Realistic Surface Scattering and Surface Bound State Formation in the High Tc Superconductor YBa$_2$Cu$_3$O$_{6+x}$

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Surface Umklapp scattering of quasiparticles, and surface roughness are shown to play essential roles in the formation of the surface bound states in realistic models for YBa$_2$Cu$_3$O$_{6+x}$. The results account for the shape, the impurity dependence of the height, and for a proposed universal width of the zero bias conductance peak.

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This article describes the formation of mid-gap surface bound states in models of YBa$_2$Cu$_3$O$_{6+x}$ (YBCO) which include realistic surface scattering of the quasiparticles. (We define realistic surface scattering to be scattering that includes surface roughness as well as surface Umklapp scattering processes and a realistic Fermi surface geometry.) More than a trivial extension of what is known about surface bound states from the study of elementary models is required. (By our definition, elementary models neglect either surface roughness or surface Umklapp scattering or both.) On the one hand, except at grazing angles, the superconducting quasiparticles are prevented from forming surface bound states because they are reflected diffusely at a rough surface, and on the other hand, the grazing incidence quasiparticles are prevented from forming surface bound states on a [110] surface (the most favorable case) when surface Umklapp scattering is considered. Surface bound states are of interest in the study of high Tc superconductors, because they probe the sign changes of the gap function $\Delta(k)$ on the Fermi surface, and also because they manifest themselves experimentally through the zero bias conductance peak (ZBCP) observed in tunneling experiments. As noted in the conclusions, our results have a considerable impact on the interpretation of experiments.

The existence of surface bound states in $d$-wave superconductors and their role in producing the ZBCP observed in tunneling experiments are well established for elementary models, e.g. in. Further studies have discussed, among other results, the existence of multiple sub-gap resonances, the surface induction of order parameters of different symmetries and the associated splitting of the ZBCP at low temperatures, the splitting of the ZBCP in a magnetic field, the effects of irradiation in suppressing the ZBCP, the effects of surface roughness in broadening the ZBCP, and the anisotropy of the ZBCP

According to the Rayleigh criterion in the theory of surface roughness (for a general discussion see), a surface is rough (reflects diffusely) or smooth (reflects specularly) according as the parameter $R_k = k_\perp \eta$ is smaller than or greater than unity. Here $k_\perp$ is the component of the incident-wave wave vector perpendicular to the surface and $\eta$ is the surface asperity. For $R_k$ small, perturbation theory (e.g. see) gives the probability of diffuse reflection as $P_D \sim R_k^2$, i.e. it goes to zero as $k_\perp^2$ for small $k_\perp$. On the other hand, for $R_k$ large, a quasi-classical approximation shows that, for a wave incident normally on the surface, the probability of specular reflection is given approximately by $P_S = exp(-4\pi R_k^2)$, i.e. there is essentially no specular reflection for $R_k$ greater than unity (e.g. see).

It follows from the above estimates that, except for quasiparticles approaching the surface at grazing incidence, the reflection is totally diffuse. These ideas have been successfully applied to the theory of the electronic surface states of a normal metal in low magnetic fields where microwave absorption experiments show that quantized magnetic surface levels exist only for electrons incident on the surface at grazing angles (so that they are specularly reflected). The application of these ideas to surface bound states in $d$-wave superconductors suggests that, except possibly for those which approach the surface at grazing angles, the quasiparticles will be diffusely reflected at a rough surface and thus will not maintain the phase coherence necessary (e.g. see the argument surrounding Eq. 25 of) to form bound states.

Surface bound states in a model which incorporates surface Umklapp scattering have recently been described in. As in, to obtain a realistic Fermi surface we use a discrete lattice model (see Fig.) including both nearest and next nearest neighbor hopping interactions in the superconductor. Also, we consider the case of a [110] surface, for which the formation of surface bound states is the most favorable. The surface bound states are eigenstates of the two-component Bogoliubov-de Gennes equations and are linear combinations of basic solutions of the form

$$U_{ki}(x) = \begin{bmatrix} \Delta_i \\ E \pm i\Omega_i \end{bmatrix} e^{i(k_i x + k_j y)} e^{-\kappa_i x}. \quad (1)$$
as in [12] and others. Here $k_i = (k_{ix}, k_{iy})$ must be on the Fermi surface, $\Delta_i = \Delta(k_i)$, $\Omega_i = \sqrt{\Delta_i^2 - E_i^2}$, and $\kappa_i = \Omega_i/(\hbar|v_{ix}|)$ with $v_{ix}$ being the $x$ component of the normal state electron velocity. The upper and lower signs in Eq. 2 correspond to $v_{ix} < 0$ and $v_{ix} > 0$, respectively. From Fig. 2 it is seen that for $k_y > k_y^0$, a line of constant $k_y$ intersects the Fermi surface at four distinct points, giving four values $k_{ix}$, $i = 1 \ldots 4$, and hence four linearly independent exponentially decaying solutions. In this case the surface bound state solutions have the form

$$U(x) = \Sigma_i C_i U_{k_i}(x).$$

From above, only grazing incidence quasiparticles, i.e. those corresponding to small values of $|k_{1x}|$ in the surface-adapted Brillouin zone of Fig. 2 of Fig. 3 will have the possibility to form surface bound states in the case of rough surfaces. However, it turns out that a detailed study of such states has shown that, at least in the case of perfectly flat surfaces, waves having $k_y > k_y^0$ in Fig. 2 (and this includes all waves of small $|k_{1x}|$) can not form surface bound states [the reason has to do with the relative signs of the gaps $\Delta(k_{1x}, k_y)$ and $\Delta(k_{2x}, k_y)$].

In summary, on the one hand, except at grazing incidence, quasiparticles (or holes) striking the surface are reflected diffusely and hence do not have the coherence necessary to form surface bound states, while on the other hand, grazing incidence quasiparticles are prevented from forming bound states in a realistic model for the Fermi surface because they do not satisfy the necessary conditions on the sign variation of the gap $\Delta(k)$. We now give a qualitative explanation of the result of our quantitative calculation presented below showing how it is possible to form surface bound states in models of YBCO which include realistic surface scattering. First, assume that the surface at $x = 0$ is perfectly flat, and consider an incoming wave of the form of Eq. 3 with (the $x$- component of its) wave vector equal to $-k_{1x}$, or equivalently $-q_1$, of Fig. 3. In order to satisfy the boundary conditions at the surface, two outgoing waves, a specularly scattered wave at $k_{1x}$ and an Umklapp scattered wave at $k_{2x}$, are required. (Note that the wave at $k_{2x}$ appears as a normal scattering process when viewed in the surface-adapted Brillouin zone of Fig. 3, but is a surface Umklapp process when viewed in the normal bulk Brillouin zone.) It is the Umklapp scattering into the state with wave vector $k_{2x}$ which prevents the formation of the surface bound state because the relative signs of the gaps at wave vectors $\pm k_{1x}$ and $\pm k_{2x}$ are incompatible with the formation of a surface bound state [3]. Thus we can only get surface bound states (or at least resonances) if the scattering from wave vectors $\pm k_{1x}$ to $\pm k_{2x}$ is sufficiently reduced.

It is the roughness of the surface which limits the Umklapp scattering of quasiparticles of wave vectors $\pm k_{1x}$ into the states of wave vector $\pm k_{2x}$. Quasiparticles in states which are linear combinations of states with wave vectors $\pm k_{2x}$ will be strongly diffusely reflected by a rough surface and will thus have short lifetimes. Their short lifetimes will spread out their density of states in energy, reducing the density of states at the energy of the quasiparticles of wave vector $k_{1x}$ and hence reducing the probability of scattering from wave vectors $\pm k_{1x}$ to $\pm k_{2x}$.

We now develop a more quantitative theory of the effects of surface roughness by assuming that surface-bound-state component states (Eq. 3) having wave vectors $\pm k_{1x}$ have a finite lifetime $\tau_i = \hbar/\gamma_i$ due to nonspecular scattering at the surface. For quasiparticles with vectors $\pm k_{2x}$ (which have a probability of unity for diffuse scattering at the surface) we take this lifetime to be the time taken for an electron to get to the surface from a distance of $(\kappa_i)^{-1}$, which, for $|E| < |\Delta_2|$ gives $\gamma_2 = |\Delta_2|$. (Similar qualitative estimates of damping rates were shown in [13] to be in excellent agreement with the results obtained from a detailed solution of the Bogoliubov-de Gennes equations.) For grazing incidence quasiparticles of wave vector $\pm k_{1x}$, which have a very small probability $P_1$ of diffuse scattering at the surface, the appropriate value of $\gamma$ is $\gamma_1 = P_1|\Delta_1|$. (The perturbation theory estimate of $P_1$ is given in the above general discussion of surface roughness.) These lifetime effects are incorporated into our model by using the phenomenological approach of replacing $E$ by $E + i\gamma_i$ in Eq. 3 for $U_{k_i}$. If we now look for solutions of the form of Eq. 2 which satisfy the appropriate boundary conditions for a superconductor to vacuum surface (corresponding to the absence of the normal metal and the insulating layer in Fig. 3), and which are valid in the limit of small $|k_{1x}|$, we find a solution having an energy $E = E_B + i\Gamma R$ where the bound state energy is $E_B = 0$ and the width due to roughness is $\Gamma_R = \gamma_1 + \Gamma_{12}$, with the component

$$\Gamma_{12}(k_y) = |\Delta_1|(|\Delta_2| + 2|\Delta_2|)\sin q_1\cot(q_2/2)/\gamma_2.$$

Here $\Delta_2 = \sqrt{\Delta_2^2 + \gamma_2^2}$ and $q_1 = k_{ix}\omega/\sqrt{2}$. Note that $\Gamma_{12}$ depends on $k_y$ through the dependences of $q_i$ and $\Delta_i$ on $k_y$. From the above result $\Gamma_R = \gamma_1 + \Gamma_{12}$, we interpret the solution as being primarily a state formed from the grazing incidence wave vectors $\pm k_{1x}$ and having a width $\gamma_1$ which is augmented by $\Gamma_{12}$ due to transitions from wave vectors $\pm k_{1x}$ to $\pm k_{2x}$. It is clear that for $\gamma_2$ having the value $|\Delta_2|$ suggested above, the width $\Gamma_{12}$ is smaller than $|\Delta_1|$ (since $q_1$ is small) and the bound state thus has a spread of energies lying within the gap $|\Delta_1|$. If $\gamma_2$ were to be small on the other hand, $\Gamma_{12}$ would be large and no well defined state would exist in the gap. Clearly it is the broadening of the quasiparticles at wave vectors $\pm k_{2x}$ by diffuse scattering that allows the formation of surface bound states for the case of realistic surface scattering.

We now proceed to a calculation of the tunneling conductance for the model NIS junction illustrated in Fig. 3 using a procedure well-established in other work, i.e. we
use the BTK formalism \cite{3} but extended to the case of d-wave superconductors \cite{2,8} and to a discrete-lattice model \cite{2,20}. The procedure is straightforward: assume a solution in the form of a linear combination of an electron moving towards the junction together with a reflected electron and reflected hole in normal state, and a linear combination of the form of Eq. 3 in the superconducting state. The coefficients in the linear combinations are found using the boundary condition implicit in Fig. 3 and the tunneling conductance is calculated following BTK \cite{2,27}. We restrict ourselves to the low temperature limit, and to the calculation of the contribution of the surface bound states to tunneling conductance, which is valid only for voltages such that eV is less than the maximum gap, and we also work in the weak transmission limit where the probability of an electron tunneling across the barrier is much less than unity, since it is only in this limit that one obtains a sharply defined ZBCP in the gap \cite{5,9}. In this way, we find that the conductance per surface unit cell (for eV smaller than the maximum gap) is given by the formula

$$G = \frac{4e^2}{h} \left( \Gamma_{SN}(k_y) \frac{\Gamma_T(k_y)}{(eV)^2 + (\Gamma_T(k_y))^2} \right)$$  \hspace{1cm} (4)$$

where the angular brackets indicate an average over \(k_y\). Here

$$\Gamma_T(k_y) = \gamma_1(k_y) + \gamma_{imp} + \Gamma_{12}(k_y) + \Gamma_{SN}(k_y)$$  \hspace{1cm} (5)$$

where the damping rate of the basics states with wave vectors \(\pm k_{1x}\), called \(\gamma_1\) above, has been replaced by \(\gamma_1 + \gamma_{imp}\), thus separating the momentum-dependent diffuse surface scattering part \(\gamma_1\) (proportional to \(q^2\)) from the momentum-independent bulk impurity scattering part, \(\gamma_{imp}\). Also

$$\Gamma_{SN} = 2\alpha_{N} \alpha_{C} \sin(q) \gamma_1 \Gamma_{2} - \sin(q) \left| \Delta_1 \right| \gamma_2$$  \hspace{1cm} (6)$$

with \(\alpha_{N} = t_{N}/V_0\), \(\alpha_{C} = t_{C}/V_0\), \(V_0\) being the additional potential on the ions in the insulating layer I of Fig. 3, and \(q \gg 0\) being the wave vector of the incident normal state electron. Our calculations are valid to the lowest nontrivial order in \(\alpha_{N}, \alpha_{C}\) (i.e. a weak transmission insulating barrier) which means that the contribution of \(\Gamma_{SN}\) to \(\Gamma_T\) should be neglected (but that \(\Gamma_{SN}\) should remain in the numerator). The fact that \(\Gamma_{SN}\) is nevertheless one of the contributions to \(\Gamma_T\) allows its interpretation as a contribution to the lifetime of the surface bound state resulting from the tunneling of the bound state excitation from the superconductor into the normal metal.

The tunneling conductance described by Eq. 3 is plotted in Fig. 3 as a function of \(eV/\Delta_0\) (charge times voltage over maximum gap). The contribution of \(\gamma_1\) to \(\Gamma_T\) is neglected since it is smaller than \(\Gamma_{12}\) at small wave vectors \(q_1\). Thus the height, width and shape of the curve of conductance versus voltage are determined by \(\Gamma_{12}, \Gamma_{SN}\), and \(\gamma_{imp}\). In particular, the cusp-shaped maximum at \(eV=0\) in the curve for \(\gamma_{imp}=0\) is due to the fact that \(\Gamma_{12}\) and \(\Gamma_{SN}\) both go to zero as \(q_1^2\) at small \(q_1\). This means that the bound states with very small \(q_1\) are very narrow and contribute all of their weight near \(eV = 0\), giving a sharp maximum there. The broader bound states at larger values of \(q_1\) give broader contributions to the conductance and are responsible for the weight in the wings. A cusp shaped ZBCP has been observed in \cite{3}.

A strong reduction of the ZBCP height with increasing disorder (i.e. increasing \(\gamma_{imp}\)) without, however, a significant increase in the ZBCP width has been found in \cite{14}. This agrees with the behavior which is predicted by our Eq. 3 and shown in Fig. 3. The qualitative explanation for this can be found in the momentum dependence of \(\Gamma_{12}\). The very small \(q_1\) quasiparticles, which are very narrow in energy, give a high ZBCP in the absence of impurity scattering. Impurity scattering broadens these quasiparticles and reduces their contribution to the peak height, but has little effect on the broader quasiparticles at less small \(q_1\) which are responsible for the overall width of the ZBCP.

Eq. (4) predicts a universal width, independent of surface asperity and impurity scattering (for impurity scattering not too strong), for the ZBCP assuming that \(\Gamma_T\) is dominated by \(\Gamma_{12}\). From Fig. 3, this universal half width at half maximum is approximately \(\Delta_0/4\). This is very different from the predictions of elementary models where the width is due to and increases in proportion to the surface asperity \cite{3} or impurity scattering \cite{4}. Our result is roughly in agreement with experiment where the widths of measurements made under widely differing conditions (for an asperity \(\eta \sim 1\) nm in \cite{14}, for \(\eta \sim 1\) to 10 nm in \cite{2} for \(\eta \sim 500\) nm in \cite{3}, and for varying \(\gamma_{imp}\) in \cite{14} all give approximately the same half width of about 2 to 2.5 meV, which is however about a factor of two smaller than our prediction. The error in the numerical factor is perhaps due to our simplistic representation of the insulating barrier by a single atomic layer, or to our simplistic treatment of the surface roughness (carried out simply by the replacement of \(E\) by \(E + i\eta\)).

Our results, in which the width of the ZBCP is due to \(\Gamma_{12}\), also resolve the problem that fitting the ZBCP to elementary models requires an inexplicably large value of the so-called smearing factor [see \cite{2}(a)].

To conclude, we note that the description of surface bound state formation and the consequent effects on the tunneling conductance in YBCO requires a realistic description of the surface scattering processes. The principal source of width of the surface bound states is their limited lifetime due to the surface Umklapp scattering from grazing incidence states to larger perpendicular momentum states, and this process hence has a determining effect on the height, width and shape of the ZBCP. These ideas give a qualitative explanation of the cusp shaped ZBCP observed in \cite{3}, the height reduc-
tion (without width increase) of the ZBCP caused by increased disorder seen in [16], and the approximately universal value (independent of surface roughness and impurity concentration) of the width of the ZBCP observed in [2,13,14,16,18].

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Fig. 1

Fig. 2

Fig. 3