by [81]:

\[
\rho_S(E) = \frac{2}{\pi} \left[ \Theta \left( 1 - \frac{E}{\Delta_0} \right) \frac{E}{\Delta_0} K \left( \frac{E}{\Delta_0} \right) \right] + \Theta \left( \frac{E}{\Delta_0} - 1 \right) \frac{K \left( \frac{\Delta_0}{E} \right)}{\frac{\Delta_0}{E}}. \tag{15}
\]

Then, if the tail-width (\( \Gamma \)) is large compared with the coherent gap amplitude, \( \Gamma > \Delta_0 \), equation (13) yields

\[
\sigma_{NS} \propto A^+ \rho_S(|eV|)|\rho_S(-eV) + \rho_N(eV)| \right. \\
+ \left. A^- \left[ 1 - \frac{2}{\pi} \arccos \left( \frac{|eV|}{\Delta_0} \right) \Theta \left( 1 - \frac{|eV|}{\Delta_0} \right) \right] \right. \\
\times \left. \left\{ \rho_N(-eV) - \rho_N(eV) \right\}. \right. \tag{16}
\]

where \( A^\pm = 1 \pm B^2 \Theta(-eV) + \frac{2}{\pi} / \rho^2 \).

As aforementioned, the doping of impurities in the cuprates causes a band tailing effect in the normal-state DOS. We have used a model DOS to reflect the shape of our DOS which is given by:

\[
\frac{\rho_N(E)}{\rho_0} = \frac{1}{2} \left[ 1 + \tanh \left( \frac{E - \Delta_\nu}{\Gamma} \right) \right]. \tag{17}
\]

This model \( \rho_N(E) \) reflects the characteristic energy dependence of the DOS in disordered doped insulators, which is a constant \( \rho_0 \) above the two-dimensional band edge, and an exponent deep in the tail (see figure 5).

No matter what symmetry the superconducting gap is, the above equations capture all the unusual signatures of the extrinsic experimental tunnelling conductance in underdoped cuprates, such as the low energy coherent SG, the high energy PG and the asymmetry, see figure 7. In the case of atomically resolved STS one should replace the averaged \( \rho_N(E) \) in the above equations with a local bandtail DOS, \( \rho_N(E, r) \), which is dependent on the position of the tip on the scanned area due to a nonuniform dopant distribution. As a result, the PG shows nanoscale inhomogeneity, while the low energy SG is spatially uniform as observed [46]. Increasing doping level tends to diminish the bipolaron binding energy, \( \Delta_p \), since the pairing potential becomes weaker due to a partial screening of EPI with low frequency phonons [82]. However, the coherent gap \( \Delta_c \), which is a product of the pairing potential and the square root of the carrier density [69], can remain about a constant or even increase with doping, as observed [46, 62].

6. SS tunnelling

For SS tunnelling there are different issues to address, in particular, tunnelling in mesas has indicated a nonzero conductance at zero voltage near and above \( T_c \), also a negative excess resistance has been observed, along with the PG and SG. All of these features are accounted for in our theory. The Hamiltonian [70]:

\[
H_{SS} = P \sum_{\nu \nu'} p^\dagger_\nu p_\nu + \frac{B}{\sqrt{N}} \sum_{\nu \nu'} \left( \sum_{\eta} p^\dagger_\nu p^\dagger_\eta p_\eta p_{\nu'} + \sum_{\eta} b^\dagger_\eta b_\eta p_\nu p_{\nu'} \right) + \text{h.c.}, \tag{18}
\]

describes the tunnelling of a single polaron from one bosonic superconductor to the other. The first term has no involvement of bipolarons and describes the annihilation of a polaron in state \( \nu \) and creation of one in state \( \nu' \). The second term involves the decay of a composed boson into two polarons, one remains in the same superconductor as the boson and is in state \( \nu \) (this is the time reversed state of \( \nu \)). The other tunnels into state \( \nu' \) in the other superconductor. The third term is the opposite to this with the annihilation of two polarons, one from each superconductor, that then combine to form a bipolaron. Again,
only single-particle tunnelling is considered, see figure 8. Following the same procedure as for NS tunnelling (applying the FDGR and equation (10)) yields:

\[
I_{SS}(V) = \frac{2\pi e P^2}{h} \sum_{\nu'\nu} (u_{\nu'}^2 u_{\nu}^2 + v_{\nu'}^2 v_{\nu}^2) (f_{\nu'} - f_{\nu}) \\
\times \delta(\epsilon_{\nu'} + eV - \epsilon_{\nu}) + u_{\nu}^2 v_{\nu}^2 (f_{\nu'} + f_{\nu} - 1)
\times [\delta(\epsilon_{\nu'} + eV + \epsilon_{\nu}) - \delta(\epsilon_{\nu'} - eV + \epsilon_{\nu})]
\left. \right] + \frac{2\pi eB^2}{h} \sum_{\nu'\nu} \left[ u_{\nu'}^2 u_{\nu}^2 \left( (1 - f_{\nu'} - f_{\nu}) \frac{x}{2} - f_{\nu} f_{\nu'} \right) \\
+ v_{\nu'}^2 v_{\nu}^2 \left( (1 - f_{\nu'} - f_{\nu}) \frac{x}{2} + (1 - f_{\nu}') (1 - f_{\nu}) \right) \right] \\
\times [\delta(\epsilon_{\nu'} - eV + \epsilon_{\nu}) - \delta(\epsilon_{\nu'} + eV + \epsilon_{\nu})]
\left. \right] + 2u_{\nu}^2 v_{\nu}^2 \left[ (f_{\nu'} - f_{\nu}) \frac{x}{2} - f_{\nu} (1 - f_{\nu'}) \right]
\times [\delta(\epsilon_{\nu'} + eV - \epsilon_{\nu'}) - \delta(\epsilon_{\nu'} - eV - \epsilon_{\nu'})].
\]

The boson energy dispersion is again dropped here, assuming that bipolarons are sufficiently heavy for their bandwidth to be relatively small.

First consider a clean bosonic superconductor, where the SS tunnelling in the BCS case for zero temperature when \(f_{\nu} = 0\). Refer back to equation (17), the normal-state DOS \(\rho_N(\xi)\) becomes a step function as \(\Gamma\), which is the width of the bandtail, tends to zero, \(\rho_N(\xi) \rightarrow \Theta(\xi - \Delta_\nu); \rho_N(\xi') \rightarrow \Theta(\xi' - \Delta_\nu).\) Thus, integrating with respect to \(\xi\) and \(\xi'\) we have for the current:

\[
I_{SS} \propto 2\Theta(eV - 2\Delta) \left\{ \left( \frac{x}{2} + 1 \right) I_0 + \frac{x}{2} (eV - 2\Delta) \\
- \sqrt{(eV - \Delta_\nu)^2 - \Delta_0^2} - \sqrt{(eV + \Delta_\nu)^2 - \Delta_0^2} \right\},
\]

such that

\[
I_0 = \frac{(eV)^2}{eV + 2\Delta_\nu} F(\arcsin(1 - \beta), \alpha) - (eV + 2\Delta_c)
\times [F(\arcsin(1 - \beta), \alpha) - E(\arcsin(1 - \beta), \alpha)],
\]

where \(\beta = \frac{2\Delta_\nu - \Delta_\nu}{2\Delta_\nu + \Delta_0}, \alpha = \frac{eV - 2\Delta_\nu}{2\Delta_\nu + \Delta_0}\), we take \(P = B, F(x, y)\) and \(E(x, y)\) are incomplete elliptic integrals of the first and second kind respectively. This is plotted in figure 9 against what is expected for SS tunnelling in the BCS theory [83]:

\[
I_{SS} \propto \Theta(eV - 2\Delta_{BCS}) \left\{ \frac{(eV)^2}{eV + 2\Delta_{BCS}} K(\alpha) \\
- (eV + 2\Delta_{BCS}) K(\alpha) - E(\alpha) \right\},
\]

where \(\alpha = \frac{eV - 2\Delta_{BCS}}{2\Delta_{BCS} + \Delta_0}\), \(K(\alpha), E(\alpha)\) are complete elliptic integrals (see [83] for more details).

Finally consider the normal-state, where \(\Delta_\nu = 0\), which means \(\epsilon_{\nu} = \sqrt{\xi_{\nu}^2 + \Delta_0^2} = |\xi_{\nu}|\), thus \(u_{\nu}^2 = 1\) and \(v_{\nu}^2 = 0\) for positive \(\xi_{\nu}\), and \(u_{\nu}^2 = 0, v_{\nu}^2 = 1\) for negative \(\xi_{\nu}\). We find:

\[
I_{SS}(V) = \frac{2\pi e P^2}{h} \sum_{\nu'\nu} (f_{\nu'} - f_{\nu}) \delta(\xi_{\nu} + eV - \xi_{\nu'}) \\
+ \frac{2\pi eB^2}{h} \sum_{\nu'\nu} \left[ (1 - f_{\nu'} - f_{\nu}) \frac{x}{2} - f_{\nu} f_{\nu'} \right] \\
\times [\delta(\xi_{\nu'} - eV + \xi_{\nu}) - \delta(\xi_{\nu'} + eV + \xi_{\nu})].
\]

Now, we can follow the same steps as [62] and neglect temperature effects by approximating the distribution function \(f_{\nu}\), with a step function \(\Theta(-\xi_{\nu})\) for temperatures near and above the transition temperature but sufficiently below the PG temperature \(T^* = \frac{\Delta_0}{k_B} > T \gtrsim T_c\), and for high enough
voltage, \( |eV| \geq k_B T \). Using the model normal-state DOS, equation (17) yields:

\[
I_{SS}(V) \propto \frac{a^2}{2(a^2 - 1)} \left[ \ln \frac{a^2(1 + b^2)}{1 + a^2 b^2} - \frac{1}{a^2} \ln \frac{a^2 + b^2}{1 + b^2} \right] + \frac{B^2(1 + x/2)}{P^2(a^2 b^4 - 1)} \ln \frac{a^2 + b^2}{a(1 + b^2)} + \frac{B^2 x a^2}{2 P^2(a^2 - b^2)} \ln \frac{a^2 + b^2}{a(1 + b^2)},
\]

(24)

where \( a = e^{-\frac{|eV|}{k_B T}} \) and \( b = e^{-\frac{|eV|}{2 k_B T}} \). Near and above \( T_c \), for high enough voltages \( eV \geq k_B T \), the conductance fits the experimental data and the gapped conductance is accounted for in underdoped mesas of Bi2212 [50], as shown in figure 10. For these voltages the shape of the conductance is almost independent of the ratio \( B'/P \) and \( x \) since the last term is much larger than all other terms in equation (24). The gapped conductance at smaller voltages can be accounted for by fully taking into account temperature effects in equation (23). One can show that the quadratic term \( f_x f_c \) in equation (23) gives negligible contribution in the relevant temperature range, so differentiating the current with respect to the voltage yields the SS conductance as:

\[
\sigma_{SS} \propto \int_{-\infty}^{\infty} d\xi \left[ \frac{\text{sech}^2\left(\frac{\xi + eV - \Delta_p}{\Gamma}\right)}{\xi - eV - \Delta_p} \right]
\]

(25)

This equation is plotted in figure 11 with \( \Gamma = 10 \) meV, the ratio \( B^2 x / 2 P^2 \) is fixed at 1.96 and we change \( \Delta_p \) to fit the experimental temperature dependence. Our theoretical results closely resemble those found experimentally by Krasnov [50]. Our comparison and other experiments [47, 60] suggests that the PG gradually decreases with increasing temperature, which could be explained by many-particle effects at significant doping. We suggest that with increasing temperature thermally excited mobile polarons screen the EPI, so the binding energy of the bipolarons drops [82] as with doping.

Negative excess resistance below the transition temperature can be seen in cuprates [84]. Our theory can account for this. Expanding equations (19) and (23) in powers of \( eV \) gives a zero-bias conductance, for low temperatures in the superconducting state this is \( \sigma_0(0) \propto T^{-1} \int_0^{\infty} d\epsilon \rho_\epsilon(\epsilon)^2 \cosh(\epsilon/2 k_B T)^{-2} \), and in the normal-state \( \sigma_0(0) \propto T^{-1} \int_0^{\infty} d\epsilon \rho_\epsilon(\epsilon)^2 \cosh(\epsilon/2 k_B T)^{-2} \). These integrals can be estimated to give respectively \( \sigma_0(0) \propto T^{-1} \exp(-\Delta_c/k_B T) \) for the s-wave coherent gap, or \( \sigma_0(0) \propto T^2 \) for the d-wave gap, and \( \sigma_0(0) \propto T^{-1} \exp(-T^*/T) \) for the latter expression is in excellent agreement with the temperature dependence of the mesa tunneling conductance above \( T_c \) [84] (see also [82]). Extrapolating this expression to temperatures below \( T_c \) yields the resistance ratio \( R_s/R_N \propto e^{(\Delta_c/k_B - T^*)/T} \) for the s-wave or \( R_s/R_N \propto \exp(-T^*/T) / T^2 \) for the d-wave. Hence in underdoped cuprates, where \( T^* > \Delta_c/k_B \), the zero-bias tunneling resistance at temperatures below \( T_c \) is smaller than...
the normal-state resistance extrapolated from above $T_c$ to the same temperatures (i.e. the negative excess resistance), as observed [84].

7. Summary

Data from tunnelling experiments is invaluable as it gives a huge insight into the low energy excitations and thus the way high-temperature superconductors work.

NS tunnelling in cuprates has indicated two energy scales, the first is the SG that vanishes above $T_c$. The second is the PG which remains a mystery, there is no general consensus as to what it is or why it exists. STM with cuprates has also shown that the tunnelling conductance of charge carriers in one direction (say tip to sample) is different to the tunnelling conduction in the other direction, this gives asymmetry in the tunnelling spectra. Again, there is no general consensus as to why this is the case. Remarkably, the position of the tip on the cuprate gives different tunnelling results.

Intrinsic tunnelling and break junction experiments have also indicated a two-gap structure. Recent experiments have provided evidence that the PG is dependent on the temperature and decreases as the temperature increases above $T_c$. Another inexplicable feature of SS tunnelling has been the negative excess resistance, where the zero-bias tunnelling resistance that is extrapolated from above to below $T_c$ is larger than that measured in the superconducting state below $T_c$.

To have a successful theory, each of these puzzles should be accounted for in both NS and SS tunnelling.

Here we have briefly reviewed theoretical understandings of two distinct gaps (PG and SG), which are one of the most puzzling phenomena in cuprate superconductors. We have discussed in more detail our theory based on the ab initio ‘LDA + GTB’ band structures of charge-transfer Mott–Hubbard insulators with the doping of impurities causing bandtails in the normal-state DOS. We have made an extension to the BCS theory in the strong-coupling regime with bosonic (bipolaronic) carriers which are the real-space pairs of polaronic electrons. While this theory has allowed us to describe the two gaps and some other unusual features in the tunnelling spectra of the cuprates, a basic question concerning the key pairing interaction in high-temperature superconductors remains open. We by no means exclude any non-phononic contribution to the pairing and different non-phononic scenarios of the PG and SG discussed in section 1. The real-space pairing seems to be a remarkable feature of (underdoped) cuprates, no matter what the pairing glue is. Overall, it seems plausible that its origin is found in a proper combination of strong electron–electron correlations with a significant EPI.

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