Theory of SIS tunnelling in cuprates

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Abstract

We show that the single-particle polaron Green's function describes SIS tunnelling in cuprates, including the absence of Ohm's law at high voltages, the dip/hump features in the first derivative of the current, a substantial incoherent spectral weight beyond quasiparticle peaks and unusual shape of the peaks. The theory allows us to determine the characteristic phonon frequencies, normal and superconducting gaps, impurity scattering rate, and the electron-phonon coupling from the tunnelling data.
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There is a number of anomalous properties of high-T_c cuprates, which seem to be intrinsic and universal. The isotope effect on the carrier mass [1], unusually high values of the static dielectric constants [2], and the non-Fermi liquid and non-BCS spectral densities observed in the angle-resolved photoemission (ARPES) [3–5], superconductor- insulator-normal metal (SIN) and superconductor- insulator-superconductor(SIS) tunnelling spectra [6–12] are among those. The isotope effect and the high values of the static dielectric constants as well as the optical spectroscopy [13] suggest that electron-phonon interaction is more than sufficient to bind carriers and phonons into small polarons and bipolarons in highly polarisable cuprates [2,14]. The bipolaron theory [15] provides a natural explanation of the normal state pseudogap (as a half of the bipolaron binding energy, Δ_p) [16,17], NMR linewidth [16], normal state kinetics [15], SIN tunnelling [18] and ARPES [19,20]. The theory accounts for two distinct energy gaps (coherent and incoherent) [21] as observed in the recent tunnelling [10–12] and Andreev reflection experiments [22,10], for the parameter-free fit of the critical temperature , upper critical field , and specific heat [23].

In this letter we present the polaron theory of SIS tunnelling in cuprates.

Within the standard approximation [24] the tunnelling current, $I(V)$, between two parts of a superconductor separated by an insulating barrier is proportional to a convolution of the Fourier component of the single-hole Green's function (GF),$G(\mathbf{k},\omega)$, with itself as

$$I(V) \propto \sum_{\mathbf{k},\mathbf{p}} \int_{-\infty}^{\infty} d\omega \Im G(\mathbf{k},\omega) \Im G(\mathbf{p}, e|V| - \omega), \tag{1}$$

where V is the voltage across the junction.

A problem of a hole on a lattice coupled with the bosonic field of lattice vibrations has a solution in terms of the coherent (Glauber) states in the strong-coupling limit, $\lambda > 1$, where the Migdal-Eliashberg theory [25,26] cannot be applied due to the broken translational symmetry [27]. For any type of electron-phonon interaction conserving the on-site occupation numbers of fermions the $1/\lambda$ perturbation technique yields (at $T = 0$) [28,29]

$$G(\mathbf{k},\omega) = Z \sum_{l=0}^{\infty} \sum_{\mathbf{q}_1,...\mathbf{q}_l} \frac{\prod_{r=1}^{l} |\gamma(\mathbf{q}_r)|^2}{(2N)^l l! (\omega - \sum_{r=1}^{l} \omega(\mathbf{q}_r) - \epsilon(\mathbf{k} + \sum_{r=1}^{l} \mathbf{q}_r) + i\delta)}, \tag{2}$$

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where $Z = \exp[-(1/2N)\sum_{\mathbf{q}}|\gamma(\mathbf{q})|^2]$, $\gamma(\mathbf{q})$ is the matrix element of the interaction with phonons of the frequency $\omega(\mathbf{q})$ [30] and $\delta- > +0$ ($\hbar = c = 1$). The hole energy spectrum, $\epsilon(\mathbf{k})$ is renormalised due to familiar polaronic narrowing of the band, and (in the superconducting state) also due to the interaction with the Bose-Einstein condensation (BEC) of bipolarons [21] as

$$\epsilon(\mathbf{k}) = \left[\xi(\mathbf{k})^2 + \Delta_c^2\right]^{1/2}. \tag{3}$$

Here $\xi(\mathbf{k}) = Z'E(\mathbf{k}) - \mu$ is the renormalised polaron band dispersion with the chemical potential μ, $E(\mathbf{k}) = \sum_{\mathbf{m}} t(\mathbf{m})exp(-i\mathbf{k}\cdot\mathbf{m})$ is the bare (LDA) disperison in a rigid lattice. The mass-renormalisation exponent is

$$Z' = \frac{\sum_{\mathbf{m}} t(\mathbf{m})e^{-g^2(\mathbf{m})}\exp(-i\mathbf{k}\cdot\mathbf{m})}{\sum_{\mathbf{m}} t(\mathbf{m})\exp(-i\mathbf{k}\cdot\mathbf{m})} \tag{4}$$

with $g^2(\mathbf{m}) = \sum_{\mathbf{q}}|\gamma(\mathbf{q})|^2[1-\cos(\mathbf{q}\cdot\mathbf{a})]$. GF, Eq.(2), is exact in the extreme strong-coupling regime, $\lambda \to \infty$ (see, for example, Ref. [24] page 294).

Quite different from the BCS superconductor the chemical potential μ is negative in the bipolaronic system, so that the edge of the single-hole band is found above the chemical potential at $-\mu = \Delta_p$. Near the edge the parabolic one-dimensional approximation for the oxygen hole is applied [18], compatible with the ARPES data [19]

$$\epsilon_{\mathbf{k}} \simeq \frac{k_x^2}{2m^*} + \Delta. \tag{5}$$

The 'global' gap $\Delta = (\Delta_p^2 + \Delta_c^2)^{1/2}$ comprises the incoherent temperature-independent (normal state) gap Δ_p, and the coherent (superconducting) gap $\Delta_c(T)$. The coherent gap disappears at T_c together with the condensation [21].

The continuous-time Quantum-Monte-Carlo simulations [31] show that the $1/\lambda$ perturbation result, Eq.(2), is practically exact in a wide range of the Fröhlich electron-phonon interaction with high-frequency phonons, including the weak-coupling regime. Different from the canonical Migdal-Eliashberg GF there is no damping ('defasing') of low-energy polaronic excitations in Eq.(2) due to the electron-phonon coupling alone (because of the

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energy conservation [32]). This coupling leads to the coherent dressing of low-energy carriers by phonons, which appears in GF as phonon sided bands with $l \geq 1$. On the other hand, the elastic scattering by impurities yields a finite life-time of the Bloch polaronic states. For the sake of analytical transparency we model this scattering as a constant imaginary self-energy, replacing $i\delta$ in Eq.(2) by a finite $i\Gamma/2$. In fact, the 'elastic' self-energy has been found explicitely as a function of energy and momentum [18,19]. Its energy/momentum dependence is essential in the subgap region of tunnelling, where it determines the value of the zero-bias conductance. However, it hardly plays any role in the peak region and higher voltages, which are of our prime interest here.

Substiting Eq.(2) into the current, Eq.(1), and performing the intergration with respect to frequency and both momenta (using Eq.(5)), we obtain the tunnelling conductance, $\sigma(V) = dI/dV$,

$$\sigma(V) \propto \sum_{l,l'=0}^{\infty} \sum_{\mathbf{q}_1,...\mathbf{q}_l} \sum_{\mathbf{q}'_1,...\mathbf{q}'_{l'}} \frac{\prod_{r=1}^{l} \prod_{r'=1}^{l'} |\gamma(\mathbf{q}_r)|^2 |\gamma(\mathbf{q}'_{r'})|^2}{(2N)^{l+l'} l! l'!} L\left[e|V| - 2\Delta - \sum_{r=1}^{l} \omega(\mathbf{q}_r) - \sum_{r'=1}^{l'} \omega(\mathbf{q}'_{r'}), \Gamma\right],$$

(6)

where $L[x, \Gamma] = \Gamma/(x^2 + \Gamma^2)$. To perform the remaining integrations and summations, we apply a model analog of the Eliashberg spectral function $\alpha^2 F(\omega)$ by replacing $\mathbf{q}$-sums, $\sum_{\mathbf{q}} |\gamma(\mathbf{q})|^2 A(\omega(\mathbf{q}))/2N$, in Eq.(6) for the integrals $(g^2/\pi) \int d\omega L[\omega - \omega_0, \delta\omega] A(\omega)$ for any arbitrarry function of the phonon frequency $A(\omega(\mathbf{q}))$. In this way we introduce the characteristic frequency ω_0 of phonons strongly coupled with holes, their avarage number g^2 in the polaronic cloud, and their dispersion $\delta\omega$. As long as $\delta\omega$ is less than ω_0, we can extend the integration over phonon frequencies from $-\infty$ to ∞ and obtain

$$\sigma(V) \propto \sum_{l,l'=0}^{\infty} \frac{g^{2(l+l')}}{l! l'!} L[e|V| - 2\Delta - (l+l')\omega_0, \Gamma + \delta\omega(l+l')].$$

(7)

By replacing the Lorentzian in Eq.(7) with the Fourier integral, we perform the summation over l and l' with the final result for the conductance as

$$\sigma(V) \propto \int_0^{\infty} dt \exp\left[2g^2 e^{-\delta\omega t} \cos(\omega_0 t) - \Gamma t\right] \cos\left[2g^2 e^{-\delta\omega t} \sin(\omega_0 t) - (e|V| - 2\Delta)t\right].$$

(8)

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From the isotope effect on the carrier mass, phonon densities of states, experimental values of the normal state pseudogap, and the residual resistivity one estimates the coupling strength g^2 to be of the order of 1 [1], the characteristic phonon frequency between 20 and 80 meV, the phonon frequency dispersion about a few tens meV, the gap Δ about 30 meV, and the impurity scattering rate of the order of 10 meV.

SIS conductance, Eq.(8), calculated with the parameters in this range is shown in Fig 1,a-d for four different values of the coupling. The conductance shape is remarkably different from the case of BCS density of states, both s-wave and d-wave. There is no Ohm's law in the normal region, $e|V| > 2\Delta$, the dip/hump features (due to phonon sided bands) are clearly seen already in the first derivative of the current, there is a substantial incoherent spectral weight beyond the quasiparticle peak for the strong coupling, $g^2 \geq 1$, and there is unusual shape of the quasiparticle peaks. All these features as well as the temperature dependence of the gap are beyond the BSC theory no matter what the symmetry of the gap is. However, they perfectly agree with the experimental SIS tunnelling spectra in cuprates [7–10,12]. In particular, the theory, Eq.(8) quantitatively describes one of the best tunnelling spetra obtained on $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals by the break-junction technique [7], Fig.2. Some excess zero-bias conductance compared with the experiment is due to our approximation of the elastic self-energy. The exact (energy dependent) self-energy provides an excellent agreement in this sub-gap region, as has been shown in Ref. [18]. A more recent dynamic conductance of Bi-2212 mesas (as shown in Fig.2 of Ref. [12]) is almost identical to our Fig. 1b as well. The unusual shape of the main peaks (Fig.1a,b) is a simple consequence of the (quasi) one-dimensional hole density of states near the edge of the oxygen band, Eq.(5). The coherent ($l = l' = 0$) contribution to the current with no elastic scattering ($\Gamma = 0$) is given by

$$I_0 \propto \int_\Delta^\infty \frac{d\epsilon}{(\epsilon - \Delta)^{1/2}} \int_\Delta^\infty \frac{d\epsilon'}{(\epsilon' - \Delta)^{1/2}} \delta(\epsilon + \epsilon' - e|V|), \qquad (9)$$

so that the conductance is a δ function

$$\sigma_0(V) \propto \delta(e|V| - 2\Delta). \qquad (10)$$

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Hence, the width of the main peaks in the SIS tunnelling, Fig.1,2 measures directly the elastic scattering rate.

The disappearance of the quasiparticle sharp peaks above T_c in Bi-cuprates has also been explained in the framework of the bipolaron theory [18,20]. Below T_c bipolaronic Bose-Einstein condensation (BEC) provides an effective screening of the long-range (Coulomb) potential of impurities, while above T_c the scattering rate might increase by many times [20]. This sudden increase of Γ in the normal state washes out the sharp peaks from the tunnelling and ARPES spectra.

Finally we would like to comment on a possible role of spin fluctuations in the tunnelling spectra. If they play a role, the peak-dip separation observed in ARPES and tunnelling should be equal to the resonance peak energy, E_r, observed in the spin-flip neutron scattering [33]. However, as discussed recently in the comprehensive review of the experimental constraints on the physics of cuprates [14], the peak-dip separation is nearly independent of T_c or the doping level, while E_r is approximately proportional to T_c. This controversy as well as the direct comparison of the electron-phonon and spin fluctuation interactions [2] suggest that the dip/hump features in ARPES and tunnelling arises from strong electron-phonon coupling (as originally proposed by one of us [18]). Recently, using high resolution ARPES data in conjuction with that from neutron, optics and local structural probes, Shen *et al* [34] provided direct evidence for strong electron-phonon coupling being important for pairing.

In conclusion, we have derived the tunnelling SIS conductance for the strongly coupled electrons and phonons in the (bi)polaronic regime. The theory describes SIS tunnelling in cuprates, including the spectral shape in the gap region, and the dip-hump incoherent features at higher voltages. It allows us to determine the characteristic phonon frequencies, the gap, impurity scattering rate, and the electron-phonon coupling from the tunnelling data.

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Figure Captures

Fig.1. SIS tunnelling conductance in the bipolaronic superconductor for different values of the electron-phonon coupling, g^2, and $\Delta =29$ meV, $\omega_0 = 55$ meV, $\delta\omega =20$ meV, $\Gamma = 8.5$ meV.

Fig.2. Theoretical conductance of Fig.1b (solid line) compared with the tunnelling spetrum obtained on $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals by the break-junction technique [7](dots).

$g^2 = .0625$

(a)

$g^2 = .5625$

(b)

$g^2 = 1.44$

(c)

$g^2 = 2.25$

(d)

dI/dV (arbitrary units)

Voltage(mV)

dI/dV(arbitrary units)

Voltage(mV)

-150 -100 -50 0 50 100 150