Failure of conductance quantization in two-dimensional topological insulators due to non-magnetic impurities

Pietro Novelli,1,2,* Fabio Taddei,3 Andre K. Geim,4 and Marco Polini1,4

1Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, I-16163 Genova, Italy
2NEST, Scuola Normale Superiore, I-56126 Pisa, Italy
3NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy
4School of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

Despite topological protection and the absence of magnetic impurities, two-dimensional topological insulators display quantized conductance only in surprisingly short channels, which can be as short as 100 nm for atomically-thin materials. We show that the combined action of short-range non-magnetic impurities located near the edges and onsite electron-electron interactions effectively creates non-collinear magnetic scatterers, and, hence, results in strong back-scattering. The mechanism causes deviations from quantization even at zero temperature and for a modest strength of electron-electron interactions. Our theory provides a straightforward conceptual framework to explain experimental results, especially those in atomically-thin crystals, plagued with short-range edge disorder.

Introduction.— In 2005, research on the impact of spin-orbit coupling in graphene led Kane and Mele1,2 to predict theoretically the existence of two-dimensional (2D) topological insulators (TIs). These are 2D electron systems with a gap in the bulk density of states (DOS) and pairs of conducting edge states displaying helicity, i.e. spin-momentum locking. Because of Kramers theorem, in the absence of many-particle effects non-magnetic impurities in a 2DTI cannot induce back-scattering within pairs of helical modes at a 2DTI edge, yielding conductance quantization against elastic disorder.3–8

All experimental measurements on 2DTIs, however, show deviations from the expected quantized value of conductance $2e^2/h$, particularly in small-gap semiconductor heterostructures such as HgTe/CdHgTe and InAs/GaSb quantum wells9–13, but also in atomically-thin crystals such as WTe$_2$.14 On the other hand, the existence of conducting edge modes was clearly demonstrated by non-local resistance measurements in Refs. 10–13. Semiconducting heterostructures were extensively studied in the low-temperature regime (below 4 K)9,13 because of their small energy gap. For channel lengths shorter than $\sim 1 \mu$m, fluctuations of the conductance around the quantized value $2e^2/h$ were observed as a function of the back gate voltage. For longer channels, even the average conductance was found to deviate from $2e^2/h$ and even totally suppressed15, when the edge was perturbed by a scanning tip. Among the 2DTIs realized by semiconducting heterostructures, the best results were obtained thanks to Si doping13. In these samples, conductance is quantized up to 1-2% at very low temperatures. Monolayers of WTe$_2$ exhibit conductance quantization up to 100 K, making them the 2DTIs existing at the highest temperatures up to date, though displaying quantization only in short channels up to length scales on the order of 100 nm.

The cause of the breakdown of conductance quantization is still poorly understood. Clearly, one possibility is the presence of an external magnetic field9,14 or of magnetic impurities16–18, which induce spin-flip scattering (thus back-scattering). Magnetic impurities, however, are rare both in materials grown by molecular beam epitaxy9–13 and in mechanically-exfoliated crystals14, but explain experimental data in the “extrinsic” case in which magnetic dopants are deliberately added to pristine three-dimensional TI samples19,20. Coupling between opposite edges of a 2DTI can also induce back-scattering21,22, with no need of time-reversal symmetry breaking. Nonetheless, due to the exponential decay of the helical modes away from an edge, such a coupling can be expected only in very narrow samples or in purposely fabricated point contacts. Finally, recalling that the topological protection of helical edge modes in 2DTIs originates from Kramers degeneracy7–8, which appears only in systems with an odd number of electrons, the breakdown of the topological phase, thus of the conductance quantization, could arise from two-body interac-
tions. In Ref. 3 it was suggested that electron-electron (e-e) interactions in 2DTIs can cause back-scattering through a scattering process which emerges in third-order perturbation theory, while the spontaneous breaking of time-reversal symmetry due to interactions was studied in Ref. 23. Interactions are also at the core of other mechanisms proposed to explain the spoiling of conductance quantization in 2DTIs. Back-scattering of helical edge modes resulting from weak e-e interactions and an impurity potential, in the absence of axial spin symmetry, was considered in Ref. 24. Deviations from the quantized conductance were found to scale like $T^4$, at low temperatures $T$. The coupling of edge modes to charge puddles naturally present in real samples was accounted for in Refs. 25 and 26. Back-scattering was found to occur by modeling the charge puddles as interacting quantum dots, thus leading to a correction to the conductance scaling like $T^4$ at low temperatures. In contrast, recent experiments\textsuperscript{37} show nearly temperature-independent conductance in 2DTIs. Another mechanism that leads to the breakdown of conductance quantization is related to the edge reconstruction\textsuperscript{37}, which can occur when the confining potential of the 2DTIs edges is not sufficiently sharp. Indeed, in order to minimize the total energy in the presence of Coulomb interactions, electronic density configurations in which time-reversal symmetry is spontaneously broken can arise. Inelastic scattering mediated by phonons was considered in Ref. 28 and shown to be irrelevant as it results in negligible corrections to the conductance in the limit of a small applied bias voltage. Finally, the effects of nuclear spins\textsuperscript{29,30}, disordered probes\textsuperscript{31}, coupling to external baths\textsuperscript{32}, and noise\textsuperscript{33} have been analyzed as well.

In this Letter we propose a simple mechanism, based on the interplay between non-magnetic scatterers and e-e interactions, which leads to the breakdown of conductance quantization in 2DTIs, even at zero temperature, and can result in the total suppression of the conductance. Starting from the single-particle Kane-Mele Hamiltonian\textsuperscript{1,2} describing a 2DTI ribbon, we consider the presence of short-range non-magnetic impurities at its edges (see Fig. 1). As expected, this leads to an enhancement of the local DOS, as in the case of midgap states in graphene\textsuperscript{34} and three-dimensional TIs\textsuperscript{35-37}. In the presence of Hubbard-like e-e interactions, using the self-consistent unrestricted Hartree-Fock method, we show that these short-range defects favor the formation of local magnetic moments, leading to the spontaneous breakdown of time-reversal symmetry and back-scattering.

**Theoretical model.**—We consider the following interacting Hamiltonian on a honeycomb lattice, known as Kane-Mele-Hubbard model\textsuperscript{38,39}:

\[
\mathcal{H} = t \sum_{\langle ij \rangle,\alpha} c_{i\alpha}^\dagger c_{j\alpha} + i\lambda \sum_{\langle ij \rangle,\alpha,\beta} \nu_{ij} c_{i\alpha}^\dagger \sigma_{\alpha\beta}^z c_{j\beta} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}.
\]

In Eq. (1), $c_{i\alpha}^\dagger$ ($c_{i\alpha}$) creates (destroys) an electron of spin $\alpha$ on site $i$ and $\sigma^z$ is a $2 \times 2$ Pauli matrix acting on spin space. The sums over $\langle ij \rangle$ ($\langle\langle ij \rangle\rangle$) are intended between $i$ and $j$ being first (second) neighbours. The parameters $t$ and $\lambda$ are hopping energies between first and second neighboring sites, respectively. The second term in Eq. (1) was introduced by Kane and Mele\textsuperscript{1,2} as a time-reversal invariant version of the Haldane model\textsuperscript{40}, and is responsible for the existence of helical edge modes. The factor $\nu_{ij}$ is equal to $\pm 1$, with $\nu_{ij} = -\nu_{ji}$, depending on the orientation of the two nearest-neighbor bonds the electron traverses in going from site $j$ to $i$: $\nu_{ij} = -1(1)$ if the electron reaches the second neighbour going (anti-)clockwise. The last term accounts for local e-e interactions and corresponds to the e-e interaction term in the standard Hubbard model. Such a two-body term will be treated within mean-field theory. The key point here is that we are not interested in dealing accurately with strong correlations in 2DTIs\textsuperscript{39}. Our aim is to utilize the simplest approach that enables us to capture an important effect stemming from local e-e interactions in the weak-coupling $U/t < 1$ regime. In this regime mean-field theory is accurate and has the great advantage of allowing us to obtain an effective single-particle Hamiltonian, which can be used in combination with Landauer-Büttiker theory\textsuperscript{41} to compute transport properties.

We consider a rectangular ribbon of width $W$ with armchair edges and length $L$, with periodic boundary conditions in the $x$-direction. In order to investigate the effect of short-range, atomic-scale defects, we assume the presence of one or two vacancies, which can be included in the model by simply dropping from the sums in Eq. (1) terms involving the lattice sites where the atoms are missing. The case of many vacancies can be tackled in a straightforward manner but lies beyond the scope of this work. Our main point, here, is to demonstrate the importance of local e-e interactions in dressing short-range non-magnetic impurities in a magnetic fashion.

We now recall that the Hartree-Fock expression for a generic two-body operator is\textsuperscript{42}

\[
c_{m\alpha} c_{m\alpha}^\dagger c_{n\beta} c_{n\beta}^\dagger \propto \langle c_{m\alpha} c_{m\alpha}^\dagger c_{n\beta} c_{n\beta}^\dagger - c_{m\alpha}^\dagger c_{m\alpha} c_{n\beta}^\dagger c_{n\beta} \rangle \equiv \langle A \rangle,
\]

where $\langle A \rangle$ denotes the expectation value of the operator $A$. Using Eq. (2), we can express (1) in the unrestricted Hartree-Fock approximation\textsuperscript{43,44} as

\[
\mathcal{H} \approx t \sum_{\langle ij \rangle,\alpha} c_{i\alpha}^\dagger c_{j\alpha} + i\lambda \sum_{\langle ij \rangle,\alpha,\beta} \nu_{ij} c_{i\alpha}^\dagger \sigma_{\alpha\beta}^z c_{j\beta} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} + \frac{U}{2} \sum_{i,\alpha,\beta} c_{i\alpha}^\dagger (n_i \mathbb{1}_{\alpha\beta} - m_i \cdot \sigma_{\alpha\beta}) c_{i\beta} - \frac{U}{4} \sum_i (n_i^2 - |m_i|^2),
\]

where $\mathbb{1}$ is the $2 \times 2$ identity matrix, $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ is a vector of $2 \times 2$ Pauli matrices acting on spin space, and
we have defined the local mean electron density

$$n_i = \langle \sum_{\alpha} c_{i\alpha}^\dagger c_{i\alpha} \rangle$$

(4)

and the local mean spin polarization

$$s_i = \frac{\hbar m_i}{2} = \hbar (m_i^x, m_i^y, m_i^z) / 2$$

(5)

which must be determined self-consistently. In order to do so, we use an iterative algorithm which involves the exact diagonalization of the Hamiltonian (3). Our calculations were performed at $T = 0$, but can easily be extended to finite temperature. Technicalities are reported in Appendix A. For $\lambda = 0$, i.e. when the second neighbour hopping term is neglected, the lattice is bipartite in the sense of Ref. 46 and Lieb theorem holds, so that a non-zero ground-state spin polarization rigorously follows from sublattice imbalance (i.e. different number of sites in the two sublattices). As we will see below, a ground-state spin polarization occurs even for $\lambda \neq 0$—i.e. in the topological phase of the model (1) with topological gap $\delta_g = |6\sqrt{3}\lambda|$ —where Lieb theorem does not apply. All numerical results below refer to a rectangular sample with $L = 45(\sqrt{3}/2)a$ and width $W = 25a$.

**Ground-state spin polarization.** — In Fig. 2 we plot the spatial profile of the three components—$m_i^x$, top panel, $m_i^y$, central panel, and $m_i^z$, bottom panel—of the dimensionless spin polarization (5), calculated at half filling for $\lambda/t = 0.09$ and $U/t = 0.1$, when a single vacancy is placed at $x = 23(\sqrt{3}/2)a$ and $y = a$, where $a$ is the lattice parameter. The ground-state electron density $n_i$ turns out to be nearly uniform.

The results show that spin polarization occurs around the vacancy, being vanishing elsewhere. This nicely agrees with the Stoner criterion, stating that a ground-state magnetization can occur in presence of a peak in the DOS. Indeed, a short-range defect generally hosts bound states localized around it, leading to an enhancement of the local DOS in proximity of the defect.

It is interesting to note that a finite spin polarization is bound to atomic-scale imperfections. Away from the vacancy the sample displays zero spin polarization. We thus expect that short-range edge roughness, which naturally occurs e.g. in atomically-thin crystals, as well can in general lead to interaction-induced spin polarization. We now move to analyze its effects on the transport properties of the system.

**Breakdown of conductance quantization.** —Due to spin-momentum locking, back-scattering is induced by spin-flip events, which, in turn, are induced by the terms proportional to $m_i^x$ and $m_i^y$ in Eq. (3). Once the mean-field theory parameters $n_i$ and $m_i$ are obtained, the conductance of the sample in a two-terminal setup (where one lead is attached to the left and the other to the right) can be calculated within the Landauer–Büttiker formalism. In particular, at zero temperature, the differential conductance $G$ is given by $G = (2e^2/h)T$, $T$ being the transmission coefficient. Quantization of conductance is a consequence of $T$ being an integer number. We have calculated the transmission as a function of energy $E$ for the mean-field Hamiltonian (3) with $n_i$ and $m_i$ calculated self-consistently by utilizing the toolkit “KWANT” 47, which implements a wave-function matching technique. The leads are defined by the same Hamiltonian (3) with $m_i = 0$ and $n_i$ uniform and equal to 1 (corresponding to half filling) for every $i$.

Figs. 3 and 4 show the transmission coefficient $T$ as a function of energy $E$ ($E = 0$ denotes the energy at which the edge-mode dispersions cross in the leads), in the presence of one vacancy and two vacancies, respectively, and for different values of the Hubbard interaction strength $U$. According to Fig. 3, relative to a single vacancy placed.
at $x = 23(\sqrt{3}/2)a$ and $y = a$, $\mathcal{T} < 2$ (thus conductance quantization is spoiled) for energies around zero. In particular, pairs of sharp dips appear where back-scattering is maximum and $\mathcal{T}$ takes its minimum value, i.e. $\mathcal{T} \approx 1$ due to the presence of an unperturbed propagating mode on the opposite edge of the sample. The main effect of increasing $U$ from 0.1$t$ to 0.5$t$ is an enhancement of the separation between the dips, while the value of $\mathcal{T}$ between the dips is slightly suppressed (by a few percent) with respect to $\mathcal{T} = 2$, virtually independently of $U$. For larger values of $U$, for example at $U = 0.8$t$, $\mathcal{T}$ is much more affected presenting, apart from the pairs of dips, a sensible suppression in a larger range of energies. A few remarks are in order here. First, due to the approximate particle-hole symmetry of the model (1) at $\lambda/t \ll 1$, the transmission is a nearly perfectly even function of $E$. As already noted, the transmission is never below 1 because the unperturbed edge mode on the opposite side of the ribbon is perfectly conducting. Notice that at the energies where the dips occur the transmission relative to one edge mode nearly vanishes. Nearly total suppression of the conductance in a 2DTI was experimentally observed in Ref. 15. Since the sample displays a finite spin polarization only around the impurity and the edge-mode wavefunctions decay exponentially away from the edge, the detrimental effects of a vacancy on the conductance rapidly vanish as this is moved towards the center of the sample (Appendix B).

The behavior of $\mathcal{T}$ for small values of $U/t$ can be understood by calculating the transmission coefficient relative to a single edge in presence of a magnetic $\delta$-like impurity. In this regime, the dips in $\mathcal{T}(E)$ can be parametrized (Appendix C) by a Breit-Wigner dependence on $E$. According to this model, such dips can be explained as anti-resonances resulting from the localization of an electron around an impurity. Indeed, local DOS calculations, reported in Appendix D, show that at the energy $E = \pm E_a$ of the dips the local DOS is localized around the impurity. This suggests that an electron with energy $E = \pm E_a$ traversing the sample gets localized in the bound state around the impurity and scattered back after a waiting time, which is inversely proportional to the full width at half height of the Breit-Wigner function.

Fig. 4 shows the transmission calculated in the presence of two vacancies. We clearly see that $\mathcal{T}$ is much more affected by the vacancies with respect to the case of a single vacancy, being suppressed in larger ranges of energy even in the weak-coupling regime. Moreover, for $U = 0.8$t$ the transmission relative to one edge mode is suppressed to zero for $-0.1t < E < 0.1t$.

Summary and discussion.—We have shown that the combined action of short-range non-magnetic impurities and onsite electron-electron interactions in two-dimensional topological insulators leads to strong back-scattering.

Strong deviations from quantization occur even in the zero-temperature limit. In contrast, all other theories\textsuperscript{23–26} including electron-electron interactions yield deviations of the conductance from its quantized value, which vanish rapidly (i.e. like $T^{\alpha}$ with $\alpha \geq 4$) as a function of temperature $T$ in the low-temperature limit. Edge reconstruction due to electron-electron interactions\textsuperscript{27}, which leads to spontaneous breaking of time-reversal symmetry, also operates down to $T = 0$ but applies only to samples with smooth confining potentials. For example, for a BHZ model applied to a HgTe/CdHgTe quantum well\textsuperscript{4}, edge reconstruction occurs\textsuperscript{27} for confining potentials that decay slower than 13 meV/nm. While certainly relevant for samples with sufficiently smooth edges, the scenario of edge reconstruction is not expected to

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{Fig3.pdf}
\caption{(Color online) Breakdown of conductance quantization for a single vacancy at the edge of a 2DTI. The transmission $\mathcal{T}$ is plotted as a function of energy $E$ (in units of $t$) at half filling and for energies lying in the gap $\delta_y$. Different curves refer to different values of $U/t$. Numerical results in this figure have been obtained by setting $\lambda/t = 0.09$ ($\delta_y \approx 0.93t$). Since on-site e-e interactions produce a spin polarization with in-plane components near the vacancy, back-scattering events occur at the same 2DTI edge and lead to the breakdown of conductance quantization, i.e. $\mathcal{T} < 2$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{Fig4.pdf}
\caption{(Color online) Same as in Fig. 3 but for the case of two vacancies placed at $x = 23(\sqrt{3}/2)a$, $y = (3/2)a$ and $x = 26(\sqrt{3}/2)a$, $y = (1/2)a$.}
\end{figure}
apply to atomically-thin crystals\textsuperscript{14}, which possess sharp
dges either created naturally by mechanical exfoliation
or deliberately by etching.

In our theory, large deviations from quantization occur
also for modest values of the dimensionless coupling con-
stant $U/t$, which determines the relative strength of on-
site electron-electron interactions. In this weak-coupling
$U/t < 1$ regime our mean-field theory is accurate and the
suppression of transmission as a function of energy can be
physically interpreted in terms of anti-resonances stem-
ing from the time spent by an electron in the bound
states formed near short-range impurities, before is back-
scattered due to spin-flipping terms in Eq. (3).

The formation of local magnetic moments in the
presence of short-range impurities and onsite electron-
electron interactions is a general feature of bipartite lat-
tices\textsuperscript{34,46}, for which the spectrum is particle-hole sym-
metric. Deep in the gap, any topological insulator poss-
sesses approximate particle-hole symmetry around the
energy at which the edge modes cross. We have shown
that small deviations from exact particle-hole symmetry (e.g. due to $\lambda \neq 0$ in our model) do not spoil the
formation of local magnetic moments near short-range
impurities. Furthermore, the same happens with the
addition of Rashba spin-orbit coupling, which introduces
extra terms breaking the exact particle-hole symmetry
of (1) at $\lambda = 0$, as shown in Appendix E. We there-
fore expect that the spontaneous formation of local mag-
netic moments near short-range impurities induced by
onsite electron-electron interactions is a general feature
of 2D topological insulators. In any event, recent work\textsuperscript{49}
has shown that a naturally occurring layered mineral (ja-
cutinaite) realizes the Kane-Mele model.

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Appendix A: Technical details on the self-consistent
numerical algorithm

Four mean-field parameters per site have to be deter-
mined self-consistently, namely the local mean electron
density $n_i$ and the three Cartesian components of the lo-
cal dimensionless mean spin polarization $m_i$ [see Eqs. (4)
and (5)].

The algorithm that we employ to determine self-consistently such mean field parameters proceeds as
follows. We start from an initial set of values $n_i^{(0)}$ and
$m_i^{(0)}$ and diagonalize exactly the Hamiltonian (3). The
obtained eigenstates are then used to calculate the ex-
pectation values $n_i^{(1)}$ and $m_i^{(1)}$ in Eqs. (4) and (5), which
are then re-inserted in the Hamiltonian. The procedure
repeats until convergence is reached, i.e., until the mean
values of the $(n-1)$-th iteration coincide, up to a desired
tolerance $\epsilon$, to the mean values of the $n$-th iteration. To
check convergence we use the uniform norm
\begin{equation}
\sup_i |X_i^{(n)} - X_i^{(n-1)}| \leq \epsilon ,
\end{equation}

where $X_i^{(n)}$ denotes the value of a mean-field parameter
at the $n$-th iteration.

Numerical results reported in the main text have been
obtained by setting $\epsilon = 10^{-10}$.

Appendix B: Dependence of the numerical results
on the position of the impurities

As the impurity is moved away from the edge into the
center of the sample, the suppression of the transmission
$T$ becomes negligible. This is shown in Fig. 5, where the
three curves refer to three different positions of a single
vacancy. The main panel shows that when $y = (3/2)a$
and $y = 2a$ the corresponding transmissions are virtually
energy-independent. A zoom of the data in the main
panel is reported in the inset. For $y = 2a$, the transmis-
sion deviates from 2 by less than 0.1%. This behavior is
easily explained by remembering that the edge-mode
wavefunctions decay exponentially away from the edge
over a length scale on the order of the lattice parameter
$a$ (see Fig. 8). If the distance between the edge and the
vacancy is larger than $a$, their overlap decreases exponen-
FIG. 6. (Color online) Numerical (red dots) and analytical (solid black line) results for the transmission $T_{SE}(E)$ relative to a single edge, as a function of energy $E$ (in units of $t$). Numerical results have been obtained for the same parameters relative to Fig. 3, and $U/t = 0.1$.

Finally, strongly reducing the chances of back-scattering events.

Appendix C: Fitting numerical data with an analytical model

Our numerical data in the weak-coupling $U/t \ll 1$ regime can be explained by utilizing a simple model proposed in Ref. 48, which describes a single edge of a 2DTI in which a pair of helical edge modes is coupled to a $\delta$-like magnetic impurity. According to Ref. 48, the transmission $T_{SE}(E)$ relative to a single edge is given by

$$T_{SE}(E) = 1 - (1 - \alpha^2) \frac{\tilde{\gamma}^2}{(E^2 - E_a^2)^2 + \tilde{\gamma}^2}. \tag{C1}$$

Here, $\pm E_a$ with $E_a = \sqrt{\Delta^2 - \gamma^2/2}$ are the positions of the dips. The parameter $\gamma$ describes coupling between the edge mode and the magnetic impurity and $\Delta$ is the strength of the magnetic impurity, while $\tilde{\gamma} = \gamma \Delta/2$ is related to the dips’ width, which in the limit $\tilde{\gamma}/E_a^2 \ll 1$ is given by $\tilde{\gamma}/E_a$. The quantity $\alpha$, which takes values in the range $-1 \leq \alpha \leq 1$, controls the depth of the dips and is given by $\alpha = \cos(\theta)$, where $\theta$ is the angle formed by the magnetization of the impurity with a vector normal to the plane of the 2DTI.

A least-square minimization procedure shows that Eq. (C1) fits very well our numerical data in the weak coupling regime $U/t \ll 1$. For example, Fig. 6 shows a comparison between the numerical data $T_{SE}(E) = T(E) - 1$ relative to a single edge for one vacancy and $U/t = 0.1$, as reported in Fig. 3, and Eq. (C1) with $\gamma = 0.0021$, $\Delta = 0.0196$, $E_a = 0.0033$, and $\cos(\theta) = 0.0362$.

FIG. 7. (Color online) Local density of states $D(E, r)$ (in units of $t^{-1}a^{-2}$) for a single vacancy, at the energy where the dip occurs in $T(E)$ in Fig. 3 of the main text, i.e. $E = -0.013t$. All parameters are the same as in Fig. 3 of the main text and $U/t = 0.1$.

FIG. 8. (Color online) Same as in Fig. 7 but for an energy $E = -0.2t$, i.e. far from the one relative to the transmission dip.

Appendix D: Local density of states

We now discuss the behavior of the local density of states $D(E, r)$ at two different representative values of energy $E$.

Fig. 7 shows $D(E, r)$ at $E = -0.013t$, which matches the energy of one of the dips for the case of a single vacancy and parameters as in Fig. 3 of the main text, with $U/t = 0.1$. It is clear that $D(E, r)$ is localized around the position of the vacancy, where the local ground-state spin polarization is also finite (see Fig. 2). On the other hand, by choosing a value of energy far from the dip in the transmission, one finds that the corresponding states are delocalized along the edge (see Fig. 8), and support transport.

Appendix E: The impact of Rashba spin-orbit coupling

The Kane-Mele Hamiltonian$^2$ can be enriched by a Rashba term of the form

$$\mathcal{H}_R = i\lambda_R \sum_{(i,j)} c_i^\dagger (s \times d_{ij})_z c_j, \tag{E1}$$
which preserves the topological phase\(^2\) for not too large values of \(\lambda_R\), with respect to \(\lambda\). Even in the presence of such term, a ground-state spin polarization still develops around a vacancy. Fig. 9 shows the resulting transmission as a function of energy, calculated for \(\lambda/t = 0.09\), \(\lambda_R/t = 0.15\), and \(U/t = 0.5\). Despite the large value of \(\lambda_R/t\), along with the dips broadening, the main difference with respect to the case where the Rashba term is absent (see Fig. 3) is that now \(T(E)\) exhibits a sizable asymmetry with respect to \(E = 0\), as a consequence of the enhanced particle-hole asymmetry.

![Graph](image)

**FIG. 9.** Transmission \(T(E)\) as a function of energy \(E\) (in units of \(t\)) for a single vacancy, obtained in presence of Rashba spin-orbit coupling. Numerical results in this figure have been obtained by setting \(\lambda/t = 0.09\), \(\lambda_R/t = 0.15\), and \(U/t = 0.5\). The position of the vacancy is as in the case of Fig. 3.

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