Preeminent role of the Van Hove singularity in the strong-coupling analysis of scanning tunneling spectroscopy for two-dimensional cuprates

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In two dimensions the non-interacting density of states displays a Van Hove singularity (VHS) which introduces an intrinsic electron-hole asymmetry, absent in three dimensions. We show that due to this VHS the strong-coupling analysis of tunneling spectra in high-$T_c$ superconductors must be reconsidered. Based on a microscopic model which reproduces the experimental data with great accuracy, we elucidate the peculiar role played by the VHS in shaping the tunneling spectra, and show that more conventional analyses of strong-coupling effects can lead to severe errors.

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Scanning tunneling spectroscopy of Bi-based cuprate high-$T_c$ superconductors (HTS) shows a $d$-wave gap and a strong dip-hump feature which is nearly always stronger for occupied than for empty states.\(^{1}\) It has been proposed that the dip-hump structure results from the interaction of electrons with a collective mode\(^2\) but the dip asymmetry has not received an explanation so far. Indeed such a coupling leads to electron-hole symmetric spectra in classical superconductors.\(^{3,4,5}\) The dip-hump was also observed by photoemission, but in those experiments it is not possible to probe the electron-hole asymmetry. Sometimes photoemission spectra are even symmetrized\(^6\) thus ignoring the relevance of the asymmetry seen in tunneling. The fact that in two dimensions the density of states (DOS) has a prominent van-Hove singularity (VHS), unlike in 3D, introduces naturally an asymmetry and thereby modifies the strong-coupling analysis and the corresponding determination of the collective mode frequency in an essential way.

Photoemission experiments have provided a detailed account of the band structure in cuprates.\(^7,8,9\) In agreement with early calculations,\(^10\) the band crossing the Fermi level presents a saddle point leading to a logarithmic VHS in the DOS. The scanning tunneling microscope (STM) is the ideal tool to look for such singularities, since under suitable conditions it probes directly the DOS with meV resolution.\(^11,12,13\) Up to now, however, there has been no report of a direct STM observation of the VHS in HTS materials, neither in the normal nor in the superconducting state. Previous interpretations of the missing VHS invoked the tunneling matrix element\(^14,15\) in planar junctions, it is indeed believed that the DOS features in the direction normal to the junction are hidden due to a cancellation with the electron velocity, and that the DOS in the plane of the junction does not show up due to focalization effects.\(^16\) These two mechanisms cannot explain the absence of VHS in $c$-axis STM/HTS tunnel junctions: the HTS materials being quasi two-dimensional have virtually no dispersion in the tunneling direction, and the STM junction, owing to its microscopic size, is qualitatively different from a planar junction and is characterized by a specific matrix element which may not lead to focalization effects.\(^11,15\) Besides, the ability of the STM to probe DOS singularities was recently demonstrated in carbon nanotubes.\(^17\)

The solution to this puzzle lies in the coupling to collective modes. Apart from inducing the dip feature,\(^18,19\) this coupling was also shown to effectively suppress the VHS peak in STM spectra.\(^20\) Here we demonstrate that the interplay of the VHS and the collective mode concludes the picture, providing a complete explanation of both the missing VHS and the pronounced electron-hole asymmetries. Our conclusions are based on a brute force fit of the STM spectra and a careful analysis of the model. The advantage of this method is to allow for unambiguous determinations of relevant physical parameters from the raw tunneling data, and to provide intuition about the relationship between trends in the spectral features and parameter variations.

As a template material we studied the three-layer com-
pound Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{8+\delta}$ (Bi2223), which has the highest $T_c$ in the Bi-based family. Reproducible spectroscopy was recently reported in single crystals of Bi2223 cleaved in situ at room temperature. The tunneling conductance measured in UHV on an optimally-doped sample is shown in Fig. 1. The spectrum presents the characteristic V shape of d-wave superconductors, strong and asymmetric coherence peaks, and an asymmetric dip-hump structure. We have deliberately selected an optimally-doped sample displaying a flat background conductance up to high energies (inset in Fig. 1). For underdoped samples the spectra acquire an asymmetric background, attributed to strong correlation effects, which can conceal other intrinsic asymmetries. By moving to optimal doping where this background is absent, we can thus exclude that the observed asymmetries result from this type of correlations.

For illustrative purposes, we plot in Fig. 1 the prediction of a conventional free-electrons BCS d-wave model (curve defined by the shaded area). This model fits the experimental data well at low energy ($\lesssim \Delta_p/2$), but fails to account for the various features present at higher energy, in particular the asymmetry of the coherence peak height. A much better description of the coherence peak height, width, and asymmetry can be achieved by taking into account the actual band structure. At energies below $\sim 200$ meV a one-band model turns out to be sufficient. We consider the two-dimensional lattice model $\xi = 2t_1(\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y + 2t_3(\cos 2k_x + \cos 2k_y) - \mu$ where $t_i$ is the $i$-th neighbor hopping energy. For this dispersion the VHS lies at energy $\xi_M = -4(t_2 - t_3) - \mu$ corresponding to the saddle point $k = (\pi,0) \equiv M$. We determined the parameters of the band through an unconstrained least-squares fit of the whole spectrum in the inset of Fig. 1 leading to $t_1 = -882$, $t_2 = 239$, $t_3 = -14$, and $\xi_M = -26$ meV, as well as a d-wave gap $\Delta_0 = 34.1$ meV. It is very encouraging that these numbers determined from nothing else than the STM tunneling conductance lead to a Fermi surface in semi-quantitative agreement with the one measured by photoemission. The Fermi energy as expected for a hole-doped material. The resulting theoretical curve (Fig. 1 dashed line) is very similar to the free-electron model at subgap energies, but performs much better up to an energy slightly above the coherence peaks. The main effect of the VHS is to provide additional spectral weight below the Fermi level and thus increase the height of the coherence peaks at negative bias. Note that in the absence of broadening factors the VHS would be visible as a secondary peak flanking the main coherence peak (see Fig. 2 below).

The “BCS plus VHS” model is nevertheless not satisfactory above $eV \sim 2\Delta_p$, where it fails to reproduce the significant transfer of spectral weight from the dip to the hump, which is strongest at negative bias in the experimental spectrum. Generically, such transfers signal a strong coupling of the quasiparticles with a collective excitation, which leads to enhanced damping of the former in a limited energy range, and to a simultaneous renormalization of the dispersion. In conventional superconductors, the electron-phonon coupling is known to induce similar features, albeit much less pronounced, at biases related to the phonon frequencies $\Omega_n$. A phonon-based interpretation of the dip-hump in HTS has been revivified recently. Another candidate is the famous $(\pi,\pi)$ magnetic excitation $\sim 41$ meV, although its energy changes from one material to the other and also with varying doping. Coupling the quasiparticles to this collective mode yields a change of the electron self-energy which can be expressed to leading order in terms of the spin susceptibility $\chi_s(q,\omega)$.

In order to estimate these parameters we again performed a least-squares fit of the whole spectrum in the inset of Fig. 1, however keeping the $t_i$’s fixed to their values determined previously. This procedure yields $\Delta_0 = 33.9$ meV and $\Omega_M = -42.4$ meV, as well as $\Omega_s = 34.4$ meV, in reasonable agreement with the properties of the magnetic resonance measured in Bi2212 at several dopings. Apart from the band-structure parameters $t_i$, $\mu$ and the d-wave gap $\Delta_0$, this model has 3 more parameters, namely the resonance energy $\Omega_s$, a characteristic length $\xi_s \sim 2a$ which describes the spread of the collective mode around $q = (\pi,\pi)$, and a coupling constant $g$.

The precise interpretation of the theoretical curve in Fig. 1 seems complicated due to the interplay of three similar energy scales: the d-wave gap $\Delta_0$, the VHS energy $\xi_M$, and the collective mode energy $\Omega_s$, all in the 30–40 meV range. Still, based on a careful study of the model we can identify the origin of each structure in the spectrum, as illustrated in Fig. 2. The bare BCS DOS $N_0(\omega)$ exhibits 5 singularities, namely (a) the V at zero energy resulting from the d-wave gap; (b) and (b’) the coherence peaks at negative and positive energies ($-\omega_b$ and $\omega_b$ respectively); (c) the VHS at energy $-\omega_s$, below the coherence peak, and (c’) the weak echo of the VHS at energy $\omega_s$, due to the BCS electron-hole mixing. The interaction with a collective mode leads to inelastic processes in which a quasiparticle of momentum $k$ and energy $\omega$ is scattered to a state with momentum $k' \neq k$ and energy $\omega - \Omega$ through emission of a collective excitation with
quantum numbers \((q, \Omega)\). The corresponding self-energy diagram is sketched in Fig. 2. If the only excitation available is a sharp-in-energy mode, all singularities of \(N_0(\omega)\) are mirrored in the self-energy, and exactly shifted by the mode energy \(\Omega_s\). Hence the DOS \(N(\omega)\) including the interaction with the mode displays 3 pairs of singularities indicated by arrows in Fig. 2, the onsets at \(\omega = \pm \Omega_s\), below which the quasiparticles do not have enough energy to excite a collective mode, a first minimum in the dip at \(-\omega_b - \Omega_s\) (resp. \(\omega_b + \Omega_s\)) corresponding to the negative-energy (positive-energy) coherence peak, and a second minimum in the dip—echoing the VHS peak in \(N_0(\omega)\)—which is more pronounced for occupied states at \(-\omega_c - \Omega_s\), but also visible at \(\omega_c + \Omega_s\). Therefore the asymmetry of the dip structure between positive and negative biases receives a natural explanation in terms of the asymmetry of the underlying BCS DOS, which in turn is due to the VHS. The appearance of a double minimum in the dip is a direct consequence of the BCS DOS having both a coherence peak at \(-\omega_c\) and a VHS peak at \(-\omega_b\). Such a double minimum is not observed in the experimental spectrum of Fig. 1. At positive bias, the various broadening effects are sufficient to smear out the two minima into one. On the other hand, we have found that if the collective mode has a finite inverse lifetime of only \(\sim 6\) meV \(\Delta\), then the two minima in the dip fade away resulting in a smooth dip also at negative bias as observed experimentally.

The exact relationship between the position of the various structures in \(N(\omega)\) and the parameters of the model is not straightforward. The peak maximum, which we have denoted by \(\frac{\Delta}{\Delta_p}\), is not related in any simple way to the structures in \(N_0(\omega)\), although it is numerically close to \(\omega_b\). Furthermore \(\omega_b\) is not given by \(\Delta_0\), but by the value of the gap function \(\Delta(k) = \frac{\Delta}{\Delta_p}(\cos k_x - \cos k_y)\) at the Fermi crossing near the M point. Hence \(\omega_b\) is slightly smaller than \(\Delta_0\). The case of \(\omega_c\) is simpler, and it can be shown that \(\omega_c = \sqrt{\xi_M^2 + \Delta_0^2}\). It follows that the first minimum in the dip at negative energy lies to a good approximation at \(-\Delta_p - \Omega_s\), and the second at \(-\sqrt{\xi_M^2 + \Delta_0^2} - \Omega_s\). In Fig. 3 we illustrate these two dependencies by varying \(\Omega_s\) and \(\xi_M\) independently in the model. Our starting point is the spectrum of Fig. 1 reproduced in bold in Fig. 3. In order to facilitate the comparison we have positioned the spectra relative to the negative-energy coherence peak. Varying \(\Omega_s\) while keeping \(\xi_M\) fixed we clearly see that the main change in the spectrum is a displacement of the dip and hump relative to the peak, consistently with the interpretation given in Fig. 2. In particular, the width of the dip at negative bias does not depend on \(\Omega_s\). As \(\Omega_s\) increases, we also observe that the coherence peaks become taller and thinner, while developing a shoulder. This shoulder carries part of the spectral weight expelled from the dip, and progressively exits the coherence peak as the difference in the energy scales \(\Omega_s\) and \(\Delta_0\) increases. Fig. 3(a) further shows that \(\Omega_s\) has not much influence on the electron-hole asymmetry of the spectra. In contrast, changing the position of the VHS by varying \(\xi_M\) dramatically affects this asymmetry. At the lowest \(\xi_M\) considered the spectrum is almost symmetric. As the VHS moves toward negative energy, the dip at \(\omega < 0\) gets wider (the first minimum in the dip does not move, as expected) and the dip at \(\omega > 0\) dies out. Inspection of Fig. 3 also shows that the maximum of the hump feature tracks the second minimum in the dip, and thus depends on both \(\Omega_s\) and \(\xi_M\). Furthermore
FIG. 4: STM conductance spectra of Bi2223 at T = 2 K. Each curve is an average of several spectra taken at different locations on the same sample, all having the indicated peak-to-peak gap Δp. Ωdip is the energy difference between the dip minimum (dot) and the peak maximum at negative bias, relative to which voltages are measured.

Having clarified the different roles of Ωs and ξM in the shape of the model DOS, we now come back to experiment. In Fig. 4 we plot a series of tunneling conductance spectra, Ωdip, also decreases with increasing Δp, but less than Ωs (from 39 to 35 meV), as can be seen in Fig. 4. From these numbers it appears clearly that Ωdip overestimates Ωs by 5 to 10 meV. Recently the energy difference between Δp and the inflection point between the dip and the hump (extremum in the d2I/dV2 spectrum) was used as an estimate of Ωp in Bi2212, resulting in an average value of 52 meV. This same estimate would give a Δp-independent result of ~57 meV for the data in Fig. 4 almost a factor of two larger that Ωs.

In summary, we have shown that the van Hove singularity plays a crucial role in shaping the spectral features induced in the STM spectra by the interaction of quasiparticles with a collective mode. As a result, determining the frequency of the mode from STM data is complicated, and cannot be done directly from simple structures in the dI/dV or d2I/dV2 spectra. This conclusion, obtained for a coupling to the (π, π) spin resonance, also applies to phonon models.

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Our theoretical curves in Figs 1 and 3 show the DOS corrected by three broadening effects: a constant scattering rate $\Gamma = 2$ meV, a 2 K thermal smearing, and a gaussian broadening of 4 meV. The latter accounts for the combined experimental uncertainty due to the lock-in ac modulation at $V_{ac} = 2$ mV, and the averaging of several slightly different spectra.

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