Quasiparticle Interference on the Surface of the Topological Insulator Bi$_2$Te$_3$

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The quasiparticle interference of the spectroscopic imaging scanning tunneling microscopy has been investigated for the surface states of the large gap topological insulator Bi$_2$Te$_3$ through the $T$-matrix formalism. Both the scalar potential scattering and the spin-orbit scattering on the warped hexagonal isoenergy contour are considered. While backscatterings are forbidden by time-reversal symmetry, other scatterings are allowed and exhibit strong dependence on the spin configurations of the eigenfunctions at $\vec{k}$ points over the isoenergy contour. The characteristic scattering wavevectors found in our analysis agree well with recent experiment results.

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I. INTRODUCTION

The theoretical proposal and experimental discovery of the topological insulators have provoked an intensive research effort in condensed matter physics. Topological insulators (TI) with time-reversal symmetry are generally characterized by a topological term in the electromagnetic action with a quantized coefficient. These states have been theoretically predicted and experimentally observed in both two and three dimensions, including the two-dimensional (2D) HgTe/HgCdTe quantum wells, and bulk three-dimensional materials Bi$_2$Te$_3$, Bi$_2$Se$_3$, and Bi$_{1-x}$Sb$_x$. They exhibit robust gapless modes at boundaries, e.g., a 1D helical edge mode for 2D TIs, and a 2D helical surface mode for 3D TIs with odd numbers of Dirac cones. Due to time-reversal symmetry, backscattering is forbidden for the helical edge and surface states, and an analysis of interaction effects for the 1D helical edge modes shows they are stable against weak and intermediate strength interactions. Bi$_2$Te$_3$ and Bi$_2$Se$_3$ have been predicted to have bulk band gaps exceeding room temperature.

Zhang et al predict that the surface states of Bi$_2$Te$_3$ consist of a single Dirac cone at the $\Gamma$ point, and that the Dirac cone evolves into a hexagonal shape at higher energy. Furthermore, near the Dirac point, the spin of the electron lies perpendicular to the momentum. Angle-resolved photo-emission spectroscopy (ARPES) measurements performed on the surface of Bi$_2$Te$_3$ have confirmed these predictions in detail. The typical shape of the Fermi surface is a snowflake-like warped hexagon. The low-energy $O(2)$ symmetry of the Dirac cone is broken due to the $C_3$ symmetry of the underlying lattice, and can be modeled by a warping term in the effective model. Another powerful surface probe, spectroscopic scanning tunneling microscopy (STM), is sensitive to quasi-particle interference (QPI) around impurities, and provides an important tool to study electronic structures in unconventional materials, such as high $T_c$ cuprates. STM experiments have yielded rich information about the QPI structure. In addition to the absence of backscattering, the STM experiments also observed recovered scattering at a wavevector $\vec{q}_{\text{nest}}$ in their, and $\vec{q}_2$ in our notation), and an extinction (i.e. near absence of scattering) at wavevectors which do not connect TR states. Below, we offer a novel explanation of this experimental puzzle. Our results are in excellent overall agreement with the QPI experiment in Bi$_2$Te$_3$.

II. SURFACE DIRAC MODEL WITH WARPING TERM

The $\vec{k} \cdot \vec{p}$ Hamiltonian for the surface Dirac cone was first derived in Ref. The bare Hamiltonian is written as $H_0 = \int d\vec{k} \psi^\dagger(\vec{k}) H(\vec{k}) \psi(\vec{k})$, where $\psi^\dagger(\vec{k}) = (c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger)$. With the addition of the cubic warping term,

$$H(\vec{k}) = v (\vec{k} \times \vec{\sigma}) \cdot \hat{z} + \lambda k^3 \cos 3\phi \sigma^z .$$ (1)
The azimuthal angle of $\vec{k}$ is $\phi_\vec{k} = \tan^{-1}(k_y/k_x)$, where the $\Gamma-K$ direction is taken as $\hat{x}$ axis. Following Ref. [17], the quadratic terms are dropped since they do not significantly change the shape of the constant energy contour, and the characteristic energy and wavevector scales are defined as: $E^* = v k_c$ and $k_c = \sqrt{\frac{v}{\lambda}}$. This Hamiltonian can be diagonalized by introducing

$$\hat{U}(\vec{k}) = \begin{pmatrix} \cos(\theta_\vec{k}/2) & ie^{-i\phi_\vec{k}} \sin(\theta_\vec{k}/2) \\ ie^{i\phi_\vec{k}} \sin(\theta_\vec{k}/2) & \cos(\theta_\vec{k}/2) \end{pmatrix},$$

where $\tan \theta_\vec{k} = k_y^2/(k_x^2 \cos 3\phi_\vec{k})$. One then finds $H(\vec{k}) = E(\vec{k}) U(\vec{k}) U^\dagger(\vec{k})$, with eigenvalues $E_{\pm} = \pm E(\vec{k})$ where

$$E(\vec{k}) = \sqrt{\left(\omega k\right)^2 + \left(\lambda k^3 \cos 3\theta_\vec{k}\right)^2}.$$ 

In fig. 1(a) we plot the isoenergy contour $E = 1.5 E^*$, which qualitatively reproduces the snowflake Fermi surface observed in the first-principles calculation and the ARPES experiment. As for the scattering process, we take

$$\mathcal{H}_{\text{imp}} = \int d^2k d^2k' V_{\vec{k}-\vec{k}'(\vec{k}')} \left[ \| + ic \hat{k} \times \vec{k}' \cdot \vec{\sigma} \right] \psi(\vec{k}').$$

For a single short-ranged scatterer we may approximate $V_{\vec{k}-\vec{k}'} \approx V_0$. The second term corresponds to the spin-orbit scattering with the coefficient $c$ describing its relative strength to the potential scattering. It is convenient to project the potential onto the eigenbasis of $\mathcal{H}_0$, so

$$\hat{V}_{\vec{k},\vec{k}'} \equiv V_0 \hat{U}^\dagger(\vec{k}') \left[ \| + ic \hat{k} \times \vec{k}' \cdot \vec{\sigma} \right] \hat{U}(\vec{k}).$$

For simplicity, we first consider the $c = 0$ case (pure scalar potential scattering), returning later to the general spin-orbit case ($c \neq 0$). Since the spectrum is particle-hole symmetric, let us focus on a definite (positive) sign of the energy. The QPI will then be dominated by scatterings inside the positive energy band, whose effective scattering potential is:

$$\hat{V}_{\vec{k},\vec{k}'}^{(1)} = V_0 \left[ \cos \frac{\theta_\vec{k}}{2} \cos \frac{\theta_\vec{k}'}{2} + \sin \frac{\theta_\vec{k}}{2} \sin \frac{\theta_\vec{k}'}{2} e^{i(\phi_\vec{k} - \phi_\vec{k}')}. \right].$$

This effect also appears in the QPI analysis of the orbital-band systems where orbital hybridization brings strong momentum dependence to the scattering process.

### III. EFFECT OF SPIN ORIENTATION ON THE QPI PATTERN

The points of extremal curvature on the Fermi surface are divided into two groups, arising from the ‘valleys’ ($k = k_L$, positive curvature) and ‘tips’ ($k = k_U$, negative curvature). We define the complexified points $A = k_L e^{i\pi/3}$, $B = k_L$, $C = k_L e^{-i\pi/3}$, $W = k_U e^{5\pi i/6}$, $X = k_U e^{-5\pi i/6}$, and $Y = k_U e^{-i\pi/2}$. Then from eqn. 6 we obtain $|V_{AB}^{(1)}|^2 = \frac{3\lambda^2}{4} \sin^2 \theta$, $|V_{AC}^{(1)}|^2 = \frac{3\lambda^2}{4} + \frac{3\lambda^2}{4} \cos^2 \theta$, and $V_{AA}^{(1)} = 0$, where $A = -A$, corresponding to scattering through the vectors $\vec{q}_3$, $\vec{q}_2$, and $\vec{q}_1$, respectively, with $\tan \vartheta = (k_c/k_L)^2$. We also find $|V_{WW}^{(1)}|^2 = \frac{3\lambda^2}{4}$, $|V_{WY}^{(1)}|^2 = \frac{3\lambda^2}{4}$, and $V_{WW}^{(1)} = 0$. These processes are depicted in fig. 1(a).

While $V_{AA}^{(1)} = V_{WW}^{(1)} = 0$ is a direct consequence of TR symmetry, the other processes through scattering vectors $\vec{q}_{2,3,5,6}$ are in general finite. Their amplitude variation may be understood in terms of the spin orientation of the eigenfunctions throughout the Brillouin zone, $S(\vec{k}) = (-\sin \theta_\vec{k} \sin \phi_\vec{k}, \sin \theta_\vec{k} \cos \phi_\vec{k}, \cos \theta_\vec{k})$, depicted in fig. 1(b). Bi$_2$Te$_3$ has the symmetry of $C_{3v}$, i.e., three-fold rotational symmetry plus the three reflection lines ($\Gamma$-M plus two equivalent lines). Therefore at the tips $S^2(\vec{k})$ must vanish since $\sigma^2$ is odd under the mirror operation. $S^2(\vec{k})$ has the largest magnitude at the valleys, but with staggered signs, as shown in the figure. Since scalar potential scattering does not flip electron spin, its matrix element is largest when $S(\vec{k}) \cdot S(\vec{k}')$ is large and positive, i.e., high spin overlap. This echoes the experimental finding of Pascual et al. that in the QPI pattern on Bi(110), only the scattering processes preserving the spin orientation are visible. One major difference, however, between Bi(110) and Bi$_2$Te$_3$ is that the former has mul-
tiple Fermi surfaces and the scattering processes preserving spin orientations do exist at finite \( \vec{q} \), while the later only has one Fermi surface and therefore no such scatterings could exist. At the tips, the spin lies in-plane, with \( \theta_{\vec{k}} = \frac{\pi}{2} \), independent of the scanning energy \( E \). It can be checked that \( \tilde{S}(\vec{k} + \vec{q}_5) \cdot \tilde{S}(\vec{k}) > \tilde{S}(\vec{k} + \vec{q}_6) \cdot \tilde{S}(\vec{k}) \), hence \( |V_{WY}^{(11)}|^2 > |V_{WY}^{(11)}|^2 \). For scatterings between the valleys, \( \tilde{S}(\vec{k}) \cdot \tilde{S}(\vec{k}') \) depends crucially on \( S^z(\vec{k}) \) and \( S^z(\vec{k}') \). Accounting for the valley-to-valley oscillation in \( \tilde{S}(\vec{k}) \), we conclude that as the scanning energy increases, \( |V_{AC}^{(11)}|^2 \) grows while \( |V_{AB}^{(11)}|^2 \) shrinks. This simple argument gives a qualitative explanation for the absence of the \( \vec{q}_5 \) scattering in the STM experiment. For typical experimental parameters, \( E/E^* \approx 1.5 \) and \( k_L/k_c \approx 1 \). In this case we estimate the scalar potential scattering gives that \( |V_{WY}^{(11)}|^2 : |V_{AC}^{(11)}|^2 : |V_{AB}^{(11)}|^2 : |V_{WY}^{(11)}|^2 \approx 6 : 5 : 3 : 2 \).

IV. NUMERICAL RESULTS

To specifically compute the QPI image, we employ a \( T \)-matrix approach for multiband systems. In the operator basis \( \Psi(\vec{k}) = U(\vec{k}) \psi(\vec{k}) \), the Green’s function is written in matrix form as

\[
\tilde{G}(\vec{k}, \vec{k}', \omega) = \tilde{G}_0(\vec{k}, \omega) \delta_{\vec{k}, \vec{k}'} + \tilde{G}_0(\vec{k}, \omega) \tilde{T}_{\vec{k}, \vec{k}'}(\omega) \tilde{G}_0(\vec{k}', \omega)
\]

where the \( T \)-matrix satisfies

\[
\tilde{T}_{\vec{k}, \vec{k}'}(\omega) = \tilde{V}_{\vec{k}, \vec{k}'} + \int d^2p \tilde{V}_{\vec{k}, \vec{p}} \tilde{G}_0(\vec{p}, \omega) \tilde{T}_{\vec{p}, \vec{k}'}(\omega),
\]

and \( \tilde{G}_{0,\sigma}(\vec{k}, \omega) \) are the bare Green’s functions. In spectroscopic imaging STM, the conductance \( (dI/dV) \) measured by the STM is proportional to the local density of states defined as

\[
\rho(\vec{r}, \omega) = \rho_{\uparrow}(\vec{r}, \omega) + \rho_{\downarrow}(\vec{r}, \omega),
\]

where \( \rho_{\sigma}(\vec{r}, \omega) = \text{Im} G_{\sigma}(\vec{r}, \vec{r}, \omega) \) is the local density of states for spin \( \sigma \). The QPI image in the Brillouin zone \( \rho(\vec{q}, \omega) \) is then obtained by performing the Fourier transform of the conductance \( dI/dV \). As a result, we can calculate \( \rho(\vec{q}, \omega) \) using the \( T \)-matrix formalism by:

\[
\rho(\vec{q}, \omega) = \int d^2r e^{i\vec{q} \cdot \vec{r}} \rho(\vec{r}, \omega) = \frac{1}{2i} \int d^2k \text{Tr} \left[ \tilde{U}(\vec{k}) \tilde{G}(\vec{k}, \vec{k} + \vec{q}, \omega) \tilde{U}^\dagger(\vec{k} + \vec{q}) \right.
\]

\[
\left. - \left( \tilde{U}(\vec{k}) \tilde{G}(\vec{k}, \vec{k} - \vec{q}, \omega) \tilde{U}^\dagger(\vec{k} - \vec{q}) \right)^* \right]
\]

where the trace is taken with respect to the matrix index. Because physically STM measures the local density of states in the spin basis of \( \psi(\vec{k}) \), while our \( T \)-matrix theory here is developed in the eigenbasis of \( \hat{\Psi}(\vec{k}) \), the SU(2) rotation matrices \( \tilde{U}(\vec{k}) \) are introduced in the last line of eq. (10) to transform back to the physical spin basis. Because the first term in eq. (10) \( \rho(\vec{q} = 0) \) contains the sum of the total density of states without the impurity, which makes it much larger than \( \rho(\vec{q} \neq 0) \), we only plot \( |\rho(\vec{q} = 0)| \) in order to reveal weaker structures of the QPI induced by the impurity scattering.

We solve eq. (10) numerically, using 2D polar coordinates. Since the dominant scattering processes are between \( \vec{k} \) points on the constant energy contour \( E_\pm(\vec{k}, \theta) = E \) (we focus on \( E > 0 \) here), we perform the integration within the range \( k_L \leq k \leq k_U \), with \( k_L \) and \( k_U \) indicated in Fig. (1a). The resulting QPI images are plotted in fig. 2 for \( c = 0 \) with \( E = 1.5 E^* \) fixed. For this choice of parameters, \( k_L/k_c = 1.029 \) and \( k_U/k_c = 1.5 \). As shown in fig. 2(a), \( \vec{q}_3 \) and \( \vec{q}_4 \) indicated by the red (dark gray) and green (light gray) circles are the strongest features while \( \vec{q}_5 \) (indicated by the white circle) is almost invisible. The reason why \( \vec{q}_5 \) is even stronger than \( \vec{q}_4 \) while they have comparable scalar scattering potential is due to the difference in the density of states. Because the tip points shown in fig. 1(a) have larger density of states than the valley points, the weights of \( \vec{q}_6 \) is larger than those of \( \vec{q}_2 \) resulting in the stronger features observed for \( \vec{q}_5 \). The strong features near \( \vec{q} = 0 \) correspond to small \( \vec{q} \) scatterings around the tips and valleys points, which have also been seen in experiments. Our results reproduce satisfactorily the experimental findings and are also consistent with the analysis from the spin-orbit selection rule discussed above.

As the scanning energy increases further, the surface states along the \( \Gamma - M \) direction start to merge into the conduction band of the bulk states. In this case, the tips of the constant energy contour will be mixed up with these bulk bands, which weakens the \( \vec{q}_6 \) scattering but enhances the small \( \vec{q} \) scatterings near \( \Gamma \) point. This is consistent with the experiments, showing that the area of the strong features near \( \Gamma \) point becomes much larger after the scanning energy exceeds the bottom of the conduction band.

V. SPIN-ORBITAL SCATTERING IMPURITY

Now we briefly comment on the effect of the spin-orbit scattering given in eq. (4) which in principle exists in any realistic system. Since surface states of the topological insulator Bi\(_2\)Te\(_3\) are two-dimensional, the spin-orbit scattering potential only has one component:

\[
\mathcal{H}_{\text{imp}}^{\text{SO}} = i\epsilon v_0 \int d^2k \int d^2k' \int d^2k'' \left( \delta(\phi_{\vec{k}} - \phi_{\vec{k}'}) \right) \sigma^z \left( \psi(\vec{k}) \right)^* \psi(\vec{k}') \psi(\vec{k}) \psi(\vec{k}'').
\]

Backscattering is still forbidden because of the \( \sin(\phi_{\vec{k}} - \phi_{\vec{k}'}) \) factor. Although \( \sigma^z \) does not flip spin, the angle-dependence \( \sin(\phi_{\vec{k}} - \phi_{\vec{k}'}) \) gives rise to an additional suppression beyond that from the spin-orientation selection rule.
FIG. 2: (Color online) The quasiparticle interference image for (a) \( c = 0 \) and (b) \( c = 0.5 \) with \( E = 1.5E^* \) and \( V_0/E^* = 0.1 \). In this case, \( k_L/k_c = 1.029 \) and \( k_U/k_c = 1.5 \). (a) The strongest large \( \vec{q} \) scatterings are \( \vec{q}_5 \) and \( \vec{q}_2 \) indicated by the red (dark gray) and green (light gray) circles (and their symmetric points). \( \vec{q}_5 \) (indicated by the white circle) is too weak to be seen. (b) For \( c = 0.5 \), new QPI features with large momenta are visible.

Nonzero \( c \) brings in new interferences which could lead to unusual suppressions or enhancements for some scattering wavevectors, depending not only on the magnitude and sign of \( c \), but also on the scanning energy \( E \). In fig. 2(b) we show the QPI image for \( c = 0.5 \). While the main features are still similar to those of fig. 2(a), new prominent features associated with larger momentum scatterings are visible. Since the matrix elements for spin-orbit scattering are larger for quasiparticles with larger momentum, this term will become more and more important as the scanning energy \( E \) increases. A detailed analysis of the spin-orbit scattering will be presented in a future publication. In comparison with the results in ref. 21, we find that spin-orbit scattering from the impurity of the Ag atom is not very important in this particular experiment.

VI. CONCLUSION

In conclusion, we have analyzed the quasiparticle interference induced by nonmagnetic impurities on the surface of the topological insulator Bi$_2$Te$_3$ using a \( T \)-matrix approach. While the backscattering is completely forbidden by time-reversal symmetry, other scatterings are allowed, resulting in the QPI patterns observed in STM experiments 20,21. We have shown further that the scattering strengths depends crucially on the spin orientations of the eigenfunctions. Since nonmagnetic impurities can not flip spin, the scalar scattering potential between two eigenstates is larger as their spin overlap is larger. Combined with the variation of the density of states, we have shown that some of the scatterings might be too weak to be seen in comparison with the strongest ones, and our results successfully reproduce the QPI pattern observed in experiments. We have further discussed the effect of the spin-orbit scattering on the QPI pattern. While the backscattering is still forbidden, we find that the spin-orbit scattering enhances several new features at large momentum, and the detailed QPI features strongly depends on the sign and strength of the spin-orbit scattering potential.

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Note added – While this paper was about completion, we learned a related work by Zhang et al. 

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