Disorder-induced splitting in quasiparticle interference of Bi$_2$Te$_3$ Dirac electrons

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August 4, 2020

Inelastic interactions of quantum systems with environment usually wash coherent effects out. In the case of Friedel oscillations, the presence of disorder leads to a fast decay of the oscillation amplitude. Here we show both experimentally and theoretically that in the three-dimensional topological insulator Bi$_2$Te$_3$, the finite lifetime of the Dirac electrons due to disorder causes a splitting of coherent scattering vectors which follows a peculiar evolution in energy. Not only this splitting enables evaluating the lifetime of Dirac quasiparticles in topological insulators, but this general phenomenon can be in play in other quantum systems, leading to non-trivial modifications of their coherent properties.

Predicted a long ago, recently discovered three-dimensional topological insulators (TIs) are characterized by conducting surface states with the linear dispersion, Dirac cones, evolving in the bulk gap. In real materials, the Dirac cones are often regular only close to their origin, the Dirac point (DP). Both theories and experiments showed that far from the Dirac point, the circular shape of the constant energy contour evolves into a hexagon and then to a snowflake with sharp tips extending along six crystallographic directions. The warping is present in Bi$_2$Se$_3$, Pb(Se,Sb)$_2$Te$_3$, and other TI materials.

The spin texture of Dirac quasiparticles in TIs is peculiar, due to momentum $k$ coupling to spin $\sigma$, it is subject of intense studies. Close to impurities, the elastic electron scattering from the state $k, \sigma$ to the state $k', \sigma'$ causes the interference between the incident and reflected waves with the wave vector $q = k - k'$ and the amplitude determined by the corresponding scattering matrix element. This gives rise to spatial variations of the local density of states (LDOS) which can be probed by Scanning Tunneling Microscopy and Spectroscopy (STM/STS). The Fourier-transformed tunneling conductance $dl/dV(x, y)$ STS maps display quasi-particle interference (QPI) patterns and reveal characteristic scattering vectors.

In search for specific scattering rules in three-dimensional TIs, the QPI patterns were studied around individual defects, steps, trigonally shaped defects are observed, originating from atomic Te-vacancies (see inset in Fig. 1b). On top of atomic corrugation, triangle-shaped defects are observed, originating from atomic Te-vacancies (see inset in Fig. 1b). On the tunneling conductance map $dl/dV(x, y)$ of the same region acquired at the sample bias $V_{bias}=90$ mV, the defects appear dark, reflecting a lower local electronic state density, Fig. 1c. Around defects, Friedel oscillations are observed; they overlap in regions of high defect density (inset in Fig. 1c).

Scanning Tunneling Microscopy/Spectroscopy of Bi$_2$Te$_3$. The crystal structure of Bi$_2$Te$_3$ consists of Te-Bi-Te-Bi-Te quintuple atomic layers in $\bar{c}$-crystallographic direction, Fig. 1a. The quintuple layers are linked to each other via van der Waals interaction, thus forming a lamellar easy-to-cleave material. Consequently, the outer (Te$_1$) and inner (Te$_2$) Te-atomic layers are not equivalent. Upon cleavage in UHV, macroscopically large atomically smooth Te$_1$-terminated terraces are obtained and revealed in STM images, Fig. 1c. On top of atomic corrugation, triangle-shaped defects are observed, originating from atomic Te-vacancies (see inset in Fig. 1b). On the tunneling conductance map $dl/dV(x, y)$ of the same region acquired at the sample bias $V_{bias}=90$ mV, the defects appear dark, reflecting a lower local electronic state density, Fig. 1c. Around defects, Friedel oscillations are observed; they overlap in regions of high defect density (inset in Fig. 1c).

Local $dl/dV(V)$ tunneling spectra taken at the position of a Te-vacancy (pointed by red arrow in Fig. 1c) look similar to those acquired away from impurities (blue arrow in Fig. 1c), as the respective curves in Fig. 1d demonstrate. Both present a low spectral weight in the window $-150$ mV to $0$ mV (in white), and a rapid raise at lower (higher) biases (in grey), consistent with previously reported results. This peculiar shape reflects the expected electronic structure of the material, Fig. 1e, where the bulk gap is crossed by topological surface bands (red curves), forming a Dirac cone. Since in the spectral window between $-100$ mV and $-50$ mV no influence of bulk states is expected, a linear extrapolation

$2\pi/|q|$ of considered Friedel oscillations. The effects related to the finite quasiparticle lifetime were not considered yet. In experiments, the QPI patterns were measured around individual impurities chosen away from other defects. In models, the finite lifetime was introduced only to avoid divergences in calculations. However, most of macroscopic electronic properties are averaged over a large collection of impurities, often considered in theories as a homogeneous disorder.

In the present paper we study the QPI from a collection of Te-vacancies - native surface defects in Bi$_2$Te$_3$. Using STM we focus on large areas where hundreds of Te-vacancies are present, dense enough to enable the overlap of Friedel oscillations from neighbouring scatters. By analysing the resulted QPI patterns, we reveal a peculiar splitting of scattering vectors in the energy window 60-120 meV above the Fermi level, that vanishes at lower and higher energies. Our numerical QPI calculations within T-matrix formalism confirm that the observed splitting at large momenta originates from the finite lifetime of quasiparticles, due to material disorder. Further inclusion into the model of the realistic triangular shape of the scattering potential strongly enhances the splitting and gives rise to the suppression of the scattering along $\Gamma-K$ direction, in agreement with experimental observations.
of $dI/dV(V)$ spectra to zero (dashed line in Fig. 1d) provides an estimate -(210±30) meV for the position of the Dirac point (DP) with respect to the Fermi level (zero-bias)$^{30}$. The main difference between red and blue spectra in Fig. 1d is their slight relative distortion and a lateral shift at negative biases. The former reflects a slight redistribution of electronic states due to impurities; the latter points towards a slightly different energies of the DP near and far from the defects, of the order of 20 meV (a more accurate estimation is difficult because of significantly different spectral weights of neighbouring bulk valence bands). Both cone distortion and variations of DP energy are more evident in Figs. 2a-h where STS maps at various biases acquired in the central part of the region Fig. 1b are presented. In all these maps, almost identical long-range variations of the contrast are observed, spatially correlated with the local concentration of defects.

The quasiparticle scattering is revealed in QPI patterns, Fig. 1f, which strongly depend on energy and nicely reflect the band structure of Bi$_2$Te$_3$, Fig. 1d. At -170 mV, the scattering vectors are very short and form a spot around Γ point, as expected for quasiparticles close to DP. At 20 mV, that is already ≈190 meV above the DP, the vectors are much longer and form a distorted contour, due to hexagonal warping of the Dirac cone. At 90 mV, the hexagon disappears, and only six scattering spots along Γ–M directions remain, witnessing for the dominant role of warping in the scattering events. An intriguing feature here is a splitting of scattering spots in doublets, which we discuss below. At 250 mV the scattering vectors form a halo, reflecting an additional contribution of the bulk conductance band in the scattering processes.

**Friedel oscillations and QPI patterns.**

We now focus on Friedel oscillations observed around triangular defects. In Fig. 2 each STS map is presented along with its QPI pattern. At large negative biases, Figs. 2a,b, no Friedel oscillations are evident. In fact, at $V_{bias} = -(140-200)$ mV the expected QPI scattering vectors are short, $q = 0.01-0.03$ Å$^{-1}$, and several effects wash the corresponding long-wave ($2\pi/q = 20-60$ nm) oscillations out: spatial variations of DP energy, short mean free path $l \sim 10$ nm (we evaluate it later), escape of Dirac electrons to the bulk valence band, etc. At positive biases however, the oscillations are visible in the real space; the characteristic scattering vectors are revealed in the QPI patterns, Figs. 2c-h. The main scattering vectors are aligned in Γ–M directions, their length and amplitude evolve with the energy. The scattering vector splitting (SVS) is observed in the spectral window 60-120 mV; it is clearly visible in QPI patterns in Figs. 2e-g. Below and above this energy window, only six spots of scattering vectors are observed. The evolution of the SVS with energy is quite odd, Fig. 2i. At $V=70$ mV, the QPI pattern is dominated by outer peaks; the amplitude of inner peaks is significantly lower. As the bias increases, the amplitude of outer peak lowers and that of the inner peak progressively increases. At 120 mV the inner peak dominates, the outer one is barely visible. At yet higher bias, the outer peak vanishes completely, and only bright inner peaks are observed. The whole dynamics looks like a transfer of the scattering probability from one scattering channel to another. At first glance, it would be tentative to assign these channels to scattering vectors $q_{\perp}$ and...
q_{qps}, Fig. 2j, as previously suggested. Due to warping however, the scattering matrix element of q_{qps}-process is weak because of a very low quasi-particle DOS of initial and final states, unlike q_{qps}, which involves high DOS (red arcs in Fig. 2) and dominates the quasiparticle scattering. The SVS phenomenon is a new interference effect related to disorder and to a specific triangular shape of the scattering potential of Te-vacancies, as we discuss now.

**QPI patterns: A model.**

To get an insight into the physical origin of the SVS and their strange evolution in energy, we examine the role of shape of the scattering potential and that of disorder on scattering processes in Bi\_3Te\_3, in the presence of a warped electronic spectrum. We consider that the QPI patterns observed by STS are mainly produced by surface electronic states, even if the bulk states are already present in the considered energy window, Fig. 1e. We then take the non-perturbed Hamiltonian, derived within k - p approach, which obeys C\_3v symmetry of the system:

\[ H_0(k) = \frac{r}{2} k^2 + \theta (1 + 3k^2) (k_x \sigma_y - k_y \sigma_x) + \lambda k_x (k_x^2 - 3k_y^2) \sigma_z, \]

where \( k = (k_x, k_y) \) is in-plane momentum, \( \sigma_{x,y,z} \) are the Pauli matrices in the spin space, \( r = 1/(2m) \) is the half inverse mass, \( \theta \) is the Fermi velocity, \( \lambda \) determines the next order correction to the Fermi velocity, and \( k \) reflects the strength of the hexagonal warping. The surface state spectrum is given by:

\[ E(k) = \frac{r}{2} k^2 + \theta |k| \sqrt{(1 + 3k^2)^2 + (\lambda/\theta)^2 (k_x^2 - 3k_y^2)^2/|k|^2}. \]

In Bi\_3Te\_3, the spectrum remains quite linear above the Dirac point (Fig. 1e), and thus the parameters \( r \) and \( \lambda \) are small. The shape of the constant energy contour at an energy \( E(k) = \omega \) is mainly determined by the parameter \( \lambda = \omega / \sqrt{\theta} \). For Bi\_3Te\_3, we take \( r/\sqrt{\lambda} = -1/2, \) \( s\theta/\lambda = 1/4 \), the warping wave vector \( k = \sqrt{\theta/\lambda} = 0.11\text{Å}^{-1}, \) and the "warping" energy \( E_c = \sqrt{\theta/\lambda} \approx 240\text{meV} \) above which the warping effects become important.

Corresponding constant energy contours \( E(k) = \omega \) are presented at different energies \( \omega \) in Fig. 2j. At low warping \( \lambda \ll 1 \), the contour is a circle; it transforms into a hexagon at the intermediate warping \( \lambda \sim 1 \), and into a snowflake at large warping \( \lambda \gg 1 \). Since \( E_c \) is counted from the Dirac point which is situated in our samples \( \sim 200\text{meV} \) below the Fermi energy, \( E_c \approx 240\text{meV} \) corresponds \( \sim 40\text{meV} \) in terms of tunneling bias. Thus, the energy window where SVS is observed corresponds to a rather strong warping \( \lambda > 1 \).

We then introduce the Green’s function of the non-perturbed Hamiltonian (1):

\[ G_0(k, \omega) = (i \delta / \omega) \delta_{\omega, H_0(k)}^{-1}, \]

in which the scattering rate \( \delta \) accounts for disorder in the material that we consider homogeneous, for the moment. The Green’s function accounting for scattering is \( G(k, \omega) = G_0(k, \omega) \delta_{\omega, H_0(k)} + G_0(k, \omega) T_{kk'}(\omega) G_0(k', \omega) \)

\[ T_{kk'}(\omega) = V_{kk'} + \sum_p V_{kp} G_0(p, \omega) T_{pk'}(\omega), \]

\[ T_{kk'}(\omega), \]

\[ T_{kk'}(\omega). \]
where \( V_{kk'}(ω) \) is a T-matrix that arises due to impurity scattering on the potential \( V_{kk'} \): the sum is taken over all wave vectors. The scattering amplitude \( ρ(q, ω) \) to be compared to experimental QPI patterns is then \( \Re \),

\[
ρ(q, ω) = \frac{i}{2π} \sum_k \text{Tr}(G(k, k - q, ω) - G^*(k, k + q, ω)),
\]

where \( \text{Tr}(M) \) means trace of a matrix \( M \). We calculate this convolution via the fast Fourier transform that significantly speeds up the process \( \Re \).

**QPI patterns: role of disorder.**

Let’s start with presenting the results of calculations for a single point-like scatter potential \( V_{kk'} = V_0 \). In Fig. 3a we present QPI patterns generated for various energies and disorder strengths for a fixed \( V_0 = 150 \text{ eVÅ} \). The energy range \( 1.1 E_v < ω < 1.6 E_v \) corresponds to the tunneling bias \( 65 \text{ mV} < V_T < 185 \text{ mV} \) and thus overlaps with the bias window where SVS was experimentally observed. These calculations confirm that the main scattering occurs indeed along Γ-M directions, in agreement with the experimental data. Moreover, two interesting features are found. The first one is the fine structure of six scattering peaks. At low \( ω \), the inner part of the peak has a higher amplitude. As \( ω \) rises, the outer peak gets stronger, indeed consistent with the experimentally revealed dynamics. Note that the effect is robust with respect to disorder. The second feature is the dependence of the calculated QPI amplitude on disorder: at higher \( δ \) the scattering peaks have stronger amplitude and larger angular extensions.

To understand the physics behind the two features, let us remind that in the considered energy window the warping is already strong and therefore the spectral density of states is strongly peaked at six tips of \( E(k) = ω \) snowflake (red arcs in Fig. 2) where warping vanishes, \( λk(k^2 - 3k^2) = 0 \). Consequently, the main scattering vectors are those linking the tips \( q_{tips} \), and the STS probes the resulting interference between these scatterings. Importantly, the tips are highly symmetric points of the contour; one point can be translated into the other by a combination of the rotational \( C_3 \) and time-reversal symmetries. In the first Born approximation, the quasiparticle scattering density can be expressed in a form:

\[
ρ(q) = \Re \int \frac{|⟨ψ_{k+δk} |ψ_{k+q}⟩|^2}{(E_k + iδ)(E_{k+q} + iδ)} d^2k,
\]

where \( \Re \) denotes the imaginary part of the integral; the energy is counted from \( ω \), for simplicity. Due to warping, the spectral DOS is localized at tips, and the integral can be substituted by the sum of two terms. One term comes from scattering process \( k → k + q \) and other term comes from scattering between Kramers partners of this states. Since this two terms are equal, we omit one of them.

\[
ρ(q) \propto \frac{δ(E_k + E_{k+q_{tips}})}{(E_k E_{k+q_{tips}} - δ^2)^2 + δ^2(E_k + E_{k+q_{tips}})^2}.
\]

Since \( E_k = E_{k+q_{tips}} = 0 \), the density vanishes, \( ρ(q_{tips}) = 0 \). This is a general result for the long wave scattering between symmetric points. It does not mean however that individual impurities do not produce Friedel oscillations around, as they locally break both translational and rotational symmetries. It just tells us that at low scattering rates one should expect the amplitude of QPI peaks at \( q_{tips} \) to be weak. The situation changes if \( δ ≠ 0 \) mixes up different energies around \( ω \) (Eq. 3). The scattering vectors \( q \) may now differ from \( q_{tips} \) by a disorder-dependent amount \( Δq \), that is \( q = q_{tips} + 2Δq \). Then, the quasiparticle scattering density becomes non-zero:

\[
|ρ(q)| \propto \left| \frac{δ(Δq)^2 E''(k)}{(E(k)^2(Δq)^2 + δ^2)^2 + δ^2(Δq)^2E''(k)^2} \right|.
\]

where \( E(k) \) and \( E''(k) \) are the first and the second derivatives of \( E(k) \), respectively. The density Eq. 6 vanishes at \( Δq → 0 \), as expected; its maximum value is reached at \( Δq_{max} \) such that \( Δq_{max}^2 = δ^2/\sqrt{E''^2 + δ^2E''^2} \), that corresponds to doublets in QPI appearing in Γ-M directions at the wave vectors \( q = q_{tips} \pm Δq_{max} \). Depending on relative weights of \( E'(k) \) and \( E''(k) \), the distance between the maxima around \( q_{tips} \) increases with increasing disorder as \( Δq \approx δ \) or \( Δq \approx \sqrt{δ} \). Thus, the disorder promotes the double-peak structure in QPI at the scattering vectors \( q \approx q_{tips} \). The present case is an example of a general phenomenon: finite quasiparticle life-time may be on the origin of non-trivial modifications of coherent scattering channels.

**QPI patterns: calculations vs experiment.**

While our calculations indeed generate SVS, the absolute value of the obtained splitting 2\( Δq_{max} \) in Fig. 3a is tiny, significantly lower than the splitting observed in the experiment, Fig. 2. This pushed us to consider a more realistic shape of the scattering potential. The STM data demonstrate that in Bi\(_2\)Te\(_3\), Te-vacancies form a triangular defect with the side about four lattice constants (see inset in Fig. 1b). It is then straightforward to model such a potential by a sum of the three scalar point potentials located at the vertices \( \Re \). The Fourier transform of this
impurity potential is written as:

$$V(k_x, k_y) = \frac{V_0}{3} \left( e^{i (k_x a + k_y b)} + e^{i (k_x a + 2k_y b)} + e^{i (2k_x a + k_y b)} \right),$$

(9)

where $a$ is the distance between point scatterers in the triangle.

We found that using the three-vertex potential of the same total strength $V_0 = 150$ eVÅ$^2$, as in the previous case of single point defects results in stronger peaks in $\Gamma$–$M$ directions and, remarkably, in a much stronger SSV. Both effects depend on $\delta$ and on size $a$ of the triangle, pointing out on their interference origin in the real space. The best match with the experimental data is obtained at $\delta = 0.1E_c$ and $a = 18$ Å. The latter is taken from $^{32}$, agrees with inset in Fig. 1b, and also matches, through the Bragg condition $q_{qpp} \sim \pi/a \approx 0.2$ Å$^{-1}$, the observed length of the scattering vectors in Fig. 2i. In Fig. 3b the calculated QPI patterns reproduce all experimentally observed features. At low energies, six single peaks are visible. The peaks appear as stripes, similarly to the experimentally observed Friedel oscillations from being experimentally observed. Therefore, limited. Indeed, it requires, from one side, the warping to be strong enough, which is fulfilled at $\omega > E_c$. From the other side, the splitting vanishes at high energies when spectral non-linearities appear, that is when the kinetic energy due to the finite mass $\sqrt{\omega^2/r}$ becomes comparable with $\omega$. Thus the splitting exists at $E_c < \omega < \sqrt{\omega^2/r}$, which is a narrow window, since both warping and mass energies have close values $\sqrt{\omega^2/\lambda} \sim \sqrt{\omega^2/r}$. It should be also mentioned that the previously predicted peaks along $\Gamma$–$K$ directions $^{28}$ do exist at larger momenta, Figs. 3; their amplitude is however lower as compared to the peaks along $\Gamma$–$M$ directions.

Finally, we estimate the scattering rate $\delta$ directly from experimental data and compare it with $\delta = 0.1E_c$, which was adjusted in Fig. 3b to fit with the experiment. Suggesting that $\delta$ occurs due to averaging the Green’s function over Gaussian randomly distributed point impurities, the scattering rate is:

$$\delta = n V_0^2 \cdot \text{Im} \int \frac{d^2k}{(2\pi)^2} G_0(k, \omega),$$

(10)

The density $n$ is estimated directly from the Fig. 1b to $n \sim 10^{-2}k^2$. With the previously used $V_0 = 150$ eVÅ$^2$, we obtain $\delta \sim 20$ meV, that is indeed not far from $0.1E_c = 24$ meV. As we can see, the scattering rate $\delta$ is quite large. Though, the corresponding mean free path $l = \hbar/\delta \sim 10$ nm looks reasonable. It is larger than $2\pi q_{qpp} \sim 3$ nm and thus does not prevent Friedel oscillations from being experimentally observed.

To conclude, in this work we studied experimentally and theoretically the effects of a moderate disorder on scattering of Dirac quasiparticles in three-dimensional topological insulator Bi$_2$Te$_3$. Low temperature Scanning Tunneling Microscopy and Spectroscopy experiments performed in-situ on in-vacuum cleaved single crystals revealed spatial oscillations of the electronic density due to coherent scattering on atomic defects. The data analysis demonstrated that in the energy window 60-120 meV above the Fermi level the scattering vectors form doublets along $\Gamma$–$M$ direction and exhibit peculiar energy evolution. These phenomena were neither observed nor theoretically predicted in previous works in which only a weak point-like disorder was considered. Our experiments demonstrate that the electronic properties of three-dimensional TIs may be strongly affected already at a moderate disorder, despite of topological protection.

An insight into the observed phenomenon is brought by a model based on T-matrix formalism which takes into account the finite quasiparticle lifetime. The model shows, that the disorder is an essential ingredient that not only predictably smeared out the oscillations but also leads to modifications of coherent scattering vectors and thus strongly affects QPI patterns. By taking into account the finite quasiparticle lifetime, energy-dependent warping and the actual form of the scattering potential we successfully reproduce the peculiar dynamics of the scattering vectors observed in the experiment.

**METHODS** The experiments were performed using Joule-Thompson low-temperature scanning tunnelling microscope TysT$^{TM}$ by SPECS$^{TM}$ GmbH operating in ultrahigh vacuum (base pressure less than $1 \times 10^{-10}$ Torr) at a temperature 1.3 K. Single crystals of Bi$_2$Te$_3$ were cleaved in ultrahigh vacuum before providing in-situ STM/STS measurements.

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**Acknowledgements**

We thank Wei-Cheng Lee for fruitful discussions. This work was supported by French-Russian (ANR - RSF) Research Grant "CrysTop" (20-42-09033). D.R. acknowledges COST Action CA16218 - Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies. A.A.G. acknowledges support by the European Union H2020-WIDESPREAD-05-2017-Twinning project SPINTECH under Grant Agreement No. 810144. A.S.V. acknowledges support from the Academic Fund Program at the National Research University Higher School of Economics (HSE) in 2018-2019 (grant No. 18-01-0016) and the Russian Academic Excellence Project 5-100. D.A.K. and R.S.A acknowledge support from the Foundation for the Advancement of Theoretical Physics and Mathematics “BASIS”, E.V.C. acknowledges support from the Saint Petersburg State University project for scientific investigations (ID No. 51126254).

**Author contribution**

VSS and DR conceived and supervised the the project; VSS realized the STM/STS measurements with contributions from DR, SV and SP; TVM and EVC provided DFT calculations; DAK, RSA, DR, VS and VSS provided the explanation of the observed phenomena; DAK and RSA did numerical modelling with contributions from DR, VS and VSS; DR and VSS wrote the manuscript with the essential contributions from DAK and RSA along with the input from VS, HA, ASV, AAG and TC.

**Competing interests:** The authors declare no competing interests.

**Additional information**

**Supplementary Information.** accompanies this paper at https://doi.org/.....

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**Peer review information:** Communication materials thanks anonymous, reviewer(s) for their contribution to the peer review of this work.

**Data availability statement**

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