Multiband quasiparticle interference in the topological insulator Cu$_{0.2}$Bi$_2$Te$_3$.

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We present angle resolved photoemission experiments and scanning tunneling spectroscopy results on the doped topological insulator Cu$_{0.2}$Bi$_2$Te$_3$. Quasi particle interference (QPI) measurements, based on high resolution conductance maps of the local density of states show that there are three distinct energy windows for quasi particle scattering. Using a model Hamiltonian for this system two new scattering channels are identified: the first between the surface states and the conduction band and the second between conduction band states. The comparison of the QPI data with self-energies extracted from photoemission indicates that spin-orbit terms are relevant for surface state → conduction band scattering.

The discovery of topological insulators (TIs)[1–3] has opened a new route to spintronic devices, whereby the surface states taking part in the charge transport are undisturbed by non-magnetic impurity scattering. Soon after the discovery of the topological phase in BiSb$_x$[4], a new family of TIs was predicted and discovered: Bi$_2$Se$_3$, Bi$_2$Te$_3$ and Sb$_2$Te$_3$[5, 6]. Recently, it has become apparent that higher order terms in the \( k \cdot p \) expansion are relevant for describing the low energy electronic states, leading to a warping of the Dirac cone away from the Dirac point [7, 8]. Such warping has been observed in angle-resolved photoemission spectroscopy (ARPES) experiments [9] and has been shown to be a source for local density of states (LDOS) oscillations observed in scanning tunneling microscopy/spectroscopy (STM/S) [7]. In terms of device applications it is important to understand and characterize such potential scattering channels, in particular in systems in which chemical potential tuning has taken place via bulk doping [9].

In this Letter we use STS, supplemented by ARPES and theoretical modeling, to uncover three different regimes of carrier scattering in Cu doped Bi$_2$Te$_3$. Firstly, scattering between the surface state (SS) and the bulk conduction band (CB) is shown to be vital in the understanding of such doped systems. Secondly, warping-assisted SS-SS scattering is also observed and thirdly quasi particle scattering between CB states completes the line-up.

Single crystals of Cu$_{0.2}$Bi$_2$Te$_3$ were grown using a Bridgman technique. The elements were sealed in a quartz tube, heated to 850 °C and held there for 10 hours. This was followed by a slow cool (1 °C/hour) to 600 °C, the samples being held at this temperature for a further 60 hours. ARPES was performed at the 1$^3$ endstation on the UE112-PGM-2b beamline at BESSYII and with a lab-based system equipped with a high intensity helium discharge source. Angular and energy resolution were set to 0.002(0.008) Å$^{-1}$ and 4(15) meV at 1$^3$ (lab-system). ARPES data were taken at 1$^3$ at a temperature of 800 mK, and the lab-based data at 18 K. UHV STM measurements were performed at 4.2 K, using Pt/Ir tips to achieve a tunneling current of 0.5 nA with junction resistances between 0.1-0.5 GΩ. Conductance maps, \( g(r,E) \), have been recorded over 60 × 60 nm$^2$ areas using a modulation frequency of 969 Hz with a bias modulation amplitude of 5 meV. In all experiments samples are cleaved in situ at room temperature.

A powerful probe of quasiparticle scattering on TI surfaces is provided by conductance mapping in...
spectroscopic-imaging STM \[10\]–\[15\]. In Fig. 1(a,b) we present representative conductance maps at two different energies. There are clear standing wave-like patterns in $g(r, E = 100 \text{ meV})$ originating at impurity sites, whose characteristic wavelength ($\approx 30$ Å) can be picked up in the Fourier Transform (FT), $\rho(q, \omega)$, shown in the inset. $\rho(q, \omega)$ at $E = -175 \text{ meV}$ \[10\] also shows a similar FT pattern, whereby the lobes arranged with six-fold symmetry are clearly closer to the origin, making the associated longer wavelength patterns difficult to spot with the naked eye in the raw LDOS data. Many such LDOS maps have been measured, generating $\rho(q, \omega)$ images spanning the bias interval -350 meV to 250 meV in 12.5 meV steps. At the energies where peaks are observed in $\rho(q, \omega)$, they always appear along the same directions in $q$-space ($\Gamma \rightarrow K$). We determine the $q$-vectors for the six quasiparticle interference (QPI) peaks and plot the average $q$-vector in Fig. 1. Error bars are determined from the spread in the peak positions in the six directions. We can identify three different regimes in the QPI patterns: (I) -300 meV to -175 meV, (II) -125 meV to 200 meV and (III) $\geq$ 200 meV. To understand the origin of these different regimes, we compare the measured $\text{d}I/\text{d}V$ to ARPES measurements presented in Fig. 2(a–d). Figure 2(a) shows the Fermi surface (FS) of as-grown Cu$_{0.2}$Bi$_2$Te$_3$. We observe a small hexagonal deviation (warping) from the perfect Dirac cone \[7\]–\[8\]. A cut along $\Gamma \rightarrow M$ is shown in Fig. 2(a). Compared to pure Bi$_2$Te$_3$, Cu doping is expected to be $p$-type and we indeed find that the chemical potential is shifted below the bottom of the CB. From Fig. 2, the energy of the Dirac point is found to be, $E_D = -180 \text{ meV}$ and the valence band maximum, $E_{VB} = -80 \text{ meV}$. Exposure to ambient conditions is known to lead to $n$-type doping of Bi$_2$Se$_3$ \[17\]–\[18\], without destroying the topologically protected surface states. Figure 2(d) shows that the same holds true for Cu-doped Bi$_2$Te$_3$ stored under ambient conditions prior to cleavage: not only is the FS area clearly greater than for the pristine crystals, but the bulk CB states are also clearly visible inside the SS features, both in the FS-map and the I($k, E$)-image. Naturally, this $n$-type ‘ambient doping’ shifts the Dirac-point to higher binding energy. Fitting the $\Gamma \rightarrow M$ dispersion using a simple linear relation shows the Dirac point in the ambient-doped system to lie at -385 meV, with a band velocity $v_k \approx 2.52 \text{ eVÅ}$. This velocity matches that in Fig. 2, further underpinning that the ambient exposure of the crystal does not significantly alter the properties of the SS.

Since the STM conductance maps were also recorded on a crystal cleaved after exposure to air, we can now relate the different regions observed in $\rho(q, \omega)$ in Fig. 1(c) to features of the bandstructure. Region I spans the energy window between the top of the valence band (VB) and the CB bottom. In this special energy interval only quasiparticle scattering between surface states (SS-SS) is possible, facilitated where relevant by the Dirac cone warping \[2\]. For energies close to the bottom of the conduction band the QPI patterns are suppressed and then a new QPI regime is encountered (dubbed region II), matching an energy window in which both SS and CB states are available for scattering. In the following, we will show that region II is indeed dominated by scattering between surface states and the bulk conduction band (SS-CB). Finally, the dispersion observed at energies above the second jump in the $q$-vector around +150 meV - indicated in Fig. 1(c) as region III - is due to scattering within the conduction bands.

To underpin the assignment of the different quasi particle interference regions, and in particular the new insight regarding the multi-band scattering underlying region II, we utilize an extension of an electronic structure model based upon the work of Ref. \[8\] and applied to simulate QPI in Refs. \[19\]–\[20\]. The electronic structure of Bi$_2$Te$_3$ and Bi$_2$Se$_3$ can be described by the Hamiltonian

$$H = \varepsilon(k)I_4 + M(k)\Gamma_5 +$$

$$+ B(k_z)\Gamma_4 k_z + A(k_{||})(k_y\Gamma_1 - k_x\Gamma_2) +$$

$$+ R_1\Gamma_3(k_z^2 - 3k_x k_y^2) + R_2\Gamma_4(3k_y k_x^2 - k_y^2)$$

where $I_4$ is the identity and $\Gamma_{1–5}$ are Dirac matrices satisfying the Clifford algebra $\{\Gamma_i, \Gamma_j\} = 2\delta_{ij}$, and the functions $\varepsilon(k) = C_0 + C_1 k_x^2 + C_2 k_y^2, M = M_0 + M_1 k_z^2 + M_2 k_z^4, B = B_0 + B_2 k_z^2$ and $A = A_0 + A_2 k_{||}$. For systems such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$, the last two terms in Eq. 1 break the in-plane symmetry, producing the Dirac cone warping.
FIG. 3: (Color online) (a): Comparison between $\rho_{exp}(\mathbf{q}, \omega)$ and $\rho_{calc}(\mathbf{q}, \omega)$ from a simple Dirac cone model (left) and a Dirac cone model with the CB included (right) for energies of -175 meV and 50 meV. In between the $\rho_{calc}(\mathbf{q}, \omega)$ data are shown the relevant constant energy contours of the spectral functions with arrows indicating the dominant scattering processes. (b, c): QPI patterns for the D-cone+CB model at selected energies: -137.5 meV, falling in between regions I and II in Fig. 1(c), and at 213 meV where intraband scattering in the CB dominates (region III).

This Hamiltonian can be reduced to an effective surface Hamiltonian, $H_{2D} = E(k) + v_{k}(k_{x}\sigma_{y} - k_{y}\sigma_{x}) + \frac{\lambda}{2}(k_{x}^{3} + k_{y}^{3})\sigma_{z}$, where $v_{k}$ and $\lambda$ are determined by comparison to ARPES experiments. The latter Hamiltonian has been used to study QPI patterns in STS experiments [19, 20] and is able to describe SS+$\uparrow$SS scattering. To include scattering between SS and the CB we need to calculate the surface Green’s function starting from the model Hamiltonian, Eq. (1), using the method outlined in [2, 21]. The Hamiltonian is split into an in-plane component depending only on $k_{||}$ and a component depending on the interlayer hopping parameters. The surface Green’s function is calculated iteratively whereby the Green’s function for N layers, $G_{N}^{-1}$, is related to the Green’s function of a single layer, $G_{0}$, through $G_{N}^{-1} = G_{0}^{-1} - H_{z}^{\dagger}G_{N-1}H_{z}$. Employing the fast iterative scheme proposed in [22], we use the resulting surface Green’s function to calculate $\rho(q, \omega)$ by means of the standard T-matrix formalism assuming ordinary impurity scattering with a momentum independent scattering potential [19, 20].

To highlight differences between the QPI patterns obtained from the full, multiband Hamiltonian (labelled ‘D-cone+CB’), Eq. (1), and the effective surface Hamiltonian (labelled ‘D-cone’), we show results obtained for both models in Fig. 3. In all calculations we used parameters chosen to reproduce the salient features of our ARPES data [23], and we added a chemical potential to fix the position of the Dirac point to match the ambient-doped ARPES data. These ingredients allow the description of the multiband QPI and ARPES data in a self-consistent manner, and Fig. 3a shows a comparison of $\rho_{calc}(\mathbf{q}, \omega)$ and the STS results. For a bias voltage of -175 meV (top panel), both simulations show six dominant scattering vectors along $\Gamma - K$ from intra SS scattering as indicated by the double-headed arrow in the constant energy contour, agreeing with the experimentally observed QPI in region I. The bottom panel shows the experimental data at a bias of 50 meV (region II) compared to both models. The simple D-cone model predicts dominant scattering along the $\Gamma - M$ direction, placing the QPI hexagon on its point, contrary to what is observed in the experimental $\rho(q, \omega)$. The main theoretical result is that this discrepancy is removed in the D-cone+CB model in which the outermost, intense features now match the orientation of the experimental QPI intensity and lie along $\Gamma - K$, as highlighted by the white arrow. The D-cone+CB model is also validated by the experimental QPI patterns at other energies. In Fig. 3b the comparison is made for an energy in between regions I and II (top panel, -137.5 meV) and panel (c) for energy in region III (213 meV). In the former, the
QPI is correctly predicted to be dominated by very small $q$-scattering due to the very large DOS associated with the bottom of the CB. In region III, the Dirac cone+CB model suggests that the dominant scattering processes seen in experiment do not involve the SS at all, and are of CB+CB character.

Fig. 3 shows we are able to successfully capture the essence of the experimental QPI behaviour by recognizing that there are three scattering regimes. Based on this insight, we close the loop by extracting the $q$-vectors for the dominant scattering processes from the two models and overlay them as solid lines on the STS results in Fig. 3. It is clear that the D-cone+CB model correctly explains both the size of the $q$-vectors and the jumps between the scattering regimes, whereas the single D-cone model is only able to describe region I. Closer inspection of Fig. 3 shows that the predicted energy dependence of the $q$-vectors in the D-cone+CB model does not match the experimental data perfectly. This points towards limitations of the $k \cdot p$-theory in providing a sufficiently accurate description of the quasi-particle dispersions away from the Dirac point. Figure 4 shows the experimental dispersion obtained from Lorentzian fits to the ARPES MDC’s. The dispersion obtained within $k \cdot p$-theory is shown in the inset of the same panel. While the warping in the experimental data appears as a reduced band velocity along $\Gamma - M$, $k \cdot p$-theory predicts that the warping leads to an increase in velocity along $\Gamma - K$. Density functional theory is able to provide a more accurate description of the true situation, correctly reproducing a lowering of the velocity along $\Gamma - M$ upon the onset of warping [24].

A final point we address is the importance of spin-orbit scattering. The effect of spin-orbit terms in QPI scattering has been studied in ref. 20. Overall, spin-orbit scattering is not needed to capture the salient features of the QPI data. However, the angle dependence of the ARPES line-widths suggests that spin-orbit scattering is relevant in these systems. The right hand panel in Fig. 4 shows the energy dependence of the imaginary part of the self energy, $\text{Im}(\Sigma(\omega))$, obtained from ARPES and the local band-velocity. We note that the SS self energy is minimal (and close to azimuthal-angle independent) for energies above the VB maxima and below the onset of warping, indicated by the purple points in Fig 4b. Once warping kicks in, $\text{Im}(\Sigma(\omega))$ increases and becomes angle dependent (Fig. 4b, black squares). Particularly this last effect calls for an angle-dependent interaction - the isotropic impurity scattering underpinning the QPI analysis will not do the trick - and the spin-orbit interaction would provide just such an anisotropic scattering mechanism [20].

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