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Quasiparticle Tunneling into High-T, Mercury-Cuprate Superconductors: Effects of $d_{x^2-y^2}$ Order Parameter Symmetry and a Two-Dimensional van Hove Singularity†

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Quasiparticle tunneling measurements of the high-T, superconductors $\mathrm{Hg_1Ba_2Ca_{n-1}Cu_nO_{2n+2+\delta}}$ (n = 1, 2, 3) are considered in the context of $d_{x^2-y^2}$ symmetry of the superconducting orderparameter and a 2-D van Hove singularity related to saddle-points in the bandstructure. We present tunneling spectra taken with a low-temperature scanning tunneling microscope on Hg-1212 epitaxial films and on polycrystalline Hg-1201 and Hg-1223. The data is analyzed with elastic tunneling formalism, using the nodal gap-function Cl(k) $= \Delta_0(\cos kr - \cos ky)/2$ and the 2D electronic dispersion E(k) $= -2t(\cos kx + \cos ky) + 4t'(\cos kx \cos ky)$. Our analysis accounts for all the generic spectral features: Gap-anisotropy introduces spectral smearing. Breakdown of the WKB-approximation near band extrema gives rise to a quasi-linear conductance background. Doping-dependence and next-nearest-neighbor interaction produce spectral asymmetry. Low c-axis dispersion enables enhancement of the spectral peaks by the van Hove singularity.

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Quasiparticle tunneling has remained a puzzling aspect of the high-T_c cuprate superconductors. Experimentally, a wide variety of spectra has been reported [1-4], typically deviating from ideal BCS behavior. Theoretically, there has been little success to explain these spectra in terms of features generic to the cuprates. The new family of Mercury-cuprate superconductors $\mathrm{Hg_1Ba_2Ca_{n-1}Cu_nO_{2n+2+\delta}}$ (Hg-12(n-1)n) with n = 1, 2, 3..., offers an exemplary system to study this problem, by virtue of their tetragonal structure, two-dimensional characteristics and low lattice-mismatch [5-7].

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High-quality samples of Hg-1201, Hg-1212 and Hg-1223 were used in our experiment. Polycrystalline samples of Hg-1201 and Hg-1223, synthesiied by a sealed-quartz-tube method, had T_c's of ~ 97 K and ~ 135 K respectively [8]. Epitaxial c-axis films of Hg-1212, made by laser-ablation on $SrTiO_3$ substrates, showed sharp transitions at ~124 K [9]. Tunneling measurements were carried out with a cryogenic scanning tunneling microscope at 5 K in helium exchange-gas. Details of the measurement apparatus and technique will be published elsewhere [10]. Tunneling spectra were taken in point-contact mode, with a platinum tip as counter-electrode. Junction resistance was typically ~ 10 $M\Omega$.

Tunneling conductance dI/dV spectra showing distinct gap-features are presented in Fig. 1. Positive voltage here means positive sample bias relative to the tip. Pronounced spectral peaks are seen at ~ ±33, ±50 and ±75 meV, respectively for Hg-1201, Hg-1212 and Hg-1223. These peaks are asymmetric in height and show considerable broadening down to very low zero-bias conductances. Quasi-linear backgrounds exist in each of the spectra! generally asymmetric in slope about zero-bias.

The tunneling data is analyzed with the nodal d-wave gap-function A(k) = $\Delta_0(\cos kx - \cos ky)/2$ and the 2D tight-binding dispersion $E(k) = -2t(\cos kx + \cos ky) + 4t'(\cos kx \cos ky)$ near half-filling. These starting assumptions are justified on both experimental and theoretical grounds [11-15]. Our analysis uses planar-junction formalism for elastic and specular tunneling [16]. At zero-temperature, the tunneling current is given by:

$$I(V) \propto \int\int d^2k_t \int_0^{eV} dE \frac{|E|}{\sqrt{E^2 - \Delta^2}} D(E_l)$$

where t and l indicate directions transverse and longitudinal to the junction, and

$$E_l = E - \hbar^2 k_t^2 / 2m$$

The matrix element $D(E_l) = ge^{-2\int \kappa dl}$ represents transmission through a square barrier: i.e.

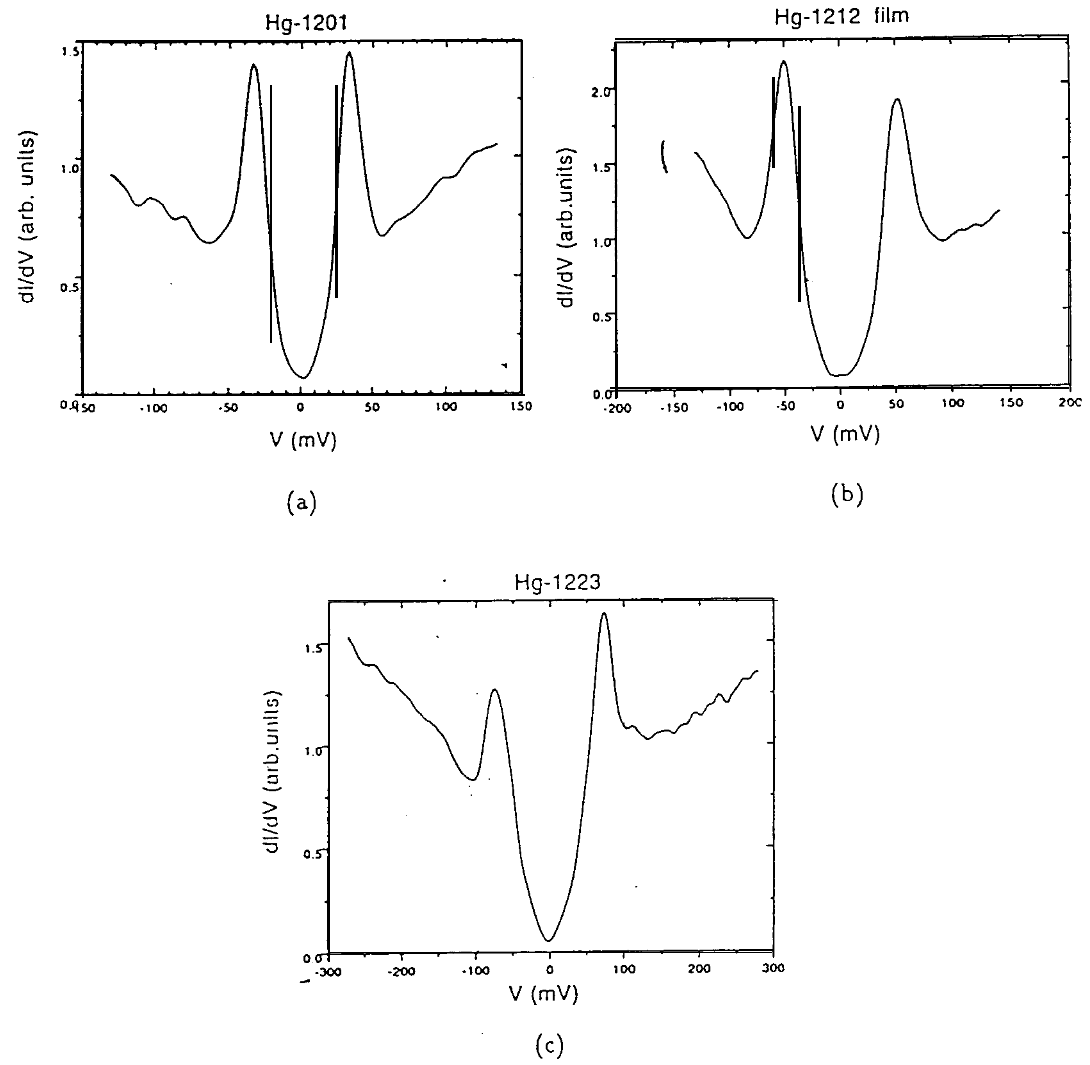
$$\kappa = \sqrt{2m/\hbar^2}\sqrt{W - E_l},$$

and wavevector-matching across the normal-insulator-superconductor junction, i.e.

$$g = \frac{16q\kappa^2 k}{(q^2 + \kappa^2)(\kappa^2 + k^2)}$$

For a simple isotropic dispersion, the integral over k_t matters little because $D(E_l)$ falls off rapidly with k_t and tunneling is collimated within a narrow momentum-cone [17]. The prefactor g can also be set to unity by invoking the WKB-approximation [18], which is valid for junction interfaces not too sharp compared with the Fermi wavelength. Therefore, tunneling should be quite insensitive to the bandstructure, and only the quasiparticle density-of-states $|E|/\sqrt{E^2 - \Delta^2}$ is expected to show up in the dI/dV spectra.

For the highly anisotropic cuprates, however, both the k_t-integral and the prefactor g are important because of the following possibilities:



(a)

(b)

(c)

FIG. 1. Experimental tunneling conductance spectra taken with an STM at 5 K. (a) Polycrystalline Hg-1201. (b) Epitaxial Hg-1212 film. (c) Polycrystalline Hg-1223. These are representative of spectra which show distinct gap-features, with pronounced peaks at $\sim\pm33, \pm50$ and ±75 meV, respectively. Positive voltage means positive sample bias relative to the tip. Junction resistance is typically 10 MΩ.

(1) The tunneling cone flattens out if the final-state has no longitudinal dispersion [19].

(2) The WKB approximation breaks down near- band extrema [20], where the wavevector k and therefore the prefactor g are effectively suppressed [22].

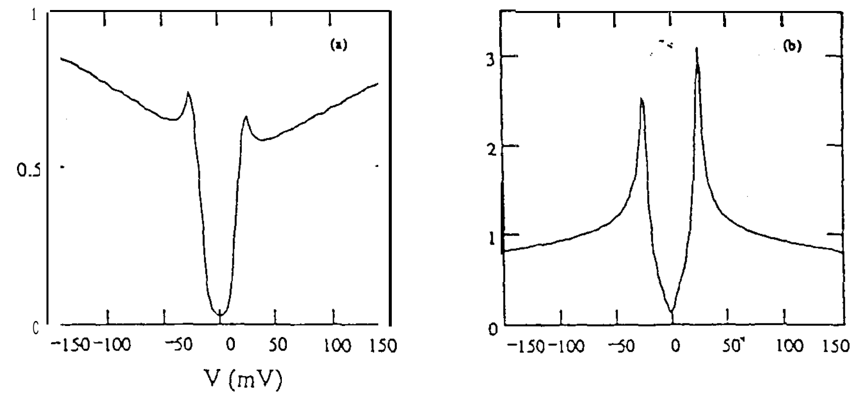


FIG. 2. Calculated tunneling conductance spectra (in arbitrary units of dI/dV), from the model described in the text. (a) For the a-axis junction. (b) For the c-axis junction. The following parameters were used: $t = 125$ meV, $t' = 30$ meV, $\Delta_0 = 25$ meV, $d = 0.1$ nm, $W = 5$ eV, $E_f = 500$ meV for the cuprate and 5 eV for the metal. A small lifetime parameter $\Gamma = 2$ meV was introduced, via $E \rightarrow E + i\Gamma$, to account for the zero-bias conductance. Slight overdoping (5 meV away from half-filling) produced considerable spectral asymmetry.

In our model, these possibilities are exemplified by c-axis and a-axis tunneling, i.e. with the junction perpendicular to the c-axis and a-axis, respectively. The first case is reminiscent of tunneling into Landau levels of electronic states localized on a semiconductor surface [21], which fully manifests the transverse 2D bandstructure. The second case has been considered theoretically by van Bentum and Tsuei for an s-wave cuprate [22], demonstrating that wavevector-suppression near saddle-points in the band-structure gives a quasi-linear weighting to the tunneling conductance. Our model combines these prior works and extends the latter to a d-wave cuprate superconductor.

Examples of our model calculations are shown in Fig. 2. Fig. 2a gives the conductance spectrum for a quasi-planar a-axis junction, i.e. with the k_t-integral limited within a $\pm\pi/4$ cone to mimic a realistic tip-to-plane geometry [22]. Fig. 2b gives the spectrum for a similar c-axis junction. As expected, a-axis tunneling shows suppressed gap-features and a quasi-linear background as a result of the WKB-breakdown near saddle-points in the $E(k)$ [22]. In contrast, c-axis tunneling looks more BCS-like, as the spectral peaks are enhanced by the transverse bandstructure in the form of a 2D van Hove singularity (vHs) near the Fermi energy. In each case, d-wave gap-symmetry introduces spectral smearing quite naturally, without the need for large broadening parameters. Spectral asymmetry follows directly from the bandstructure, by moving the Fermi surface away from the vHs (doping off half-filling) or away from perfect nesting (through the next-nearest-neighbor interaction t') [22].

Qualitatively speaking, each of the measured tunneling spectra shown in Fig. 1 can be described as some superposition of the a-axis and c-axis models shown in Fig. 2. Such a superposition is justified for point-contact tunneling, especially in the case of polycrystalline samples where the exact junction orientation and geometry are not known. Our tunneling model quite reasonably reproduces all the generic features observed in the spectra: gap-edge smearing, quasi-linear conductance profile, enhancement of the spectral peaks and overall spectral asymmetry. Detailed spectral fitting involves finely tuning the model parameters. Fitting results for the energy-gap Δ_0 and implications of the gap-size will be the focus of an upcoming paper [23].

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