Interplay between destructive quantum interference and symmetry-breaking phenomena in graphene quantum junctions

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(Dated: October 29, 2018)

Quantum junctions with organic functional units exhibit antiresonances in the electronic transmission function, originating from completely destructive quantum interference (QI). We report a remarkable interplay between destructive QI and the electronic spin and valley degrees of freedom in graphene nanoflakes with zigzag edges. When the spin or valley symmetry is intact, electrons with opposite spin or valley display the same interference pattern and degenerate QI transmission antiresonances. On the contrary, when a symmetry is broken (either spontaneously or due to an external field) the degeneracy of the QI antiresonances is lifted, resulting in a dramatic differentiation in the transport properties in the different channels. This phenomenon is at the origin of the recently proposed QI-assisted spin-filtering effect [A. Valli et al. Nano Lett. 18, 2158 (2018)]. We support numerical calculations with analytic results, establishing a relation between the analytical structure of the electronic Green function and the symmetries of the microscopic model. We speculate that this is a generic and robust feature that can be exploited in different ways for the realization of novel nanoelectronic QI devices.

I. INTRODUCTION

Quantum interference (QI) effects in the electronic transport in nanostructures is a direct evidence of the particle-wave duality of electrons, which roots deep in the fundamentals of quantum mechanics. From the theoretical point of view, it is well established that ballistic electron transport in molecular junctions characterized by multiple transmission paths display clear signatures of QI. The prototype of completely destructive QI is the meta-benzene molecular junction, in which the electrons propagating along the short- and the long-arms of the ring acquire a relative phase difference $\Delta \phi = \pi \frac{2n}{m}$ yielding a complete cancellation of the transmitted wave amplitude. The presence of a QI antiresonance close to the Fermi level drastically influences the transport properties of quantum junctions and results in huge ON/OFF ratios which can be exploited for the realization of nanoelectronic devices, such as transistor and spin filters with organic functional units.

Recently, experimental evidence of destructive QI has been clearly observed in molecular junctions involving benzene, anthracene, antraquinone and several other molecules with an organic backbone where the agreement between experiments and density functional theory calculations as well as with predictions made by graphical rules is remarkable. Poly-phenyl molecules represent the natural platform for QI effects, as multiple transmission paths are naturally provided by the topology of the constituent organic rings.

Remarkably, also graphene nanostructures, being alternant hydrocarbons with delocalized $\pi$ orbitals on a honeycomb lattice, fall into this category. Recent experiments reported QI patterns in quantum junctions involving graphene nanoconstrictions or bridges as well as relatively large molecules paving the way to the realization of atomic-scale engineered quantum coherent devices. What is more important, quantum junctions with graphene functional blocks benefit of all the extraordinary properties of graphene. Their chiral nature enables the manipulation of spin and valley degrees of freedom, while appropriate engineering of the substrate and gating offer the possibility to realize superlattices and to tune the properties of the junction. Furthermore, the presence of edges and reduced dimensionality offer the possibility to enhance correlation effects and to induce magnetic order, absent in pristine graphene thus opening the way to a wide range of applications. Very recently, for instance, edge magnetism has been stabilized in graphene nanoribbons functionalized with stable magnetic radical groups, demonstrating spin coherence times in the range of microseconds at room temperature.

The present work is related to all these aspects. By means of numerical calculations and a detailed symmetry analysis, we show that QI effects can be used to control spin and valley polarization of ballistic transport in graphene quantum junctions in the absence of external magnetic fields. In particular, we show that both spin filtering and valley filtering can be achieved in the same device by simply tuning the coupling with a substrate to switch the nature of the site-site correlations in the functional element between ionic and antiferromagnetic.

The paper is organized as follows. In Sec. we discuss the model and the method used to tackle the problem of correlated transport and QI effects in graphene nanostructures. In Sec. we discuss the interplay between destructive QI and different kinds of symmetry-breaking, and we provide a unified description of the phenomenon. In Sec. we explore the origin of the QI anti-resonances from a Green’s function perspective, which allows us to pinpoint the origin of the phenomenon. Finally, Sec. contains an outlook and our conclusions.
II. GRAPHENE QUANTUM JUNCTIONS

The quantum junction Hamiltonian ($H$) can be decomposed in three terms describing the nanoflake ($H_F$), the leads ($H_L$), and the leads-flake tunnel coupling ($H_T$), respectively

$$H = H_F + H_T + H_L. \quad (1)$$

The nanoflake can be described by the following low-energy effective Hubbard model for the delocalized $\pi$ electrons

$$H_F = -t \sum_{\langle ij \rangle \sigma} p_{i \sigma}^{\dagger} p_{j \sigma} - \mu \sum_i n_{i \sigma} + U \sum_i n_{i \sigma} n_{i \bar{\sigma}} + \epsilon \sum_{\sigma} \left( \sum_{i \in A} n_{i \sigma} - \sum_{i \in B} n_{i \sigma} \right), \quad (2)$$

where $p_{i \sigma}^{\dagger}$ ($p_{i \sigma}$) create (annihilate) an electron at lattice site $i$ with spin $\sigma$, with $n_{i \sigma} = p_{i \sigma}^{\dagger} p_{i \sigma}$. The parameter $t$ denotes the nearest-neighbor hopping amplitude on the honeycomb lattice, $\mu$ is the chemical potential, the Hubbard $U$ describes the onsite Coulomb repulsion, and $\epsilon$ is an onsite energy which explicitly breaks the chiral symmetry between the A and B graphene sublattices, which can be induced, e.g., by a substrate.

The metallic electrodes and the tunneling terms, $H_L$ and $H_T$, are instead given by

$$H_L = \sum_{\alpha k \sigma} \epsilon_{\alpha k \sigma} c_{\alpha k \sigma}^{\dagger} c_{\alpha k \sigma},$$

$$H_T = \sum_{\alpha i \sigma} \left( V_{\alpha i i \sigma} c_{\alpha i \sigma}^{\dagger} p_{i \sigma} + V_{\alpha i i \sigma}^{*} p_{i \sigma}^{\dagger} c_{\alpha i \sigma} \right), \quad (3)$$

where the operators $c_{\alpha k \sigma}^{\dagger}$ ($c_{\alpha k \sigma}$) create (annihilate) an electron with energy $\epsilon_{\alpha k \sigma}$ in lead $\alpha$, and $V_{\alpha i i \sigma}$ denotes the hopping amplitude between lattice site $i$ of the nanoflake and state $k$ of lead $\alpha$. As shown in Figure 1, we consider a hexagonal zig-zag edge graphene nanoflake with $N = 54$ C atoms and a $C_3$ rotation symmetry around the center. As discussed in Ref. [4], destructive QI effects arise in contact configurations analogue to the meta configuration of a benzene molecular junction. In the meta configuration for the nanoflake, the leads are connected at edge sites that belong to the same graphene sublattice. As depicted in Fig. 1, there are two possibilities to realize such a configuration, i.e., when the edges belong to either the A or the B sublattice.

The Green’s function of the nanoflake in the presence of the leads is obtained by solving the Dyson equation

$$G_{ij}^{-1}(\omega) = G_{0,ij}^{-1}(\omega) - \Sigma_{ij}^{L}(\omega) - \Sigma_{ij}^{R}(\omega) - \Sigma_{ij}(\omega), \quad (4)$$

where $G_{0,ij}(\omega)$ is the bare Green’s function of the isolated nanoflake, which is renormalized by three self-energy contributions: $\Sigma_{ij}^{L}(\omega)$ and $\Sigma_{ij}^{R}(\omega)$, which describe the embedding of the nanoflake with the left (L) and right (R) lead, respectively, and $\Sigma_{ij}(\omega)$, which describe the electronic correlations stemming from the Hubbard interaction $U$ within the nanoflake.

The leads contribution to the self-energy is given by

$$\Sigma_{ij}^\alpha(\omega) = \sum_k \frac{V_{\alpha ik} V_{\alpha jk}^*}{\omega + \eta - \epsilon_{ak\sigma}}, \quad (5)$$

where $\eta > 0$ regularizes the analytic continuation. The parameter $V_{\alpha ik} V_{\alpha jk}^*$ in Eq. (5) describes virtual hopping processes in which an electron from site $i$ of the nanoflake is injected into state $k$ of lead $\alpha$ and (after a certain time) returns to site $j$ of nanoflake. In the following, we restrict to local hybridization processes, i.e., $\Sigma_{ij}^\alpha \propto \delta_{ij}$, without affecting the qualitative results presented below. Moreover, since the QI properties originate from the topology of the nanoflake, and are independent of the details of the coupling with the leads, it is reasonable to assume a wideband limit (WBL) approximation for the leads, in which $\Sigma_{ii}^\alpha = -i\Gamma$ and it is independent on energy for each contact site $i$.

The effects of electronic correlations within the nanoflake are taken into account within the dynamical mean-field theory (DMFT), in a real-space extension suitable to deal with systems where the translational symmetry is broken in one of more spatial dimensions. Within real-space DMFT, the nanoflake is mapped onto a set of self-consistent auxiliary Anderson impurity problems, which are solved with a Lánzos exact diagonalization procedure, yielding a local yet site-dependent self-energy $\Sigma_{ij}(\omega) = \Sigma_{ij}(\delta_{ij})$. Within this approximation, local quantum fluctuation are treated non-perturbatively, whereas non-local spatial correlations are retained at a static mean-field level.
Starting from the Green’s function of the nanoflake, under appropriate assumptions\textsuperscript{40,41} the transmission of the junction can be estimated with the following Landauer-Büttiker expression\textsuperscript{42,43}

\[
T(\omega) = \text{Tr} \left[ \Gamma^L G^{\sigma} \Gamma^R G^{\sigma} \right],
\]

where \( G^{\sigma(\ell)} \) is the retarded (advanced) Green’s function obtained from Eq. (1), while the matrix \( \Gamma^\sigma = i \Sigma^\sigma - \Sigma^{\sigma\sigma} \) encloses the spectral information of the leads. Within our description of the leads, the transmission in Eq. (6) can be recast as

\[
T(\omega) = \sum_\ell \sum_r \Gamma^R_{r\ell} \Gamma^L_{\ell r} |G^R_{\ell r}(\omega)|^2,
\]

which represents a sum over independent transmission channels, with \( \ell \) and \( r \) labelling the lattice sites of the nanoflake connected to the L and R leads, respectively.

As evident from Eq. (7), the energy dependence of the transmission is controlled entirely by the Green’s function, thus establishing a direct relation between the transport properties of the junction and the electronic properties of the graphene nanoflake. It can be explicitly shown that corrections to the transmission function beyond the WBL do not change qualitatively the results presented in the following\textsuperscript{44}. This is particularly relevant because it is possible to link the existence of destructive QI to the symmetries and the analytic properties of the Green’s function (see Sec. IV and Appendix A). This suggests that the extraordinary filtering properties of the device in the spin- and valley- channels are robust features, which depend neither on the details of the nanoflake and of the lead-flake hybridization, nor on the approximation employed in the calculations\textsuperscript{3}.

III. RESULTS AND DISCUSSION

In the following we discuss the electronic and transport properties of the hexagonal graphene nanoflake quantum junction. In particular, we focus on the interplay between the destructive QI in the meta configuration and the symmetry breaking phenomena involving the spin- and valley- degrees of freedom.

A. Effects of the symmetry breaking on a destructive QI antiresonance

In order to realize the scenario we are interested in, the minimal requirement for the transmission function \( T_\lambda(\omega) \) are: (1) \( T_\lambda(\omega) \) displays a QI antiresonance at \( \omega^QI_\lambda \) in a given channel, denoted by \( \lambda \), which has two (or more) components; (2) \( T_\lambda(\omega) \) is the same for each component of \( \lambda \), at least close to \( \omega^QI_\lambda \), when the symmetry associated to \( \lambda \) is not broken.

\[
\begin{align*}
\text{(a)} & \quad \text{valley-split} & \quad U/t = 2.75 \quad \epsilon/t = 0.05 \\
\text{(b)} & \quad \text{spin- & valley-degenerate} & \quad U/t = 2.75 \quad \epsilon/t = 0 \\
\text{(c)} & \quad \text{spin-split} & \quad U/t = 3.25 \quad \epsilon/t = 0.25 \\
\text{(d)} & \quad \text{spin- & valley-split} & \quad U/t = 3.25 \quad \epsilon/t = 0.2
\end{align*}
\]

FIG. 2. (Color online) Evolution of \( T_\lambda(\omega) \) in the spin- and valley- transmission channels. By breaking the spin-SU(2) or the chiral symmetry (or both) the four-fold degeneracy \( (g_\lambda = 4) \) of the QI antiresonance at \( \omega^QI = 0 \) is lifted, and \( g_\lambda = 2 \) or \( g_\lambda = 1 \) QI antiresonances at \( \omega^QI \neq 0 \) appear in the corresponding channel. The curves of each case are shifted vertically for clarity. Parameters: \( \Gamma/t = 0.02 \), \( T/t = 0.05 \), while \( U/t \) and \( \epsilon/t \) as labelled.

In the present case, the previous requirements are fulfilled, in any of the meta contact configurations of the junction, for both the spin and valley pseudo-spin (i.e., \( \lambda = \{\sigma, \tau\} \), with \( \sigma = \pm 1 \) and \( \tau = \pm 1 \)). When the SU(2) symmetry associated with the two degrees of freedom is intact, we observe a QI antiresonance with multiplicity \( g_\lambda = 4 \), while breaking the spin-SU(2) or the chiral symmetry (or both) results in a lifting of the degeneracy of \( \omega^QI_\lambda \) and a strong differentiation of the transport properties due to the destructive QI. We summarize our findings in Fig. 2, where we show how the transmission \( T(\omega) \) changes when breaking the \( \sigma \)- and \( \tau \)-symmetries of the Hamiltonian. When neither the spin nor the valley degeneracy is lifted, \( T(\omega) \) is the same in all channels and displays a four-fold antiresonance at \( \omega^QI = 0 \), signature of destructive QI. This scenario is depicted in Fig. 2(b), while Fig. 2(a, c, and d) correspond to all the different symmetry-breaking scenarios, that we are going to discuss below in details.

B. Spin-split scenario

The ground state of the nanoflake changes from PM to antiferromagnetic (AF) when the local repulsion overcomes a critical threshold \( (U > U^{AF}) \). The AF state breaks the spin-SU(2) symmetry, with a Néel-like pattern of ordered moments \( \langle S^z_i \rangle = (n_{it}) - (n_{it}) \), which have op-
The local magnetic moments are spatially inhomogeneous, and increase with the distance from the centre of the nanoflake.\(^{35,45,46}\) The magnetic pattern is stabilized by short-range antiferromagnetic correlations, which are stronger at the edges and weaker in the bulk.\(^{35}\) In the spin-$SU(2)$ symmetry-broken state, the transmission for a given valley is no longer the same in the spin-$\uparrow$ and spin-$\downarrow$ channels. The spin-resolved transmission $T_\sigma(\omega)$ still exhibits destructive QI, but the antiresonances are separated in energy and located at $\omega^{QI}_\sigma \propto \bar{U}_\sigma \langle S^z \rangle$, as shown in Fig. 2(c).

The selective suppression of the transmission in one of the spin channels, due to destructive QI, can be exploited to obtain a nearly perfect QI-assisted spin-filtering device, as recently proposed in Ref. 4, which demonstrates the potential impact of the investigated phenomenon for technological applications.

Note that, since the two sublattices have opposite magnetization, the transmission is still symmetric under the simultaneous inversion of the spin ($\sigma \rightarrow \bar{\sigma}$) and valley pseudospin ($\tau \rightarrow \bar{\tau}$) i.e., $T_{\tau \sigma}(\omega) = T_{\bar{\tau} \bar{\sigma}}(\omega)$, as specified in the legend of Fig. 2. This means also that the QI antiresonance is still two-fold degenerate $\omega^{QI}_\sigma = \omega^{QI}_{\bar{\sigma}}$.

The transport properties of the junction in this scenario are shown in details in Fig. 3. The top panels show the heatmap of $T_\sigma(\omega)$ for valley $B$ and $T_{\bar{\sigma}}(\omega)$ for valley $A$, which identify the charge spectral gap, and in particular, the HOMO and LUMO, closest to the Fermi level, corresponding to the spin-$\uparrow$ channel, but the situation is analogous for valley $A$, as discussed above. One can follow the evolution of: (1) the resonances (darker shades of color), and in particular, the closest to the Fermi level, corresponding to the HOMO and LUMO, which identify the charge spectral gap, and (2) the QI antiresonance (in the middle of the white area). At $U/t < U_{AF}/t \lesssim 3$, the gap is reduced with respect to its non-interacting value as $\Delta \approx \langle Z \rangle \Delta_0$, where $\langle Z \rangle$ is the average over the nanoflake of local quasi-particle residue, extracted from the local DMFT self-energy as

$$Z_i = \left(1 - \frac{\partial \Sigma_i(\omega)}{\partial \omega} \right|_{\omega \rightarrow 0} \right)^{-1}. \quad (9)$$

The QI antiresonance $\omega^{QI}_\sigma = 0$ is pinned at the Fermi level due to the particle-hole symmetry of the spectrum.\(^{45}\) Instead, when AF sets in, the gap is no longer controlled by...
quantum confinement effect, but by the staggered magnetization, and it increases with $U$, while $\omega_{\sigma}^{QI}$ shifts below or above the Fermi level, proportionally to the average staggered magnetization $\langle S^z \rangle$, depending on the spin channel. This clearly demonstrates the behavior sketched in Fig. 2(c) for the spin-split scenario.

As a consequence of the different behavior of $T_\uparrow(\omega)$ and $T_\downarrow(\omega)$, the spin-polarization of the transmission

$$\zeta_\sigma(\omega) = \frac{T_\uparrow - T_\downarrow}{T_\uparrow + T_\downarrow}, \quad (10)$$

is not zero in a wide frequency range above and below the Fermi level. This is demonstrated in the bottom panels of Fig. 3 where we show the heatmap of $\zeta_\sigma(\omega)$ as a function of $\omega/t$ and $U/t$, as well as cuts of $\zeta_\sigma(\omega)$ for specific values of $U/t$. The maxima (or minima) of the polarization are always located in correspondence of $\omega_{\sigma}^{QI}$, where the transmission probability in one spin channel is strongly suppressed and the transport is dominated by the other channel.

C. Valley-split scenario

Let us consider the case in which both the spin-SU(2) and the chiral symmetry are broken. It is more intuitive to take the spin-split scenario above as a starting point and break the chiral symmetry with $\epsilon$. As shown in Fig. 2(d), the QI antiresonance of each valley splits under the effect of $\epsilon$, further reducing the degeneracy of $\omega_{\sigma}^{QI}$ to $g_\lambda = 1$. It is obvious that a completely equivalent description is obtained by taking the valley-split scenario as a starting point and increasing $U$ above $U^{AF}$ to induce magnetic order. Let us just note that the there is a non-trivial feedback between charge- and spin-correlations, resulting in (weak) dependence of critical threshold for spin order on the chiral symmetry-breaking field, i.e., $U^{AF} = U^{AF}(\epsilon)$. In fact, the formation of a charge-density wave requires to locally drive the C atoms away from half-filling. This is detrimental to the formation of the AF state, and results in a partial quench of the local magnetic moments. A consequence of this interplay is that, if the system is at the verge of magnetic ordering, tuning $\epsilon$ could allow to drive the system through the PM$\leftrightarrow$AF crossover, and ideally working as a switch between spin-filtering and valley-filtering effects.

D. Spin- and valley-split scenario

Last, we consider the case in which both the spin-SU(2) and the chiral symmetry are broken. It is more intuitive to take the spin-split scenario above as a starting point and break the chiral symmetry with $\epsilon$. As shown in Fig. 2(d), the QI antiresonance of each valley splits under the effect of $\epsilon$, further reducing the degeneracy of $\omega_{\sigma}^{QI}$ to $g_\lambda = 1$. It is obvious that a completely equivalent description is obtained by taking the valley-split scenario as a starting point and increasing $U$ above $U^{AF}$ to induce magnetic order. Let us just note that the there is a non-trivial feedback between charge- and spin-correlations, resulting in (weak) dependence of critical threshold for spin order on the chiral symmetry-breaking field, i.e., $U^{AF} = U^{AF}(\epsilon)$. In fact, the formation of a charge-density wave requires to locally drive the C atoms away from half-filling. This is detrimental to the formation of the AF state, and results in a partial quench of the local magnetic moments. A consequence of this interplay is that, if the system is at the verge of magnetic ordering, tuning $\epsilon$ could allow to drive the system through the PM$\leftrightarrow$AF crossover, and ideally working as a switch between spin-filtering and valley-filtering effects.

IV. ORIGIN OF THE QI ANTIRESONANCES

In order to understand what is the mechanism leading to the $\omega^{QI}$ degeneracy lifting, we look explicitly at the structure of the Green’s function.

As already discussed, the general Landauer expression for the transmission function can be recast as in Eq. (7), which establishes a direct link between $T(\omega)$ and $G_{\ell r}(\omega)$ for the generic $\ell \rightarrow r$ channel. In particular, in the WBL, all the frequency dependence of $T(\omega)$ comes from the Green’s function. This means that a QI antiresonance (i.e., a zero of the transmission) necessarily implies a zero of the Green’s function. At energies $|\omega|<\Delta$ (i.e., within the spectral gap) $\Im G_{\ell r}(\omega)\approx 0$ for every pair $(\ell, r)$, where the exact relation holds at $T=0$. Therefore the zeroes of the Green’s function coincide with the zeroes of $\Im G_{\ell r}(\omega)$. 

While an analytic expression for $\omega^{QI}_\lambda$ in the generic case cannot be easily obtained, in Appendix A we provide an argument that explains the relation between $\omega^{QI}_\lambda$ and the order parameters $(S^z)$ and $(n_A-n_B)$, which is shown in Figs. 5 and 6 for the two symmetry-broken states.

V. CONCLUSIONS & OUTLOOK

We investigated the interplay between destructive QI and symmetry-breaking phenomena involving the spin and valley degrees of freedom in graphene nanoflakes. Specifically, by establishing a relation between the analytic structure of the nanoflake’s Green’s function and the symmetries of the Hamiltonian, we provide a clear understanding of the origin of the antiresonances and of their effects on ballistic transport.

In Ref. 4, we showed that destructive QI can be used to generate pure spin currents in the absence of magnetic fields or spin-orbit coupling, simply exploiting the spontaneous breaking of the $SU(2)$ spin-rotational symmetry induced by electronic correlation in the presence of the edges. The symmetry analysis presented here allows us to explain and extend the results of Ref. 4 showing that by coupling the nanoflake to a substrate, it is possible to switch the nature of the electronic correlations between antiferromagnetic and ionic, and turn the spin filter into a valley filter.

Interestingly, our analysis works both in the symmetric and in the symmetry-broken case. Indeed we show that, under the appropriate assumptions, breaking a symmetry shifts the position of the antiresonance, without spoiling the destructive QI. The approach developed in the present work points at a general scheme to design selective electronic transport devices in chiral lattice structures, relying on two essential ingredients: i) the identification of a symmetry and of a symmetry-breaking control parameter, and ii) the presence of destructive QI effects. As such, the protocol can be applied to different situations, e.g., in graphene bilayers it could be employed to engineer destructive QI between electronic waves propagating in the two layers. Even more intriguing would be the possibility of a similar interplay between destructive QI and superconductivity.

Appendix A: Impact of symmetries on the real-space Green’s function and the transmission

1. Symmetric state

At half-filling, the Hamiltonian of the flake $H_F$ given in Eq. (2) is symmetric under the following particle-hole transformation

\[
\begin{align*}
    p^\dagger_{A\sigma} &\rightarrow p_{A\sigma} \quad p_{A\sigma} &\rightarrow p^\dagger_{A\sigma}, \\
    p^\dagger_{B\sigma} &\rightarrow -p_{B\sigma} \quad p_{B\sigma} &\rightarrow -p^\dagger_{B\sigma}.
\end{align*}
\]

FIG. 5. (Color online) Zeros of the $\Re G(r)(\omega)$ for the sites in the middle of the edges of the meta configuration, without and with symmetry breaking. In the spin-split scenario for valley A (upper panel) and in the valley-split scenario for spin-$\uparrow$ (lower panel), the two-fold degeneracy of the zero at $\omega=0$ is lifted, yielding two zeros at $|\omega_0^A|=|\omega_0^B|\approx (S^z)\approx 0.33$, and two zeroes at $|\omega_0^A|=|\omega_0^B|\approx (n_B-n_A)\approx 0.19$, respectively. The grey shaded area indicates the energy window lying outside the broken-symmetry gaps. Parameters: $U/t=3.75$, $\epsilon/t=0$, $\Gamma/t=0.02$ and $T=0.05t$ (upper panel); $U/t=1.5$, $\epsilon/t=0$ and $\epsilon/t=0.4$, $\Gamma/t=0.02$ and $T=0.05t$ (lower panel).

It can be shown (see Appendix A1 for the derivation) that when neither the spin-$SU(2)$ nor the chiral symmetry are broken, the zero of the Green’s function is pinned at the Fermi level ($\omega=0$) by the particle-hole symmetry. Instead, any symmetry-breaking term shifts the zeroes of $\Re G(r)(\omega)$, and hence the destructive QI antiresonance at finite frequency (see Appendix A2).

In order to demonstrate this effect, in Fig. 5 we explicitly show the low-energy structure of $\Re G(r)(\omega)$, for a given transmission channel, in which $t$ and $r$ are sites in the middle of the $\ell$ and $R$ edges in the meta configuration (of sublattice B). The case of sublattice A can be obtained from this one by symmetry. In the upper panel of Fig. 5 we show the effect of the spin-$SU(2)$ symmetry breaking. In the PM state, the zero of $\Re G(r)(\omega)$ is found at $\omega=0$ for both the spin-$\uparrow$ and spin-$\downarrow$ channels, while in the AF state we observe an opposite shift of the zeroes to finite frequency which correlates with the behavior of the destructive QI antiresonance found at $\omega^{QI}_\sigma$, as shown in Fig. 2 (sublattice B). In the lower panel of Fig. 5 we demonstrate the analogous effect in for the chiral symmetry breaking. Differently from the previous case, at $\epsilon=0$, $\Re G(r)(\omega)$ is not identical for the two valleys, but both display a zero at $\omega=0$. At finite field $\epsilon$, the zeroes split symmetrically with respect to the Fermi level, yielding different $\omega^{QI}_\lambda$ for the two valleys.
The pinning of the destructive QI antiresonance at the Fermi level can be demonstrated by considering the definition of the Green’s function

\[ G_{ij\sigma}(\omega) = -i \int \theta(t) \left\langle \left\{ p_{i\sigma}(t), p_{j\sigma}^\dagger(0) \right\} \right\rangle e^{-i\omega t} dt, \]  

(A2)

where \( \theta(t) \) is the Heaviside function, \( \{\cdot,\cdot\} \) is the anticommutator for the fermionic operators, and the average is taken over the ground state at \( T = 0 \), while it is replaced by the usual thermal average at \( T \neq 0 \). The invariance of the above expression under particle-hole transformation implies

\[ G^r_{ij\sigma}(\omega) = -i(-1)^{i+j} \int \theta(t) \left\langle \left\{ p_{i\sigma}^\dagger(t), p_{j\sigma}(0) \right\} \right\rangle e^{-i\omega t} dt \]  

(A3)

where the prefactor \((-1)^{i+j}\) equals \pm 1 depending on whether \( i \) and \( j \) belong to the same or to different sublattices. On the other hand, taking the complex conjugate of Eq. (A2) one obtains

\[ (G_{ij\sigma}(\omega))^* = i \int \theta(t) \left\langle \left\{ p_{i\sigma}^\dagger(t), p_{j\sigma}(0) \right\} \right\rangle e^{i\omega t} dt. \]  

(A4)

A comparison of equations Eq. (A3) and Eq. (A4) demonstrates that in the presence of particle-hole symmetry the following relation holds

\[ (G_{ij\sigma}(\omega))^* = (-1)^{i+j+1} G_{ij\sigma}(\omega). \]  

(A5)

This implies that, in the meta configuration, \( \Re G_{ij\sigma}(0) \) is vanishing due to the particle-hole symmetry. Since \( \Im G_{ij\sigma}(0) \) is suppressed by the presence of the spectral gap, the transmission from Eq. (7) becomes

\[ \Gamma_{\ell\ell}^{\text{meta}}(0) = \sum_{\ell r} \Gamma_{\ell\ell} \Gamma_{rr} |G_{\ell r \sigma}(0)|^2 \approx 0, \]  

(A6)

where \( \ell \) and \( r \) span the proper subsets for the meta configuration. This demonstrates the pinning of the destructive QI at the Fermi level in the particle-hole symmetric case. Moreover, this implies that a destructive QI is expected for any transmission channel \( \ell \rightarrow r \) connecting sites from the same sublattice, which allow to predict the occurrence of antiresonances in complex graphene nanostructures.

It is interesting to notice that the situation is drastically different in the other possible transport configurations. In both the ortho and para configurations, the sites \( i \) and \( j \) belong to different sublattices. Hence, Eq. (A5) implies that \( \Im G_{ij\sigma}(0) \) is vanishing, while \( \Re G_{ij\sigma}(0) \) is not. As a consequence, both \( T_{\sigma}^{\text{ortho}}(0) \) and \( T_{\sigma}^{\text{para}}(0) \) do not display any destructive QI antiresonance at the Fermi level.

Let us note that, in principle, an asymmetric coupling between the leads and the flake explicitly breaks the particle-hole symmetry. However, in the WBL approximation, the leads introduce an additional lifetime \( \Gamma_{\ell\ell} \) and \( \Gamma_{rr} \), but do not induce any energy shift to the poles, so that the excitation spectrum remains particle-hole symmetric. Furthermore, even in the case when the particle-hole is broken, the QI antiresonance would still exist at a finite frequency \( \omega_Q \).

2. Symmetry-broken state

In the presence of AF short-range order with a Néel pattern, the particle-hole transformation Eq. (A1) has to be modified as follows, to leave the ground-state invariant

\[ p_{Ai\sigma}^\dagger \rightarrow p_{Bi\sigma}, \quad p_{Ai\sigma} \rightarrow p_{Bi\sigma}^\dagger, \]  

\[ p_{Bi\sigma}^\dagger \rightarrow -p_{Bi\sigma}, \quad p_{Bi\sigma} \rightarrow -p_{Bi\sigma}^\dagger \]  

(A7)

where \( \bar{\sigma} = -\sigma \). In this case, Eq. (A5) becomes

\[ (G_{ij\sigma}(\omega))^* = (-1)^{i+j+1} G_{ij\sigma}(\omega), \]  

(A8)

which yields the following relation for the spin-dependent conductance

\[ T_{\sigma}(\omega) = T_{\bar{\sigma}}(-\omega). \]  

(A9)

in all transport configurations.

Since the AF order and the graphene sublattices share the same real-space pattern, we can equivalently define the particle-hole transformation as

\[ p_{Ai\sigma}^\dagger \rightarrow p_{Bi\sigma}, \quad p_{Ai\sigma} \rightarrow p_{Bi\sigma}^\dagger, \]  

\[ p_{Bi\sigma}^\dagger \rightarrow -p_{Bi\sigma}, \quad p_{Bi\sigma} \rightarrow -p_{Bi\sigma}^\dagger \]  

(A10)

where, with respect to Eq. (A7), we only exchanged the role of spin and sublattice indices.

Let us now analyze the consequences of the invariance of the Green’s function under the particle-hole transformation in Eq. (A10). When the Green’s function connects sites belonging to different sublattices, as in the ortho and para configurations, the invariance under Eq. (A10) implies

\[ G_{ij\sigma}(\omega) = i \int \theta(t) \left\langle \left\{ p_{i\sigma}^\dagger(t), p_{i\sigma}(0) \right\} \right\rangle e^{-i\omega t} dt \]  

(A11)

that compared with Eq. (A4) yields

\[ [G_{ij\sigma}(\omega)]^* = -G_{ij\sigma}^A(-\omega). \]  

(A12)

where the superscript \( AB \) indicate that \( i \) and \( j \) belong to different sublattices. Eq. (A12) in turn implies for the total transmission in the ortho and para configurations

\[ T_{\sigma}(\omega) = T_{\bar{\sigma}}(-\omega) \]  

and along with Eq. (A9) eventually prevents the spin-filtering effect, yielding

\[ T_{\sigma}^{\text{ortho}}(\omega) = T_{\bar{\sigma}}^{\text{ortho}}(\omega), \quad T_{\sigma}^{\text{para}}(\omega) = T_{\bar{\sigma}}^{\text{para}}(\omega). \]  

(A13)

On the contrary, in the meta configuration, similar reasoning shows that invariance under Eq. (A10) implies

\[ [G_{ij\sigma}(\omega)]^* = G_{ij\sigma}^{BB}(-\omega) \]  

(A14)

where the \( AA \) and \( BB \) superscripts indicate the two possible meta configurations, i.e., where only sites of sublattice A or only sites of sublattice B are connected.
Eq. (A14) implies the following relation for the transmission
\[ T_{\sigma AA}^{\text{meta}}(\omega) = T_{\sigma BB}^{\text{meta}}(-\omega), \]
that along with Eq. (A9) yields
\[ T_{\sigma AA}^{\text{meta}}(\omega) = T_{\bar{\sigma} BB}^{\text{meta}}(\omega). \] (A16)
Hence, provided that \( \omega^{\text{QI}} \neq 0 \), the above relations imply the spin- and sublattice-structure observed in the numerical simulations.

The last step consists in the identification of the mechanism that shifts the QI antiresonance. Within DMFT, the spin-\textit{SU}(2) symmetry breaking is a spontaneous phenomenon. It is induced by the sort-range AF correlations due to the local repulsion \( U \), resulting in a dynamical spin-dependent self-energy \( \Sigma_\tau(\omega) \). The static contribution of the self-energy \( \Sigma_\sigma(0) \propto U \langle S^\sigma \rangle \), acts as an effective chemical potential, with opposite sign for the two spin polarizations, and shifts the zeroes of the Green’s function to \( \omega^{\text{QI}} \). This effect is ultimately at the origin of the behavior observed in Fig. 5 (upper panel) for the spin-split case. The chiral symmetry is instead explicitly broken by the field, so that the effective correction to the zero of the Green’s function is given by \( \epsilon_\tau + \Sigma_\sigma(0) \propto (n_A - n_B) \). Both terms have opposite sign for the two valleys, and induce the symmetric shift of the zeroes to \( \omega^{\text{QI}}_\lambda \), as observed in Fig. 5 (lower panel) for the valley-split case. Finally, in the spin- and valley-split case, the combination of the above self-energy corrections in the different channels result in the complete lifting of the four-fold degeneracy of the QI antiresonance.

In general, the exact value of \( \omega^{\text{QI}}_\lambda \) in a given transmission channel depends on the details of the real-space magnetization and charge redistribution pattern. Moreover, since the transmission through the junction is given by the contributions of different channels, one should expect a distribution of antiresonances, which result in a broadening of the minima of the transmission, with respect to the one pinned at the Fermi level and controlled by the particle-hole symmetry alone.

ACKNOWLEDGMENTS

We thank R. Stadler and C. Lambert for valuable discussions. We acknowledges financial support from MIUR PRIN 2015 (Prot. 2015C5SEJ001) and SISSA/CNR project "Superconductivity, Ferroelectricity and Magnetism in bad metals" (Prot. 232/2015). A.A. acknowledges support from the H2020 Framework Programme, under ERC Advanced Grant No. 692670 "FIRSTORM". A.V. acknowledges financial support from the Austrian Science Fund (FWF) through the Erwin Schrödinger fellowship J3890-N36.

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See also the extended discussion in the Supporting Information of Ref. 4, at https://pubs.acs.org/doi/abs/10.1021/acs.nanolett.8b00453.

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