Beyond the constant-mass Dirac physics: Solitons, charge fractionization, and the emergence of topological insulators in graphene rings

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The doubly connected polygonal geometry of planar graphene rings is found to bring forth topological configurations for accessing nontrivial relativistic quantum field (RQF) theory models that carry beyond the constant-mass Dirac-fermion theory. These include the generation of sign-alternating masses, solitonic excitations, and charge fractionization. The work integrates a RQF Lagrangian formulation with numerical tight-binding Aharonov-Bohm electronic spectra and the generalized position-dependent-mass Dirac equation. In contrast to armchair graphene rings (aGRGs) with pure metallic arms, certain classes of aGRGs with semiconducting arms, as well as with mixed metallic-semiconducting ones, are shown to exhibit properties of one-dimensional nontrivial topological insulators. This further reveals an alternative direction for realizing a graphene-based nontrivial topological insulator through the manipulation of the honeycomb lattice geometry, without a spin-orbit contribution.

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I. INTRODUCTION

Research endeavors aiming at the realization [1–9] of vaunted relativistic quantum field (RQF) behavior [10] in “low-energy” laboratory setups were spawned by the isolation of graphene [1,3], whose low-energy excitations behave as massless Dirac-Weyl (DW) fermions (moving with a Fermi velocity $v_F$ instead of the speed of light $c$; $v_F \sim c/300$), offering a link to quantum electrodynamics [2,3,11,12] (e.g., Klein tunneling and Zitterbewegung).

Here we show that planar polygonal graphene rings with armchair edge terminations (aGRGs) can provide an as-yet unexplored condensed-matter bridge to high-energy particle physics beyond both the massless Dirac-Weyl and the constant-mass Dirac fermions. Due to their doubly connected topology (supporting Aharonov-Bohm (AB) physics [13]), aGRGs bring forth condensed-matter realizations for accessing ac-claimed one-dimensional (1D) RQF models involving the emergence of position-dependent masses and consideration of interconnected vacua (or topological domains). As a function of the ring’s arm width, one finds two general outcomes: (i) the formation of soliton/antisoliton fermionic complexes [14–16] studied in the context of charge fractionization [17] and the physics of trans-polyacetylene [14,15] and (ii) the formation of fermion bags introduced in the context of the nuclear hadronic $\sigma$ model [18] and in investigations of nontrivial Higgs-field mass acquisition for heavy quarks [19].

A principal result of our study is that it reveals an emergent alternative direction for realizing a graphene-based nontrivial topological insulator (TI) [4,5] through the manipulation of the honeycomb lattice geometry, without a spin-orbit contribution. In particular, in contrast to armchair graphene rings with pure metallic arms, certain classes of aGRGs with semiconducting arms, as well as with mixed metallic-semiconducting ones, are shown to exhibit properties of one-dimensional nontrivial TIs.

II. METHODOLOGY

The energy of a particle (with one-dimensional momentum $p_x$) is given by the Einstein relativistic relation $E = \sqrt{(p_x v_F)^2 + (M v_F^2)^2}$, where $M$ is the rest mass. In gapped graphene or graphene systems, the mass parameter is related to the particle-hole energy gap $\Delta$, as $M = \Delta/(2v_F^2)$. In RQF theory, the mass of elementary particles is imparted through interaction with a scalar field known as the Higgs field. Accordingly, the mass $M$ is replaced by a position-dependent Higgs field $\phi(x)$ to which the relativistic fermionic field $\Psi(x)$ couples through the Yukawa Lagrangian [19,20] $\mathcal{L}_Y = -\phi \Psi^\dagger \beta \Psi$ (with $\beta$ being a Pauli matrix). In the elementary-particles standard model [10], such coupling is responsible for the masses of quarks and leptons. For $\phi(x) \equiv \phi_0$ (constant), $M v_F^2 = \phi_0$, and the massive fermion Dirac theory is recovered.

We exploit the generalized Dirac physics governed by a total Lagrangian density $\mathcal{L} = \mathcal{L}_f + \mathcal{L}_\phi$, where the fermionic part is given by

$$\mathcal{L}_f = -i \hbar \Psi^\dagger \frac{\partial}{\partial t} \Psi - i \hbar v_F \Psi^\dagger \alpha \frac{\partial}{\partial x} \Psi + \mathcal{L}_Y,$$

and the scalar-field part has the form

$$\mathcal{L}_\phi = -\frac{1}{2} \left( \frac{\partial \phi}{\partial x} \right)^2 - \frac{\xi}{4} (\phi^2 - \phi_0^2)^2,$$

with the potential $V(\phi)$ (second term) assumed to have a double-well $\phi^2$ form; $\xi$ and $\phi_0$ are constants.

Henceforth, the Dirac equation is generalized as

$$E \Psi + i \hbar v_F \alpha \frac{\partial \Psi}{\partial x} - \beta \phi(x) \Psi = 0.$$

In one dimension, the fermion field is a two-component spinor $\Psi = (\psi_u, \psi_l)^T$; $u$ and $l$ stand, respectively, for the upper and lower component and $\alpha$ and $\beta$ can be any two of the three Pauli matrices.

Each arm of a polygonal ring can be viewed as an approximation of an armchair graphene nanoribbon (aGR). The excitations of an infinite aGR are described by the 1D

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massive Dirac equation [see Eq. (3)], with \( \alpha = \sigma_2, \beta = \sigma_1 \), and 
\( \phi(x) \equiv \phi_0 = \Delta/2 \equiv |t_1 - t_2| \). The two (in general) unequal 
hopping parameters \( t_1 \) and \( t_2 \) are associated with an effective 
1D tight-binding problem (see Appendix A) and are given 
[21] by 
\( t_1 = -2t \cos[p \pi/(N_w + 1)], \ p = 1, 2, \ldots, N_w \) and 
\( t_2 = -t; \ N_w \) is the number of carbon atoms specifying the 
width of the nanoribbon and \( t = 2.7 \ eV \) is the hopping 
parameter for 2D graphene. The effective [21] TB Hamiltonian 
of an aGR has a form similar to that used in \( \textit{trans}-\text{polycrylate} \), 
the inequality of \( t_1 \) and \( t_2 \) (referred to as dimerization) is 
a consequence of a Peierls distortion induced by the electron-
onphonon coupling. For an aGR, this inequality is a topological 
effect associated with the geometry of the edge and the width 
of the ribbon. We recall that as a function of their width, \( N_w \), 
the armchair graphene nanoribbons fall into three classes: 
(I) \( N_w = 2l \) (semiconducting, \( \Delta > 0 \)), (II) \( N_w = 2l + 1 \) 
(semiconducting, \( \Delta > 0 \)), and (III) \( N_w = 2l + 2 \) (metallic, 
\( \Delta = 0 \)), \( l = 1, 2, 3, \ldots \).

We adapt the "crystal" approach [13] to the AB effect 
and introduce a virtual Dirac-Kronig-Penney [22] (DKP) 
relativistic superlattice (see Appendix B). Charged fermions 
in a perpendicular magnetic field circulating around the ring 
behave like electrons in a spatially periodic structure (period 
\( D \)) with the magnetic flux \( \Phi/\Phi_0 = \hbar c/e \) playing the role 
of the Bloch wave vector \( k \), i.e., \( 2\pi \Phi/\Phi_0 = kD \) [see the cosine 
term in Eq. (B5)].

III. RESULTS

A. Rings with semiconducting arms

Naturally, nanorings with arms made of nanoribbon seg-
ments belonging to the semiconducting classes I and II may 
be expected to exhibit a particle-hole gap (particle-antiparticle 
gap in QRF theory). Indeed this is found for class-I aGRGs 
[see gap \( \Delta \) in Fig. 1(a)]. Surprisingly, the class-II nanorings 
demonstrate a different behavior, showing a "forbidden" 
band in the middle of the gap region [see Fig. 1(b)]. This 
forbidden band is dissected by the zero-energy axis and its 
members cross this axis at regular-magnetic-flux intervals 
\( \Phi = (\pm j + 1/2)\Phi_0, \ j = 1, 2, 3, \ldots \), manifesting semimetallic 
behavior.

This behavior of class-II aGRGs can be explained through 
alogies with QRF theoretical models, describing single zero-
energy fermionic solitons with fractional charge [14,17] or 
their modifications when forming soliton/antisoliton systems 
[14,16]. [A solution of the equation of motion corresponding to 
Eq. (2) is a \( Z_2 \) kink soliton, \( \phi_k(x) \). The solution of Eq. (3) with 
\( \phi = \phi_k(x) \) is the fermionic soliton.] We model the hexagonal 
ring with the use of a continuous 1D Kronig-Penney [22,23] 
model (see Appendix B) based on the generalized Dirac 
equation (3), allowing variation of the scalar field \( \phi(x) \) along 
the ring’s arms. We find that the DKP model reproduces [see 
Fig. 1(d)] the spectrum of the class-II ring (including the 
forbidden band) when considering alternating masses \( \pm m_0 \) 
associated with contiguous arms [see inset in Fig. 1(b)].

The sign-alternating mass regions, separated by six regions 
of vanishing mass centered at the corners, correspond to a 
Higgs field composed of a train (or a so-called crystal 
[24–26]) of three kink/antikink soliton pairs. In analogy with 
the physics of \( \textit{trans}-\text{polycrylate} \), the positive and negative 
masses correspond to two degenerate domains associated 
with the two possible dimerization patterns [14,15] 
\( \cdots - t_1 - t_2 - t_3 - t_2 - - \cdots \) and 
\( \cdots - t_2 - t_1 - t_2 - t_1 - \cdots \), which are possible in a single-atom chain. The transition zones between 
the two domains (here the corners of the hexagonal ring) are 
referred to as the domain walls.

For a single soliton, a (precise) zero-energy fermionic 
excitation emerges, localized at the domain wall. In the 
case of soliton-antisoliton pairs, paired energy levels with 
small positive and negative values appear within the gap. 
The TB spectrum in Fig. 1(b) exhibits a forbidden band 
of six paired \( +/− \) levels, a property fully reproduced by
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These alternating localization patterns (trains of solitons) are faithfully reproduced [see Fig. 2(b)] by the upper, $\psi_u$, and lower, $\psi_l$, spinor components of the DKP model. The three soliton-antisoliton trains in Fig. 2(b) generate an unusual $e/6$ charge fractionization at each corner, which is unlike the $e/2$ fractionization familiar from polyacetylene. Moreover, the fractionization patterns in topological graphene structures may be tuned. For example, as illustrated below, the more familiar $e/2$ fraction [15,17,27] can be realized in the case of an aGRG with mixed class-I and class-III arms.

The absence of a forbidden band (i.e., solitonic excitations within the gap) in the spectrum of the class-I hexagonal nanorings [see Fig. 1(a), $N_w = 16$] indicates that the corners in this case do not induce an alternation between the two equivalent dimerized domains (represented by $\pm m_0$ in the DKP model). Here the corners do not act as topological domain walls. The inset in Fig. 1(c) portrays the DKP spectrum when a constant mass $M = 0.13\hbar$ is assumed to encircle the ring. This spectrum conforms with that expected from a free massive Dirac fermion, and it clearly disagrees with the TB spectrum in Fig. 1(a). However, direct correspondence between the TB and DKP spectra is achieved here too by using a variable Higgs field defined as $\phi(x) = m_1^{(n)}(x)$ with $m_1^{(n)} = m_3^{(n)} = 0.06\hbar/v_F^2$ and $m_2^{(n)} = 0.13\hbar/v_F^2$ [see the schematic inset in Fig. 1(a); the DKP spectrum is plotted in Fig. 1(c)]. $\phi(x)$ now exhibits depressions at the hexagon corners, instead of the aforementioned sign alternation; compare insets in Figs. 1(a) and 1(b). This variation of $\phi(x)$ resembles that of the field used in the theory of polarons in conducting polymers [28] and in the theory of fermion bags in hadronic [18] and heavy-quark physics [19].

B. Rings with mixed semiconducting/metallic arms

The pure metallic-aGRG (class-III) wave functions do not exhibit any localization features and are thus devoid of any topological-insulator characteristics; see Fig. 2(c). Unique TI configurations, however, can be formed in mixed rings, i.e., with arms belonging to different classes. Figure 3 portrays a mixed ring, with four arms belonging to class-III ($N_w = 17$; metallic) and the two remaining ones belonging to class-I ($N_w = 15$; semiconducting) ribbons. The TB spectra are displayed in Fig. 3(a), and Fig. 3(b) schematically describes the Higgs field $\phi(x) = m_1^{(n)}(x)$, which yields the best DKP reproduction of the TB spectra (see caption). The TB spectrum in Fig. 3(a) reflects the loss of sixfold symmetry of the Higgs field (in contrast to Fig. 1). Furthermore, five states in the energy range $0.01\hbar/v_F^2 < \varepsilon < 0.13\hbar/v_F^2$ exhibit a magnetic-field-independent flat profile, corresponding to the behavior of a particle in a box. Namely, the practically $(m_{0,1} = 0.01\hbar/v_F^2)$ massless Dirac fermion is confined in the potential well formed by the four arms $n = 1$ to 4, unable to penetrate under the high barrier represented by the larger masses $\pm m_2 = \pm 0.20\hbar/v_F^2$ associated with the fifth and sixth arms of the hexagon. The twofold braid band around $\varepsilon = 0$ exhibits a clear Aharonov-Bohm dependence on the magnetic flux $\Phi$. The TB wave function of one state in this band (with $\varepsilon = 0.1995 \times 10^{-2}\Phi$) is plotted in Fig. 3(c). It describes the emergence of a fermionic soliton (with $e/2$ fractional charge) localized at the domain wall (corner denoted by an arrow) between the

![Fig. 2. (Color online) Wave functions for an excitation belonging to the “forbidden” solitonic band. (a) A-sublattice (red) and B-sublattice (blue) components of the TB state with energy $e = 0.12507 \times 10^{-2}$ at $\Phi = \Phi_0/3$, belonging to the forbidden solitonic band of the class-II nanoring with $N_w = 16$ [see Fig. 1(b)]. (b) Upper (red) and lower (blue) spinor components for the corresponding state (forbidden band) according to the DKP spectrum [see Fig. 1(d)], reproducing the TB behavior of the class-II nanoring with $N_w = 16$ ($m_0 = 0.18\hbar/v_F^2$). The TB and DKP wave functions for all states of the solitonic band are similar to those displayed here. The wave functions here represent trains of solitons. For contrast, see Fig. 10 in Ref. [20] which schematically portrays the spinor $\Psi_S$ for a single fermionic soliton attached to a Higgs field with a smooth kink-soliton analytic shape $\phi_S(x) = \phi_S(\sqrt{x}/2\phi_0,x)$. $\phi_S(x)$ is a solution [14,20] of the Lagrangian in Eq. (2). (c) A-sublattice (red) and B-sublattice (blue) components of the TB state with energy $e = 0.55636 \times 10^{-2}$ at $\Phi = \Phi_0/3$, associated with the metallic (class-III) nanoring with $N_w = 14$ (see corresponding spectrum in Fig. 1(b) of Ref. [20]). In contrast to the localized-at-theorners topological-insulator wave functions of the semiconducting (class-II) ring in (a), the metallic-aGRG (class-III) wave functions in (c) do not exhibit any localization features and are thus devoid of any TI characteristics. DKP densities in units of $10^{-3}/d$, where $d = 0.35\alpha_0$.](image)
two-band nontrivial one-dimensional TI. In particular, the topological domain with a positive mass $m_0 > 0$ is a trivial insulator with a Chern number equal to zero, while the topological domain with $m_0 < 0$ is a nontrivial TI with a Chern number equal to unity. The localized fermionic kink solitons [Figs. 2(a), 2(b), and 3] at the domain walls (corners of the hexagonal aGROs connecting adjacent arms, i.e., domains with different Chern numbers) correspond to the celebrated TI edge states (end states [31] for 1D systems), used as a fingerprint for the emergence of the TI state. Usually, realization of a TI requires consideration of the spin-orbit coupling, which, however, is negligible for planar graphene. Currently, attempts to enhance the spin-orbit coupling of graphene via adatom deposition are attracting attention [33]. The present findings point to a different direction for realizing a graphene-based TI through the manipulation of the geometry of the honeycomb lattice, which is able to overcome the drawback of negligible spin-orbit coupling.

IV. SUMMARY

In summary, we have advanced and illustrated that the doubly connected, polygonal geometry of graphene rings brings forth, in addition to the celebrated Aharonov-Bohm physics [13,34], an as-yet unexplored platform spawning topological arrangements (including, in particular, the realization of 1D nontrivial topological insulators) for accessing acclaimed one-dimensional relativistic quantum field models [14,17–19]. These include the generation of position-dependent masses, solitonic excitations, and charge fractionization, beyond the constant-mass Dirac and DW fermions. These intriguing phenomena, coupled with advances in the preparation of atomically precise graphene nanostructures [35,36], artificial forms of graphene [8,37], topological insulators [4,5], and graphene mimics in ultracold-atom optical lattices [7], provide impetus [38,39] for further experimental and theoretical endeavors.

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APPENDIX A: TIGHT-BINDING METHOD

To calculate the single-particle spectrum [the energy levels $\varepsilon_i(\Phi)$] of the graphene nanorings in the tight-binding approximation, we use the Hamiltonian

$$H_{\text{TB}} = -\sum_{\langle i,j \rangle} \tilde{t}_{ij} c_i^\dagger c_j + \text{H.c.},$$

with $\langle \cdot \rangle$ indicating summation over the nearest-neighbor sites $i,j$. The hopping parameter

$$\tilde{t}_{ij} = \tau \exp \left[ \frac{ie}{\hbar c} \int_{r_i}^{r_j} ds \cdot A(r) \right],$$

where $r_i$ and $r_j$ are the positions of the carbon atoms $i$ and $j$, respectively, and $A$ is the vector potential (in the Landau gauge) associated with the constant magnetic field $B$ applied perpendicularly to the plane of the nanoring. $\Phi = BS$ is the magnetic flux through the area $S$ of the graphene ring and

the fourth and fifth arms of the hexagon. The DKP modeling closely reproduces this TB solitonic wave function, as seen from the densities of the upper (red) and lower (blue) spinor components of the fermionic field $\Psi$.

A central finding of the paper concerns the emergence of topological-insulator [4,5] aspects in certain classes of semiconducting, as well as of mixed metallic-semiconducting, armchair graphene nanorings. Indeed, it is well established that the Su-Schrieffer-Heeger (SSH) model [15] for polyacetylene (and its Jackiw-Rebbi RQF counterpart [17]) is [29–32] a two-band nontrivial one-dimensional TI.
Φ₀ = ℏc/e is the flux quantum. t = 2.7 eV is the hopping parameter of the two-dimensional graphene.

The derivation of the effective 1D tight-binding equation for an aGR, given in Ref. [21] [see Eq. (6) therein], starts with the 2D TB Hamiltonian here [Eq. (A1) above] and involves Fourier expansions of the wave functions of the A and B sublattices.

**APPENDIX B: DIRAC-KRONIG-PENNEY SUPERLATTICE MODEL**

The building block of the DKP model is a 2 × 2 wave-function matrix Ω formed by the components of two independent spinor solutions (at a point x) of the one-dimensional, first-order generalized Dirac equation [see Eq. (3) above]. Ω plays [22] the role of the Wronskian matrix W used in the second-order nonrelativistic Kronig-Penney model. Following Ref. [22], we use the simple form of Ω in the Dirac representation (α = σ₁, β = σ₃), namely,

\[
\Omega_K(x) = \begin{pmatrix} e^{ikx} & e^{-ikx} \\ \Lambda e^{ikx} & -\Lambda e^{-ikx} \end{pmatrix}
\]

where

\[
K^2 = \frac{(E - V)^2 - m^2 v_F^2}{h^2 v_F^2}, \quad \Lambda = \frac{h v_F K}{E - V + m v_F^2}.
\]

The transfer matrix for a given region (extending between two matching points x₁ and x₂ specifying the potential steps m⁽ⁿ⁾) is the product \( M_K(x_1, x_2) = \Omega_K(x_2) \Omega_K⁻¹(x_1) \); this latter matrix depends only on the width \( x_2 - x_1 \) of the region, and not separately on \( x_1 \) or \( x_2 \).

The transfer matrix corresponding to the \( n \)th arm of the hexagon can be formed [20] as the product

\[
t_n = \prod_{i=1,3} M_K(x_i, x_{i+1}), \quad x_1 = 0, \quad x_4 = L,
\]

with \( L \) being the (common) length on the hexagon arm. The transfer matrix associated with the complete unit cell (encircling the hexagonal ring) is the product

\[
T = \prod_{n=1}^{6} t_n.
\]

Following Refs. [13] and [20], we consider the superlattice generated from the virtual periodic translation of the unit cell as a result of the application of a magnetic field \( B \) perpendicular to the ring. Then the Aharonov-Bohm energy spectra are given as solutions of the dispersion relation,

\[
\cos[2\pi (\Phi/\Phi₀ + 1/2)] = \text{Tr}[T(E)]/2,
\]

where we have explicitly denoted the dependence of the right-hand side on the energy \( E \).

The energy spectra and single-particle densities do not depend on a specific representation. However, the wave functions (upper and lower spinor components of the fermionic field \( \Psi \)) do depend on the representation used. To transform the initial DKP wave functions to the \( (\alpha = \sigma_2, \beta = \sigma_1) \) representation, which corresponds to the natural separation of the tight-binding amplitudes into the A and B sublattices, we successively apply the unitary transformations \( D_{23} = (\sigma_2 + \sigma_1)/\sqrt{2} \) and \( D_3 = \exp(i\pi \sigma_3/4) \).

[23] For nanoribbons with widths in the range considered by us here (see also Ref. [36]), use of the continuous 1D DKP model is appropriate. We note recent broad interest in one-dimensional systems exhibiting topological properties; see, e.g., F. Grusdt, M. Honig, and M. Fleischhauer, Phys. Rev. Lett. 110, 260405 (2013); also Y. E. Kraus, Y. Lahini, Z. Ringel, M. Verbin, and O. Zilberberg, ibid. 109, 106402 (2012).
[36] The experimental challenge of growing armchair nanoribbons with a uniform width has been met by the “bottom-up atomically precise” fabrication approaches; see, e.g., Ref. [35]. Reference [35] not only described the fabrication of atomically precise armchair nanoribbons with a width of seven carbon atoms (semiconductor), but also that of chevron (W-shaped nanowiggles) nanoribbons which include multiple corners. For a theoretical work describing the band structure of atomically precise W-shaped nanoribbons, see E. Costa Girão, L. Liang, E. Cruz-Silva, António Gomes Souza Filho, and V. Meunier, Phys. Rev. Lett. 107, 135501 (2011). The bottom-up fabrication of atomically precise armchair nanoribbons with a width of 7, 14, and 21 carbon atoms has been reported in H. Huang, D. Wei, J. Sun, S. L. Wong, Y. P. Feng, A. H. Castro Neto, and A. T. S. Wee, Sci. Rep. 2, 983 (2012).
[38] Our methodology and analysis can also be applied to bilayer graphene systems, where lattice domain inversions and the formation of solitons have been very recently observed along single and multiple defect lines; see J. S. Alden, A. W. Tsen, P. Y. Huang, R. Hovden, L. Brown, J. Park, D. A. Muller, and P. L. McEuen, Proc. Nat. Acad. Sci. 110, 11259 (2013).