LOCAL PAIR MODEL FOR THE ANALYSIS OF TUNNELING AND PHOTOEMISSION EXPERIMENTS IN THE NORMAL STATE OF HIGH TC SUPERCONDUCTORS

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Abstract

We analize tunneling and high resolution photoemission results in the normal phase of high Tc superconductors. The analysis is based on a "mixed Fermion-Boson" model, in which a band of paired states overlaps the Fermi level of a wider fermion band. In this model the possibility that a tunnel electron joins an electron in the band to enter a paired state arises quite naturally and gives rise to the V-shaped form of the tunnel conductance. The opposite process accounts for the shape of the photoemission spectrum near the Fermi level.

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The normal properties of high Tc superconductors (HTS) show peculiarities that are not found in ordinary metals. Based on a careful analysis of the experiments showing anomalies common to a number of HTS compounds several authors have proposed a set of phenomenological constraints to the theory of these materials [1,2]. One of these constraints applies to the imaginary part of the self-energy of the one-particle propagator whose energy dependence takes a V-shaped form centered at the Fermi level at zero temperature. At higher temperatures, the vertex of the V is truncated at an energy proportional to the temperature. This feature takes care of one of the most discussed peculiarities of HTS : the linear dependence of resistivity with temperature (which extrapolates to zero in the best samples) [1,6,10].

We have recently shown that this behaviour of the self-energy can be derived quite straightforwardly from the assumption that a band of paired states overlaps the Fermi level of a broader electron band [3]. This picture of "mixed Fermion-Boson fields" has been studied first by Ranninger and Robaszkiewicz [4] and proposed as the scenario for HTS by Kulik [5], Eliashberg [6] and others (see Ref.[11]).

Another crucial point in the phenomenological analysis of the normal phase of HTS is represented by the experiments that probe directly into the density of states of these materials near the Fermi level : tunneling [7] and high resolution photoemission experiments [8].

Both experiments reveal a non analytic V-shaped form of the density of states centered at the Fermi level (E_F) in several of the HTS (including the three dimensional compounds based on $BaBiO_3$) : $D(w) = D(E_F) + K * |w-E_F|$. The absolute values of the parameters $D(E_F)$ and K cannot be determined these experiments. However, the ratio between them as obtained from tunneling [7] is quite consistent with that obtained from photoemission experiments [8].

This peculiar form of the density of states can be linked to the imaginary part of the self-energy [1], however the procedure is not free from arbitrariness. In fact, if the density of states is calculated from the one particle Green function using for the self-energy only the proposed V-shaped imaginary part and its Kramers-Kronig consistent logarithmic real part, one obtains a cusp at the Fermi level instead of a minimum.

Here we want to show that the same assumption that lead us to the correct form of the self-energy [3], the mixed Fermion-Boson system, leads to a different interpretation of the tunneling and photoemission results which explains their peculiarities in a very simple way.

To this end, consider first the following mixed states Hamiltonian :

$$H = \sum_{k,\sigma} (\varepsilon_k-\mu)\, c^{+}_{k\sigma} c_{k\sigma} + \sum_{j,\sigma} (E_j-\mu)\, d^{+}_{j\sigma} d_{j\sigma} - \frac{U}{2} \sum_{j,\sigma} n^{d}_{j\sigma} n^{d}_{j\bar{\sigma}}$$

$$+ \sum_{j,k,\sigma} (V_{kj}\, c^{+}_{k\sigma} d_{j\sigma} + V^{*}_{kj}\, d^{+}_{j\sigma} c_{k\sigma}),$$

(1)

where $c^{+}_{k\sigma}$ creates an electron with crystal momentum k, spin σ and energy ε_k in a broad uncorrelated band, $d^{+}_{j\sigma}$ is the electron creation operator in another set of states labeled by the quantum numbers $(j\sigma)$ with energies E_j. To fix ideas in the following we will consider the latter as localized states, so that we can take $V_{kj} = \frac{W}{\sqrt{N}} e^{-ikR_j}$. We assume that particles in d-states are strongly correlated by an attractive potential $-U$ ($U>0$). $n^{d}_{j\sigma}=d^{+}_{j\sigma}d_{j\sigma}$ is the d-state number operator, N the total number of sites, μ denotes the chemical potential. The last term in (1) represents the hybridization between localized and extended states.

We assume U>W and reduce the Hilbert space eliminating the high energy singly occupied d-electron states. This is achieved by a generalized Schrieffer-Wolff transformation [4,9]. The transformed Hamiltonian reads:

$$\tilde{H} = \sum_{k,\sigma}(\varepsilon_k-\mu)\ c^{+}_{k\sigma}c_{k\sigma} + \sum_{j} 2(\Delta_j-\mu)\ A^{+}_{j}A_{j} +$$

$$+ \frac{W}{2N} \sum_{j,k,k'} g_{jk}\ [e^{-i(k+k').R_j}\ (\ c^{+}_{k'\downarrow}c^{+}_{k\uparrow} + c^{+}_{k\downarrow}c^{+}_{k'\uparrow}\ )\ A_j + \text{H.c.}], \tag{2}$$

where $A^{+}_{j}=d^{+}_{j\uparrow}d^{+}_{j\downarrow}$ is the creation operator for the electron pair at site j with energy $2\Delta_j=(2{*}E_j-U)$, $g_{jk} = \dfrac{W\,U}{\left[(U/2)^2+(\Delta_j-\varepsilon_k)^2\right]}$. The elimination of the electron hybridization term of Eq (1) gives rise to a new mixing term in which two electrons from the uncorrelated band simultaneously enter a paired state and viceversa.

From the transformed Hamiltonian we can obtain several of the thermodynamic quantities of the system and also quantities like the one particle self-energy [3,6]. The self-energy thus calculated has the phenomenological V-shape described above if the energies of the paired states are assumed to be uniformly distributed around the Fermi level.

To analize the results from tunneling and photoemission experiments it is necessary to add to the Hamiltonian terms that represent the interaction of the system with : i) the tunnel electrons, or with ii) the incident radiation.

i)To describe the tunneling process we add to Hamiltonian (1) the following terms :

$$H_T = \sum_{k,\sigma} (\varepsilon'_k-\mu)\ b^+_{k\sigma} b_{k\sigma} + \sum_{k,k',\sigma} (\ T_{kk'}\ c^+_{k\sigma} b_{k'\sigma} + T^*_{kk'}\ b^+_{k'\sigma} c_{k\sigma}\ ) + \\ + \sum_{j,k,\sigma} (\ G_{kj}\ b^+_{k\sigma} d_{j\sigma} + G^*_{kj}\ d^+_{j\sigma} b_{k\sigma}\ ). \tag{3}$$

Here $b^+_{k\sigma}$ denotes the creation operator for tunnel electrons with crystal momentum k , spin σ and energy ε'_k . The first term in (3) corresponds to the band of tunnel electrons, while the next two terms represent the interaction of that band with the HTS system.

ii)In order to describe the photoemission processes we add to

Hamiltonian (1) the following terms describing the interaction of the HTS with the incident radiation :

$$H_X = \hbar w_q a_q^+ a_q + \sum_{k,\sigma} E_k f_{k\sigma}^+ f_{k\sigma}$$

$$+ \sum_{k,k',\sigma} (a_q + a_{-q}^+) [R_{kk'}(q) f_{k\sigma}^+ c_{k'\sigma} + H.c.] +$$

$$+ \sum_{j,k,\sigma} (a_q + a_{-q}^+) [F_{kj}(q) f_{k\sigma}^+ d_{j\sigma} + H.c.],$$

(4)

where a_q^+ denotes the operator which creates a photon of momentum q and energy $\hbar w_q$, while $f_{k\sigma}^+$ is the creation operator for an emitted photoelectron of energy E_k.

To evaluate the tunneling conductance or the photoemission spectrum we again use the canonical transformation that reduces the dynamical space to paired d-states.

In case i), the transformed of the tunneling Hamiltonian (3) reads :

$$\tilde{H}_T = \sum_{k,\sigma} (\varepsilon_k' - \mu) b_{k\sigma}^+ b_{k\sigma} + \sum_{k,k',\sigma} (T_{kk'} c_{k\sigma}^+ b_{k'\sigma} + T_{kk'}^* b_{k'\sigma}^+ c_{k\sigma}) +$$

$$+ \sum_{j,k,k'} \frac{g_{jk}}{\sqrt{N}} \left[G_{k'j} (b_{k'\downarrow}^+ c_{k\uparrow}^+ + c_{k\downarrow}^+ b_{k'\uparrow}^+) A_j + H.c. \right],$$

(5)

where the first term corresponds to a normal tunneling process, while the second gives rise to a new tunneling process in which an added electron can join one of the electrons in the fermion band to enter a paired state.

In case ii), the transformed photoemission Hamiltonian (4) reads :

$$\tilde{H}_X = \hbar w_q a^+_q a_q + \sum_{k,\sigma} E_k f^+_{k\sigma} f_{k\sigma} +$$
$$+ \sum_{k,k';\sigma} (a_q + a^+_{-q}) [R_{kk'}(q) f^+_{k\sigma} c_{k'\sigma} + \mathrm{H.c.}] +$$
$$+ \sum_{j,k,k'} \frac{g_{jk}}{\sqrt{N}} (a_q + a^+_{-q}) \Big[F_{k'j}(q) (f^+_{k\downarrow} c^+_{k\uparrow} + c^+_{k\downarrow} f^+_{k'\uparrow}) A_j + \mathrm{H.c.} \Big]. \tag{6}$$

Here again a new process arises : an electron from a paired state can be ejected out of the sample by a photon, while the other electron from the pair is pushed into the hole states of the HTS fermion band. The transformed Hamiltonians (5) and (6) agree with those used by Kulik [5].

We will proceed now to evaluate the contributions of these new terms to the tunneling current and the photoemission spectra.

Using Hamiltonian (5), the Fermi Golden Rule allows us to calculate the probability per unit time for an electron to tunnel through the two possible processes into the HTS. From it one can calculate the tunneling current J_t . Assuming constant densities of states for the localized and extended bands (see Fig.1), we obtain for the conductance ($g(V)=dJ_t/dV$) the following result :

$$\frac{g(V)}{g(0)} = 1 + \frac{\rho_b\, 8(W/U)^2}{\beta}\left[\coth(eV\beta/2)\right]\ln\left[\frac{\cosh(\beta B)\ \cosh[\beta(A+eV/2)]}{\cosh(\beta A)\ \cosh[\beta(B-eV/2)]}\right], \tag{7}$$

where the first term corresponds to the normal tunneling contribution, while the second originates from the new tunneling process. To obtain this result we have assumed $g_{jk} \simeq 4\ W/U$ and considered the coupling parameters $T_{kk'}$ and G_{kj} as constants of the same order of magnitude.

We display in Fig.2 the ratio $g(V)/g(V_0)$, V_0=0.1V, for the temperatures T=0,100,500 K. In order to fit this curve to experimental results [7] we have taken $[\rho_b\ 8(W/U)^2]$= 3.5/eV. The value of the conductance at V=0 and T=0 K corresponds entirely to the normal tunneling process, while the $|V|$ dependence of the conductance arises from the anomalous tunneling process. The energy-width of this V-shaped dependence extends from (-2A) to (2B).

Regarding photoemission, which is described by Hamiltonian (6), Fermi's Golden Rule allows us to calculate the probability per unit time to collect photoelectrons of given energy produced in the two possible types of photoemission processes. This quantity is proportional to the photoemission spectrum. With the previous assumptions for the densities of states (Fig.1) and coupling parameters, we obtain for the photoemission spectrum :

$$I(E) \; \alpha \; \frac{1}{1+e^{\beta E}} + \frac{\rho_b \, 8(W/U)^2}{\beta} \, \frac{1}{e^{\beta E}-1} \; \ln\left[\frac{\cosh(\beta B) \cosh[\beta(A+E/2)]}{\cosh(\beta A) \cosh[\beta(B-E/2)]}\right], \tag{8}$$

where E is the photoelectron initial-state energy, restricted to values around the Fermi level. The first term in (8) is the normal photoemission contribution and the second corresponds to the processes in which a localized pair is broken.

In Fig 3 we plot our result for the photoemission spectrum at T= 0, 100, 500 K, having taken $[\rho_b \, 8(W/U)^2] = 8/eV$ to fit the experimental data of reference [8]. Again, the intensity value at the Fermi level and T=0 K corresponds to normal photoemission processes, while the (-E) dependence obtained for initial-state energies below the Fermi level, and extending through an energy range of the width of the localized band, arises from the processes in which a localized pair is broken.

In order to obtain results consistent with experimental values we have had to assume that the density of paired states has a rather large value ($\rho_b \simeq$ 10states/eV/cell). Since the width of this band has to be larger than $\simeq$ 0.15eV [7,8], this implies that the number of paired states is of the order of the number of unit cells. This fact excludes the possibility that the paired states arise from non-intrinsic properties of the material. The density of paired states is also consistent with the magnitude of the linear term in the resistivity [1,10](taking reasonable values for the parameters involved : $n_e \simeq 10^{22}/cm^3$, $m/m_e \simeq 5$, $W \simeq 0.6eV$, ρ_c= 1state/eV/cell).

To go further in the interpretation of these results and to clarify the origin of the paired states, it would be highly useful to have measurements of different quantities made on the same sample, and then compare results from different samples. The results from tunneling and photoemission can be linked to thermodinamic results through the formalism presented here.

The arguments presented here are based on the existence of a distribution of paired states. Neither the exact nature of these states nor their origin in the different compounds is clear. In this sense, this paper advances on a possible scenario for the phenomenology of the HTS but does not provide a microscopic theory. The strength -and weakness- of the ideas based on the mixture of local pairs and fermions lies in the fact that they do not rely on dimensionality or magnetic properties. Even though they provide a satisfactory explanation to peculiarities of HTS, this does not rule out other possibilities. The beautiful ideas based on magnetism [12] also lead to the prediction of anomalies in the properties of HTS consistent with the observed results [13]. In this sense the most clarifying information could come from further observations in the $BaBiO_3$-based HTS alloys, which could establish how close the properties of these diamagnetic three-dimensional materials are to those of the two-dimensional "magnetic" related cuprates.

In conclusion, our calculations show that the peculiar results found in tunneling and photoemission experiments in HTS are consistent with the "mixed Fermion-Boson" picture of these materials and provide a way to connect these results to other properties of HTS.

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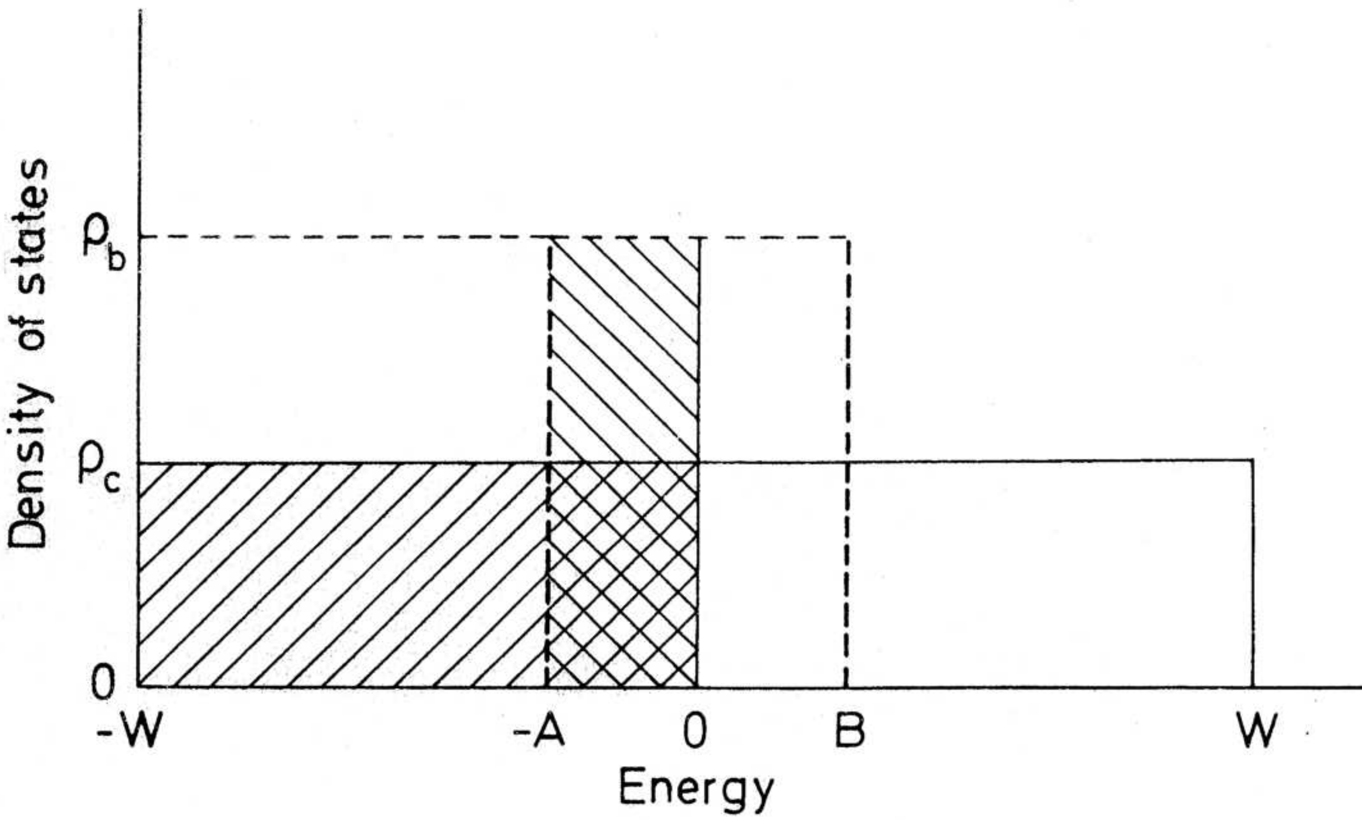
Figure Captions

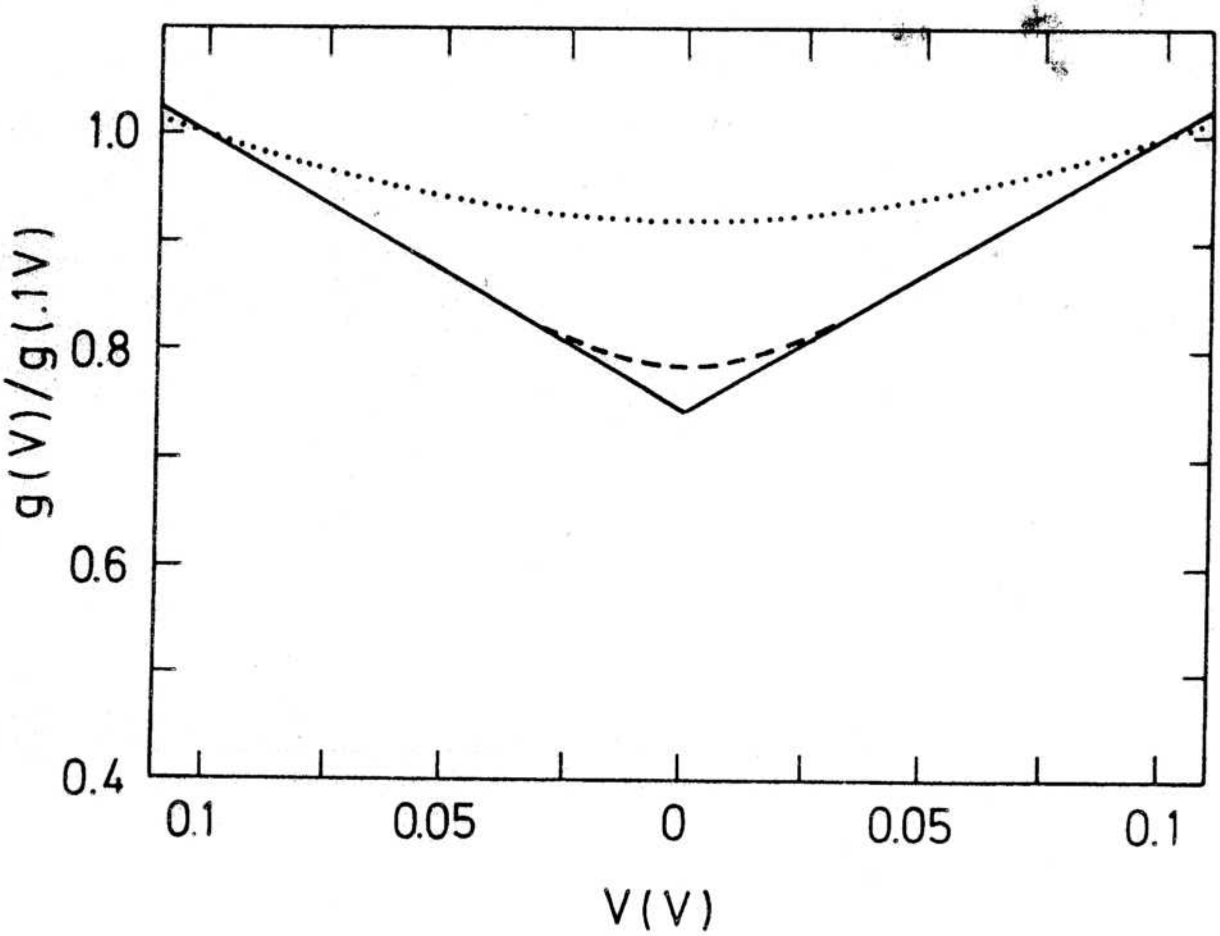
Fig. 1) Schematic drawing of the band configurations used to calculate the tunneling conductance and the photoemission spectrum.

Fig. 2) The ratio of tunneling conductances $g(V)/g(V_0)$, V_0=0.1eV, for temperatures T=0 (full line), 100 K (dashed line) and 500 K (dotted line), taking A=B=0.1eV.

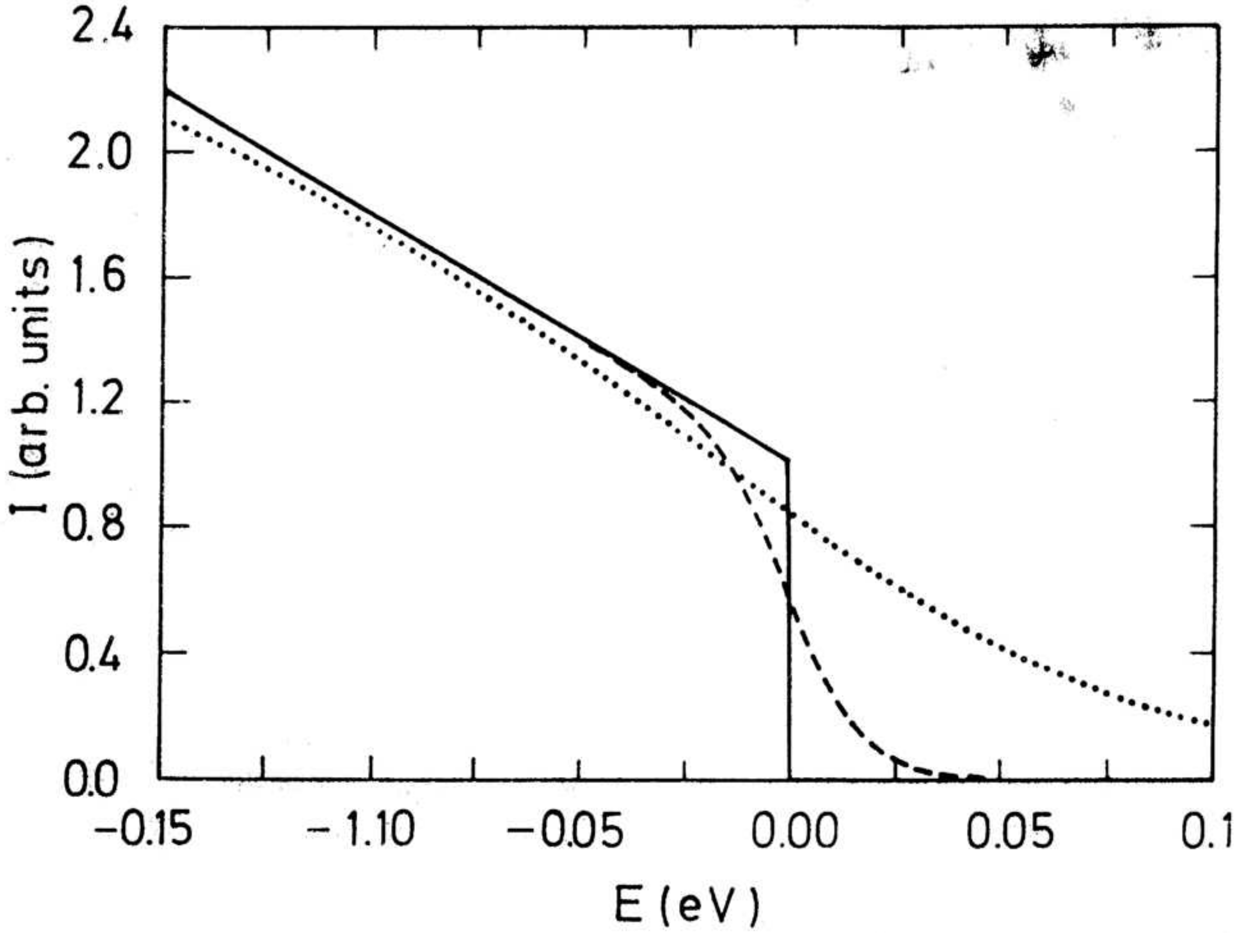
Fig. 3) Photoemission spectrum plotted as a function of initial-state energy for temperatures T=0 (full line), 100 K(dashed line) and 500 K (dotted line), taking A=B=0.1eV.



Density of states
ρ_b
ρ_c
0
-W
-A
0
B
W
Energy



1.0
0.8
0.6
0.4
g(V)/g(.1V)
0.1
0.05
0
0.05
0.1
V(V)



2.4
2.0
1.6
1.2
0.8
0.4
0.0
I (arb. units)
-0.15
- 1.10
-0.05
0.00
0.05
0.1
E (eV)