

Impurity effects on Dirac modes in graphene armchair nanoribbons

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We consider finite ribbons of graphene with armchair orientation of their edges to study in detail impurity effects on specific Dirac-like modes. In the framework of Anderson hybrid model of impurity perturbation, a possibility for Mott localization and for opening of a mobility gap under local impurity perturbations is found and analyzed in function of this model parameters: the impurity energy level, its hybridization with the host Dirac modes, and the impurity concentration. Possible electronic phase states in such disordered system and subsequent phase transitions between them are discussed.

Keywords: graphene nanoribbons, armchair edge states, impurity disorder, Anderson model

I. INTRODUCTION

Between electronic properties of two-dimensional (2D) graphene layer, the presence of linear gapless quasiparticle modes, or 2D Dirac modes, is especially notable by defining unusual physical effects in graphene [1–3]. These modes are also a source for even finer, 1D Dirac modes, in graphene nanoribbons [4–6] with special orientation of their edges and special adjustment of their atomic width [7].

A broad family of Dirac semi-metals is of great interest for modern electronics, in particular, their behavior under doping by different impurities and the resulting restructuring of quasiparticle spectrum. Comparing with the known impurity effects in common semiconductors and in 2D graphene, the doped graphene nanoribbons can be expected to permit even higher sensitivity to various external controls and their study may deepen our general knowledge of disorder physics.

This work continues the recent study of impurity effects in graphene nanoribbons [8], focusing on their armchair edge orientation and their width adjusted for presence of Dirac-like modes in the electronic spectrum. In this course, we study various regimes of spectrum restructuring under impurity perturbation in function of perturbation parameters and compare the obtained results with the known such effects in other electronic materials.

The following consideration begins from the description of an armchair graphene nanoribbon (AGNR) and its spectral structure in terms of the second quantization Hamiltonian (Sec. II) and the related Green functions (GFs, Sec. III). The perturbation of Hamiltonian by impurity adatoms within the Anderson hybrid model is

introduced in Sec. IV, giving the solutions for perturbed GFs in the T-matrix form and checking for Mott localization of perturbed quasiparticles. The analysis of possible electronic phase states in doped AGNR in function of perturbation parameters is developed in Secs. V, VI and compared with the known behaviors of analogous electronic materials. The final discussion of the obtained results with suggestions for their possible practical use is presented in Sec. VII. An additional check of the solutions for 1D modes, beyond the T-matrix framework, is done in Appendix.

It is our honour to dedicate this paper to 95th birthday of a prominent solid state theorist Emmanuel Iosifovich Rashba. His brilliant scientific career began in his native city Kyiv, Ukraine's capital, where he studied, worked for a long time and formed as a physicist under an outstanding supervise by S.I. Pecar. Rashba's results in non-ideal molecular crystal optics, in semiconductors theory, and, especially, in spintronics the very emergence of which was mostly due to his discovery of a new type spin-orbit coupling, essentially promoted the understanding of processes and phenomena in electronic systems of various dimensionalities.

II. HAMILTONIAN AND GREEN FUNCTIONS

Graphene armchair nanoribbon can be seen as a periodic sequence of N segments where each segment is a slant stack of M layers (collinear between the segments) and each layer consists of two atomic sites (of graphene a - and b -types, see Fig. 1). The respective local electronic states in m th layer of n th segment are generated by the local operators $a_{n,m}^\dagger$ and $b_{n,m}^\dagger$. Longitudinal translational invariance is imposed through the Born-von Karman closure of the N th to the 1st segment. For an AGNR with M layers (M -AGNR) and the nearest neighbor hopping

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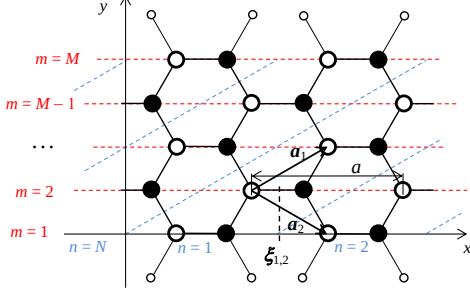


FIG. 1: Graphene nanoribbon with armchair orientation of its edges. Blue dashed lines delimit slant segments $n = 1, \dots, N$. Each segment extends along the graphene elementary translation vector $\mathbf{a}_1$ and includes $m = 1, \dots, M$ layers (red dashed lines) with a -type (white) and b -type (black) atomic sites. The sequence of segments has its longitudinal period $a = |\mathbf{a}_1 + \mathbf{a}_2|$. The carbon dangling bonds at the edges are passivated by hydrogens (small circles).

t , the related tight-binding Hamiltonian reads:

$$H_{tb} = t \left\{ \sum_{n=1}^N \left[\sum_{m=2}^M a_{n,m}^\dagger (b_{n,m} + b_{n-1,m+1} + b_{n,m-1}) + a_{n,1}^\dagger (b_{n,1} + b_{n-1,2}) \right] + \sum_{m=1}^{M-1} a_{1,m}^\dagger b_{N,m+1} + h.c. \right\}. \quad (1)$$

The last sum in Eq. 1 just generates the longitudinal translation invariance and suggests the Fourier-transform to 1D-wave operators. The longitudinal coordinates of a - and b -sites in units of the longitudinal period $a = |\mathbf{a}_1 + \mathbf{a}_2|$ define this transform as:

$$\alpha_{k,m} = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{i(2\pi k/N)(\xi_{n,m}-1/6)} a_{n,m},$$

$$\beta_{k,m} = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{i(2\pi k/N)(\xi_{n,m}+1/6)} b_{n,m}, \quad (2)$$

where $\xi_{n,m} = n + (m + 1)/2$ is the longitudinal coordinate of the center of m th layer from n th segment (see an example in Fig. 1). This readily diagonalizes the Hamiltonian, Eq. 1, in the k numbers. If the AGNR is macroscopically long, $N \rightarrow \infty$, one can pass to a quasi-continuous momentum variable: $2\pi k/N \rightarrow k$ (measured in a^{-1} units). Also, for simplicity, the energy ε will be measured in units of t .

Then the system dynamics in the transversal m -index can be considered at a fixed longitudinal k -momentum, and the overall spectrum structure results qualitatively defined by the AGNR width M . In the known analytic approach by Wakabayashi *et al* [7, 9, 10], $2M$ eigen-states

at given k are taken as running k -waves superposed by standing waves in the transversal q -momentum, subject to the open edge condition (reaching a node when continued by a half-period beyond an AGNR edge). Namely, they are pairs of standing waves with discrete momentum values:

$$q_j = \frac{\pi j}{M+1}, \quad j = 1, \dots, M, \quad (3)$$

being just the combinations (symmetric and antisymmetric in a - and b -sites) of 1D-projected graphene states.

The related eigen-energies are simple uniform 1D-projections of the 2D graphene spectrum for transversal momentum values q_j by Eq. 3:

$$\varepsilon_{j,k} = \sqrt{1 + 4 \cos \frac{k}{2} \cos q_j + 4 \cos^2 q_j}, \quad (4)$$

for conduction sub-bands (and $-\varepsilon_{j,k}$ for valence sub-bands). The 1D Brillouin zone (BZ) for all the $2M$ sub-bands is defined within the $0 \leq k \leq 2\pi$ range and the respective secular determinant reads:

$$\det(\varepsilon - \hat{H}) = \prod_{j=1}^M (\varepsilon^2 - \varepsilon_{j,k}^2). \quad (5)$$

The eigen-state associated to the (j,k) -mode is a combination of the running k -wave and the standing q_j -wave [10] with its amplitudes on a - and b -sites in m -layer:

$$A_m^{(j,k)} = -\frac{e^{-i\varphi_{j,k}}}{\sqrt{M+1}} \sin m q_j,$$

$$B_m^{(j,k)} = \frac{e^{i\varphi_{j,k}}}{\sqrt{M+1}} \sin m q_j, \quad (6)$$

where the phase is defined by the relation:

$$\varphi_{j,k} = \frac{1}{2} \arctan \frac{\sin \frac{k}{2}}{\cos \frac{k}{2} + 2 \cos q_j} + \frac{k}{6}. \quad (7)$$

The standing waves are orthonormalized through the relations:

$$\sum_{j=1}^M \sin m q_j \sin m' q_j = \frac{M+1}{2} \delta_{m,m'},$$

$$\sum_{m=1}^M \sin m q_j \sin m q_{j'} = \frac{M+1}{2} \delta_{j,j'}. \quad (8)$$

Then we construct the eigen-mode operators $\psi_{\pm j,k}$ from the wave operators $\alpha_{m,k}$ and $\beta_{m,k}$ by Eq. 2 in order to reproduce the mode amplitudes by Eq. 6:

$$\psi_{\pm j,k} = \frac{1}{\sqrt{M+1}} \sum_{m=1}^M \sin m q_j (e^{i\varphi_{j,k}} \beta_{m,k} \mp e^{-i\varphi_{j,k}} \alpha_{m,k}). \quad (9)$$

In their basis, the Hamiltonian, Eq. 1, turns fully diagonal:

$$H_{tb} = \sum_{j,k} \varepsilon_{j,k} \left(\psi_{j,k}^\dagger \psi_{j,k} - \psi_{-j,k}^\dagger \psi_{-j,k} \right). \quad (10)$$

By inversion of Eqs. 2, 9, the local operators are expanded in the eigen-mode operators:

$$\begin{aligned} a_{n,m} &= \frac{1}{\sqrt{(M+1)N}} \sum_{j,k} e^{i(k\xi_{n,m} - \varphi_{j,k})} \sin mq_j \\ &\quad \times (\psi_{-j,k} - \psi_{j,k}), \\ b_{n,m} &= \frac{1}{\sqrt{(M+1)N}} \sum_{j,k} e^{i(k\xi_{n,m} + \varphi_{j,k})} \sin mq_j \\ &\quad \times (\psi_{-j,k} + \psi_{j,k}), \end{aligned} \quad (11)$$

which is helpful for the next treatment of AGNR perturbations by local impurity centers.

The notable feature of the spectrum by Eq. 4 is that it contains gapless modes if the AGNR width satisfies a special condition [7]:

$$M+1 = 3\nu, \quad \nu = 1, 2, \dots \quad (12)$$

For such $M = 3\nu - 1$, the mode with $j = 2\nu$ reaches zero energy at the BZ edge $k = 0$ as:

$$\varepsilon_{2\nu,k} = 2 \left| \sin \frac{k}{4} \right| \approx \frac{|k|}{2} \quad (13)$$

(see Fig. 2), and the mode with $j = \nu$ reaches zero energy at the opposite BZ edge $k = 2\pi$ as:

$$\varepsilon_{\nu,k} = 2 \left| \cos \frac{k}{4} \right| \approx \frac{|k - 2\pi|}{2}. \quad (14)$$

The dispersion laws by Eqs. 13, 14 formally coincide

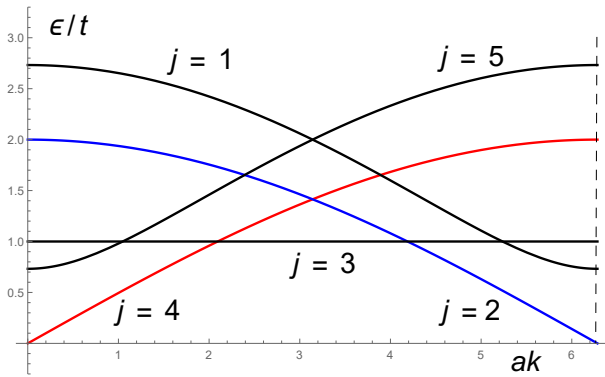


FIG. 2: Energy bands dispersion in 5-AGNR ($\nu = 2$ by Eq. 12), showing the Dirac-like modes with $j = 2, 4$.

with the standard linear dispersion near the Dirac points of 2D graphene, hence they can be seen as definitions of effective 1D Dirac points in $(3\nu - 1)$ -AGNR spectra. All other modes there (with $j \neq \nu, 2\nu$) have finite energy gaps.

III. GREEN FUNCTIONS AND OBSERVABLES

The following consideration goes in the framework of two-time GFs [11, 12] defined by their Fourier transforms:

$$\langle\langle A|B \rangle\rangle_\varepsilon = \frac{i}{\pi} \int_0^\infty dt e^{it(\varepsilon+i0)} \langle\{A(t), B(0)\}\rangle \quad (15)$$

where $A(t) = e^{iHt} A e^{-iHt}$ is a Heisenberg picture operator for the system Hamiltonian H , $\{.,.\}$ is the anti-commutator and $\langle\ldots\rangle$ is the quantum-statistical average. In what follows, the GF's energy subindex is mostly omitted.

Practical calculation of GFs is done through the general equation of motion:

$$\varepsilon \langle\langle A|B \rangle\rangle = \langle\{A(0), B(0)\}\rangle + \langle\langle [A, H] | B \rangle\rangle, \quad (16)$$

involving the commutator $[.,.]$. So found GFs generate the physical observable quantities (the averages of operator products) through the spectral relation:

$$\langle AB \rangle = \frac{1}{\pi} \text{Im} \int_0^\infty \langle\langle B|A \rangle\rangle_\varepsilon d\varepsilon. \quad (17)$$

In the present case, the system electronic properties can be obtained from the $2M \times 2M$ GF matrix $\hat{G}(k, k')$ with its matrix elements $G_{j,j'}(k, k') \equiv \langle\langle \psi_{j,k} | \psi_{j',k'}^\dagger \rangle\rangle$ built from the eigen-mode operators by Eq. 9 where the j -indices count the transversal momenta as by Eq. 3 and also their opposites $-j$ ($2M$ altogether).

For the unperturbed AGNR system with its diagonal Hamiltonian, Eq. 10, the above defined GF matrix results also diagonal: $G_{j,j'}^{(0)}(k, k') = \delta_{j,j'} \delta_{k,k'} G_{j,k}^{(0)}(\varepsilon)$, with its diagonal elements called propagators:

$$G_{j,k}^{(0)}(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_{j,k}}. \quad (18)$$

They define an important observable, the density of quasiparticle states (DOS), as a sum $\rho(\varepsilon) = \sum_{j=1}^M \rho_j(\varepsilon)$ where a partial contribution from $(j, -j)$ subbands is:

$$\rho_j(\varepsilon) = \frac{2}{\pi} \sum_k \text{Im} \left[G_{j,k}^{(0)}(\varepsilon) + G_{-j,k}^{(0)}(\varepsilon) \right] \quad (19)$$

(including the implicit factor 2 for electron spins). Using Eqs. 4, 18 and passing from sum in k to integral:

$$\frac{1}{N} \sum_k f(k) = \frac{1}{2\pi} \int_0^{2\pi} f(k) dk, \quad (20)$$

gives this contribution as:

$$\rho_j(\varepsilon) = \frac{8|\varepsilon|}{\pi(M+1) \sqrt{(\varepsilon^2 - \varepsilon_{-,j}^2)(\varepsilon_{+,j}^2 - \varepsilon^2)}}, \quad (21)$$

where $\varepsilon_{\pm,j} = 1 \pm 2 \cos q_j$ are the j th subband energy limits.

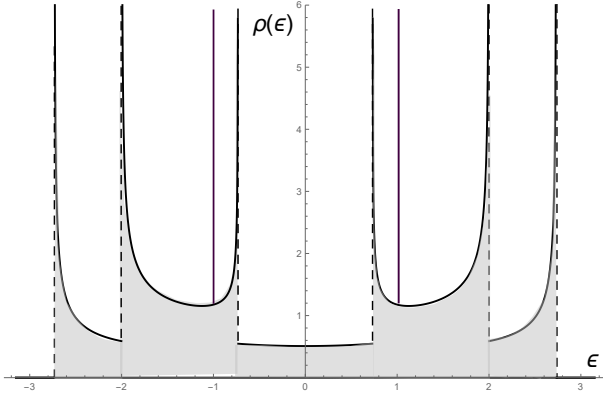


FIG. 3: Density of states in 5-AGNR. Almost constant value $\approx 4/(3\pi)$ within the low energy range, $|\varepsilon| \leq \sqrt{3} - 1$, comes from the Dirac-like ($j = 2, 4$) subbands.

In particular, for the most relevant here Dirac-like modes with $\varepsilon_{+, \nu} = \varepsilon_{-, 2\nu} = 2$, $\varepsilon_{+, 2\nu} = \varepsilon_{-, \nu} = 0$, we have:

$$\rho_{\nu}(\varepsilon) = \rho_{2\nu}(\varepsilon) = \frac{4}{3\pi\nu\sqrt{1 - (\varepsilon/2)^2}}, \quad (22)$$

so DOS results almost constant at low energies: $\rho(\varepsilon) \approx \rho(0) \equiv \rho_0 = 8/(3\pi\nu)$ at $|\varepsilon| \ll 1$, as seen in the case of 5-AGNR presented in Fig. 3.

IV. IMPURITY PERTURBATIONS

The local impurity perturbations in graphene nanoribbons of both zigzag and armchair types were recently considered within two basic impurity models: the one-parameter Lifshitz model (LM) [13], more adequate for substitutional impurities, and the two-parameter Anderson hybrid model (AM) [14], for impurity adatoms [8]. For zigzag structures, the overall conclusion was about their eigen-modes stability (topological protection) against quasiparticles localization by the impurity disorder, both in LM and AM models.

However such localization was found in AGNRs with LM impurities, though reduced in that case to a narrow vicinity of the Dirac point (zero energy). But this already opens a possibility for Mott's metal/insulator phase transitions in a nanosystem and generates the next interest for studying AGNR behavior under more diversified AM perturbations. In the latter case, a more complicated intermittence of conducting and localized states in other ranges of energy spectrum and a broader variety of related phase states for this 1D system can be expected. Then it would be also of interest to compare such effects with the known analogs for 3D and 2D electronic systems under impurity disorder.

The following consideration is focused on special $(3\nu - 1)$ -AGNRs and restricted to only their Dirac-like modes. Since these modes with $j = \nu$ and 2ν give identical and

independent contributions to the spectrum, one can next focus on a single Dirac-like mode, say $j = 2\nu$, then denoting $\psi_{2\nu, k} \equiv \psi_{+, k}$ and $\psi_{-2\nu, k} \equiv \psi_{-, k}$. Consequently, the above introduced $\hat{G}(k, k')$ matrix gets reduced to the 2×2 form in the basis of $\psi_{\pm, k}$ operators. In particular, the non-perturbed solution, Eq. 18, presents here as $\hat{G}^{(0)}(k, k') = \delta_{k, k'}(\varepsilon - \varepsilon_k \hat{\sigma}_3)^{-1}$ with $\varepsilon_k \equiv \varepsilon_{2\nu, k}$ by Eq. 13 and the Pauli matrix $\hat{\sigma}_3$ in $\pm$ indices.

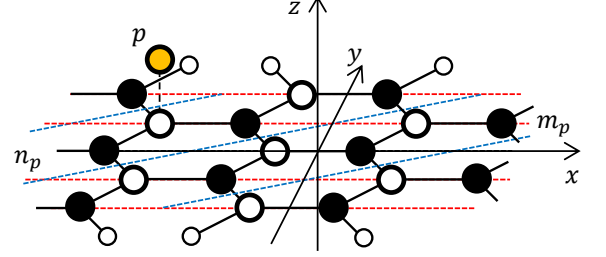


FIG. 4: Position p of a top impurity adatom over an a -site in m_p -layer from n_p -segment of 5-AGNR.

Then we consider the impurity adatoms location restricted to the simplest top-positions: p_a over an a -type host atom in m_p layer from n_p segment (see Fig. 4) or p_b over a b -type host atom.

In these notations, the AM perturbation Hamiltonian reads:

$$H_{AM} = \sum_p \left\{ \varepsilon_{res} c_p^\dagger c_p + \frac{\omega}{\sqrt{3\nu N}} \sum_k \left[\sin \frac{\pi m_p}{3} \times e^{i(k\xi_p \mp \phi_k)} c_p^\dagger (\psi_{-, k} \mp \psi_{+, k}) + \text{h.c.} \right] \right\}, \quad (23)$$

where a local impurity operator c_p with its resonance level ε_{res} is coupled to the Dirac-like modes $\pm \varepsilon_k$ through the hybridization ω with the neighbor host atom at the longitudinal position $\xi_{n_p, m_p} - 1/6$ for its a -type as in Fig. 4 (or $\xi_{n_p, m_p} + 1/6$ for its b -type).

Then the complete Hamiltonian $H_{tb} + H_{AM}$ generates a perturbation of the GF matrix: $\hat{G}^{(0)} \rightarrow \hat{G}$. In its simplest form, this is given by the T-matrix approximation:

$$\hat{G} = \left(\varepsilon - c\hat{T}(\varepsilon) - \varepsilon_k \hat{\sigma}_3 \right)^{-1}, \quad (24)$$

where $c = (2MN)^{-1} \sum_p 1$ is the impurity concentration and the T-matrix in this case results diagonal:

$$\hat{T}(\varepsilon) \equiv T(\varepsilon) = \frac{\omega^2}{2} \left(\varepsilon - \varepsilon_{res} - \frac{i\omega^2}{4f\sqrt{1 - (\varepsilon/2)^2}} \right)^{-1}. \quad (25)$$

Then the modified dispersion law $\tilde{\varepsilon}_k$ follows from the standard GF secular equation $\text{Re}[\det(\hat{G})^{-1}] = 0$ [15] as:

$$\tilde{\varepsilon}_k = \sqrt{\varepsilon_k^2 + (c \text{Im} T(\varepsilon))^2 + c \text{Re} T(\varepsilon)}, \quad (26)$$

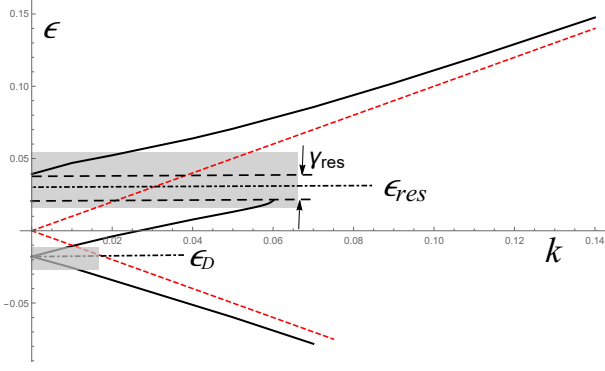


FIG. 5: Dispersion law for the Dirac-like modes in 5-AGNR having AM impurities with their parameters $\varepsilon_{res} = 0.03$, $\omega = 0.3$, and concentration $c = 0.02$. For comparison, the unperturbed Dirac-like modes are shown by the red dashed lines.

and its solution for 5-AGNR at the choice of AM impurity parameters $\varepsilon_0 = 0.03$ and $\omega = 0.3$, corresponding to Cu adatoms in top position [16], is presented in Fig. 5. Here the characteristic impurity effects are seen as:

1) the shift of the Dirac point from its initial zero energy position down to

$$\varepsilon_D \equiv \tilde{\varepsilon}_{k=0} \approx \frac{\varepsilon_{res} - \sqrt{\varepsilon_{res}^2 + 2c\omega^2}}{2}, \quad (27)$$

2) the resonance splitting between the initial linear ε_k law and the impurity resonance level ε_{res} until its vicinity of width

$$\gamma_{res} \approx \omega \sqrt{\frac{c - c_0}{2}}. \quad (28)$$

where $c_0 \sim \omega^2/(8\nu^2)$ is the critical concentration value for this splitting to appear.

Also an anomalous negative dispersion formally appears inside this vicinity, at $|\varepsilon - \varepsilon_{res}| \lesssim \gamma_{res}$, but this range occurs unphysical when validity of the modified dispersion law is checked with the Ioffe-Regel-Mott (IRM) criterion for conducting states [17, 18]:

$$k \frac{\partial \tilde{\varepsilon}_k}{\partial k} \gtrsim c \text{Im } T(\tilde{\varepsilon}_k). \quad (29)$$

This simply means that the quasiparticle lifetime (inverse of the r.h.s) is longer than its oscillation period (inverse of the l.h.s) and such quasiparticles are conductive indeed, otherwise they are localized near impurity sites. The explicit form of the IRM criterion for the dispersion law by Eq. 26 and the T-matrix by Eq. 25 reads:

$$\frac{2}{\partial \ln \text{Re} [\varepsilon - cT(\varepsilon)]^2 / \partial \varepsilon} \gtrsim c \text{Im } T, \quad (30)$$

All the energy ranges where this inequality does not hold are attributed to localized states so the dispersion law by Eq. 26 for conducting states does not apply there.

The mobility edges between conducting and localized states can be qualitatively estimated as the ε values that make the relation of Eq. 30 an equality. The results of such numerical estimation at the choice of AM parameters as for Cu top impurities are shown in Fig. 6a. They illustrate formation of two mobility gaps (ranges of localization), one around ε_{res} and another around ε_D . Their width grows with the impurity concentration c : the first as $\sim 2\gamma_{res}(c)$ (by Eq. 28) and the second as $\gamma_D \approx c\omega^4/[8\nu(\varepsilon_D - \varepsilon_{res})^2]$.

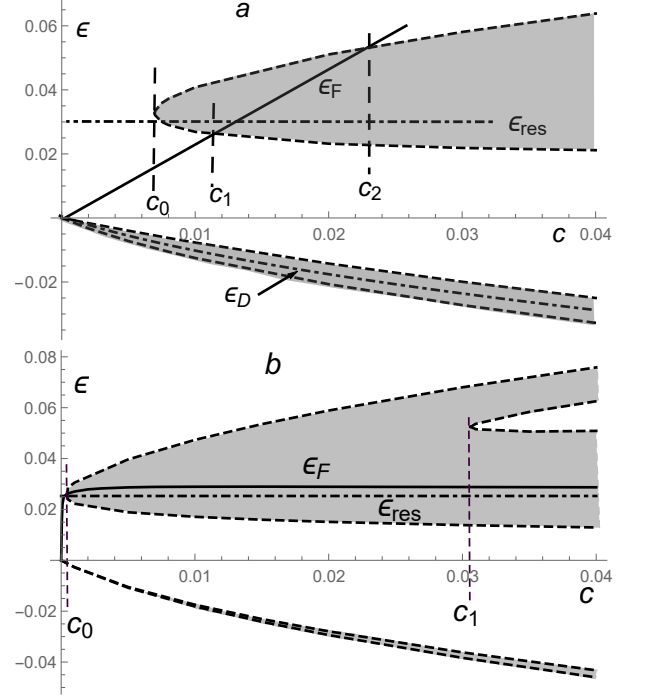


FIG. 6: a) Mobility gaps (in meV scale) in function of impurity concentration c at the choice of AM parameters as in Fig. 5. Special concentration values refer respectively: c_0 to opening of mobility gap near the resonance level ε_{res} , c_1 to metal/insulator, and c_2 to insulator/metal transitions (see below). b) Analogous developments for the same impurities in 2D graphene, note here opening of a spectrum quasi-gap inside the mobility gap at c_1 , absent in AGNR.

Validity of the above T-matrix description is confirmed with an additional check beyond the frame of this simplest approximation (see in Appendix).

An important issue for such disordered AGNRs is how the positions of mobility edges compare with that of the Fermi level *vs* impurity concentration, $\varepsilon_F(c)$. The latter results from an extra amount of c charge carriers by impurities (per host atom) being filled into the relevant subbands:

$$\int_0^{\varepsilon_F(c)} \rho(\varepsilon) d\varepsilon = c. \quad (31)$$

Notably, the above indicated low energy DOS, $\rho(\varepsilon) \approx \rho_0$, holds its constancy even under impurity disorder, as seen

from stability of Eq. 22 at the passing $\varepsilon \rightarrow \varepsilon - cT(\varepsilon)$ since $|\varepsilon - cT(\varepsilon)| \ll 1$ for all $|\varepsilon| \ll 1$, one of the main specifics of this 1D-like system.

Then from Eq. 31 we come to a simple linear relation $\varepsilon_F(c) \approx c/\rho_0$. Such behavior superposed onto the diagram of mobility gaps in Fig. 6a shows a possibility for ε_F to cross the mobility edges near ε_{res} , both into and out of this mobility gap. Then an intermittency of the related metal/insulator transitions (MIT) can be expected.

It is of interest to compare these AGNR results with their analogs for the same impurities in 2D graphene (Fig. 6b). Besides a general similarity of two pictures, they also present substantial differences. First of all, the estimated critical concentration for localization on Cu impurities in 5-AGNR, $c_0 \approx 7 \cdot 10^{-3}$, is more than an order of magnitude higher than its analog for the 2D case, $c_0^{(2D)} \approx 4 \cdot 10^{-4}$ [16]. This can be explained by the higher and almost constant low-energy DOS for the 1D Dirac-like modes: $\rho_0 \sim 1$, compared to its linear in ε smallness for the 2D Dirac modes: $\rho_{2D}(\varepsilon) \approx 4\varepsilon/(\pi\sqrt{3}) \ll 1$.

Another difference is in behaviors of $\varepsilon_F(c)$ for each system, also caused by that of DOS. From Eq. 31, its almost linear growth in AGNR: $\varepsilon_F(c) \approx c/\rho_0$ is much slower than the very fast, square root initial growth of $\varepsilon_F^{(2D)}(c) \approx \sqrt{c\pi\sqrt{3}/2}$ in 2D graphene. This defines a much higher threshold in c for occurrence of MIT in AGNR: $c_1 \sim \varepsilon_{res}\rho_0$, than in 2D graphene: $\sim c_0^{(2D)}$. But the constancy of AGNR DOS, even in presence of impurities, permits the linear $\varepsilon_F(c)$ growth to persist also for $c > c_1$ and then an inverse MIT to occur at its emergence from the mobility gap at $c = c_2 \sim \varepsilon_{res}\rho_0 + (\omega\rho_0)^2$. In contrary, the 2D graphene DOS presents a sharp resonance peak near ε_{res} and the Fermi level, when approaching this peak at $c \rightarrow c_0^{(2D)}$, gets fixed here, defining insulating phase for all $c > c_0^{(2D)}$.

At least, the critical concentration c_0 by Eq. 28 that defines the onset of localization near ε_{res} , indicates it to occur earlier for weaker impurity-host coupling ω .

V. ELECTRONIC PHASE STATES AND THEIR TUNING

An important physical issue is to determine the system electronic phase states. For the considered nanoribbons, this refers first of all to their electric conductivity.

In the limit of zero temperature, it is fully defined by the Fermi level position with respect to the spectrum mobility edges: implying the metallic state for ε_F out of the mobility gaps and the insulating state for ε_F inside them. Thus, from the diagram in Fig. 6, the system of 5-AGNR with given concentration c of Cu impurities is expected to be metallic if $0 < c < c_1$ or $c > c_2$ and insulating if $c_1 < c < c_2$.

But a practical interest arises in an effective tuning of possible MIT's at a given impurity composition (in analogy with the common gate controls in doped semi-

conductors). First of all, the initial composition can be chosen to set the Fermi level close enough to a mobility edge, for instance, $\varepsilon_F < \varepsilon_g < \varepsilon_{res}$ and $\varepsilon_F - \varepsilon_g \ll \varepsilon_{res}$. Then several factors can be considered for MIT tuning: 1) temperature (in terms of its inverse β), 2) magnetic field, $\mathbf{h}$, and 3) electric field, $\mathbf{E}$.

The temperature control will result from the interplay between the metallic conductivity $\sigma_{met}(\beta)$, due to extended states, and the hopping conductivity $\sigma_{hop}(\beta)$, due to localized states.

The first type refers to the Kubo-Greenwood formula written here as:

$$\sigma_{met}(\beta) \approx \rho_0 \int_0^{\varepsilon_g} [1 - (\varepsilon/2)^2] \tau(\varepsilon) \frac{\partial n(\varepsilon, \beta)}{\partial \varepsilon} d\varepsilon, \quad (32)$$

where $n(\varepsilon, \beta) = [e^{\beta(\varepsilon - \varepsilon_F)} + 1]^{-1}$ is the standard Fermi function and the lifetime $\tau(\varepsilon) = [\tau_{imp}^{-1}(\varepsilon) + \tau_{ph}^{-1}(\varepsilon)]^{-1}$ involves:

$\tau_{imp}^{-1}(\varepsilon) = c|\text{Im } T(\varepsilon)|$ (β -independent) due to impurities, and

$\tau_{ph}^{-1}(\varepsilon) \sim 1/\beta\Theta_D$, due to 1D phonons (with the Debye temperature Θ_D).

The second type refers to the Mott formula written for an 1D system:

$$\sigma_{hop}(\beta) \propto e^{-\sqrt{\beta T_0}}, \quad (33)$$

where $T_0 \sim \tau^{-1}(\varepsilon_F)/\rho(\varepsilon_F)$. Interplay of this decreasing $\sigma_{hop}(\beta)$ and the growing $\sigma_{met}(\beta)$ by Eq. 32 results in an overall conductivity maximum at $\beta \sim 1/|\varepsilon_F - \varepsilon_g|$, but having a comparable temperature width. So, this crossover between the types of conductivity is not yet a canonical phase transition.

But a true electronic phase transition at zero temperature can be realized, for instance, applying a uniform static magnetic field $\mathbf{h}$ to AGNR. This will produce a spin splitting of the Dirac-like subbands defined in Sec. III and also of the impurity levels, implying respective splitting of IRM critical points for spin subbands.

At the same time, the position of overall Fermi level for a given impurity concentration c will stay the same as it was for $h = 0$, due to the persisting constancy of the overall DOS. Then, in the situation of several overlapping subbands, the overall mobility edges are determined by the Mott principle: if, at a given energy, there is at least one state extended, all other states at this energy are also extended. Then the overall mobility gap is formed by the intersection of partial (formal) gaps for each spin projection and it gets reduced with growing splitting $\mu_B h$. In this way, the overall mobility edges are tuned by the applied field and MIT is realized at its critical value $h_{cr} \sim |\varepsilon_F - \varepsilon_g|/\mu_B$ (see Fig. 7a). But for the relevant energy scales of several meV, this may require high enough h values of several tens Tesla.

An alternative way may be sought in applying a static electric field $E_y \equiv E$ across the nanoribbon (along the y -axis in Figs. 1, 4) to produce linearly growing local potentials $V_m = meE$ on m -layers. This can be shown not

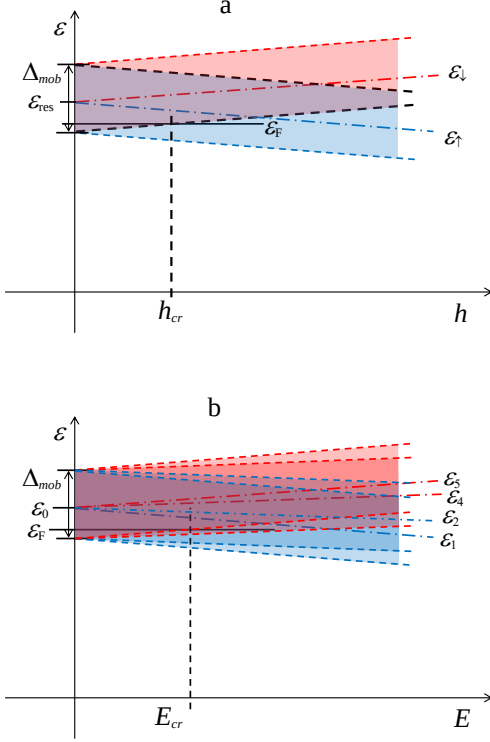


FIG. 7: Realization of MIT in AGNR with Cu top impurities by tuning of the composed mobility edges: a) with an applied magnetic field or b) with an applied electric field (here for $M = 5$).

to influence the relevant Dirac-like subbands, however to produce an M -fold splitting between the local energy levels for impurities on different m -layers and so between the respective mobility gaps, with a subsequent decrease of the resulting mobility gap (as in Fig. 7b). The critical fields to achieve MIT in this case, $E_{cr} \sim |\varepsilon_F - \varepsilon_g|/(eM)$ of some mV/nm, could be reached with no experimental difficulties.

VI. SPIN-ORBIT EFFECTS ON ELECTRONIC PHASE STATES

Yet one more tuning mechanism can result from the spin-orbit (SO) effect, including the Rashba spin-orbit coupling [19]. The latter is generally known to lift the spin degeneracy in the systems with broken mirror symmetry, for instance, under electric field E_z , applied normally to the crystal surface [20] or to the 2D graphene plane (along the z -axis in Fig. 4) [21, 22]. A similar effect can be achieved in graphene nanotubes [23, 24] and also in AGNRs [25].

For the AGNR case, we note that the relevant Dirac-like $\psi_{\pm,k}$ modes (from Eq. 23) have their amplitudes $\sin m\frac{\pi}{3}$ equal zero at each third m -layer, so the interlayer

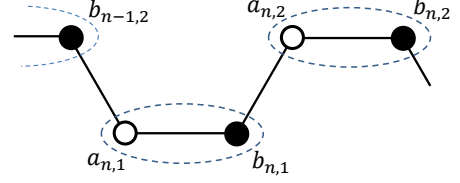


FIG. 8: Coupled pair of $m = 1, 2$ layers in AGNR.

couplings through these modes are restricted to the m -pairs: $(1, 2), (4, 5), \dots, (M-1, M)$, and their overall effect on AGNR can be represented by a single pair, for instance, with $m = 1, 2$ (see Fig. 8). All the couplings in such a pair of layers are suitably presented in terms of local operators, now equipped with explicit $\uparrow\downarrow$ spin indices and then composed into 4-spinors:

$$f_{n,m} = \begin{pmatrix} a_{n,m,\uparrow} \\ a_{n,m,\downarrow} \\ b_{n,m,\uparrow} \\ b_{n,m,\downarrow} \end{pmatrix}. \quad (34)$$

In the basis of these local spinors, the SO Hamiltonian reads:

$$H_{SO} = \sum_n \left[f_{n,1}^\dagger \hat{H}_{SO} (f_{n,1} + f_{n,2} + f_{n-1,2}) + f_{n,2}^\dagger \hat{H}_{SO} (f_{n,2} + f_{n,1} + f_{n+1,1}) \right], \quad (35)$$

where the 4×4 matrix:

$$\hat{H}_{SO} = \Delta \hat{\sigma}_z + \lambda (\hat{\sigma}_x \hat{\tau}_y - \hat{\sigma}_y \hat{\tau}_x).$$

includes the Pauli matrices $\hat{\sigma}_j$ in spin $\uparrow, \downarrow$ -indices and $\hat{\tau}_j$ in sublattice a, b -indices and also the parameters Δ for standard SO and λ for Rashba SO (the latter being E_z -dependent). The estimates for these local SO couplings in 2D graphene (also plausible for nanoribbons) show the standard $\Delta \sim 10^{-4}$ [21], fixed and much smaller of the relevant energy scales for MIT crossing. Otherwise, the Rashba λ can be strongly enhanced [26] and yet tunable [21], so it is taken as an effective SO variable below.

Next, we pass to the basis of chain-wave 4-spinors:

$$\psi_k = \begin{pmatrix} \psi_{+,k,\uparrow} \\ \psi_{+,k,\downarrow} \\ \psi_{-,k,\uparrow} \\ \psi_{-,k,\downarrow} \end{pmatrix}, \quad (36)$$

which are related to the local spinors by Eq. 34 (with $m = 1, 2$) through a $\hat{\tau}$ -rotation:

$$f_{n,m} = \frac{(-1)^{m-1}}{2\sqrt{\nu N}} \sum_k e^{ik\xi_{n,m}} \hat{U}_k \psi_k. \quad (37)$$

Here the rotation matrix:

$$\hat{U}_k = \cos \phi_k (\hat{\tau}_x - \hat{\tau}_z) + \sin \phi_k (\hat{\tau}_y + i\hat{\tau}_0), \quad (38)$$

results from Eq. 11 (restricted to single $j = 2\nu$) for the components of $f_{n,m}$. At relevant $|k| \ll 1$, the phase $\phi_k \equiv \phi_{2f,k}$ is approximated as $\phi_k \approx \phi_0 = -\pi/4$. Then the Dirac-like part of SO Hamiltonian reads:

$$H_{SO} = \sum_k \psi_k^\dagger [-\Delta \hat{\sigma}_z \hat{\tau}_x + \lambda (\hat{\sigma}_x \hat{\tau}_z + \hat{\sigma}_y \hat{\tau}_y)] \psi_k, \quad (39)$$

and, together with the Dirac-like part of H_{tb} by Eq. 10, it defines the SO-split dispersion laws (in neglect of impurity disorder):

$$\varepsilon_{\pm,k} = \sqrt{\varepsilon_k^2 + \Delta_{\pm}^2}. \quad (40)$$

Here the non-zero bandgaps:

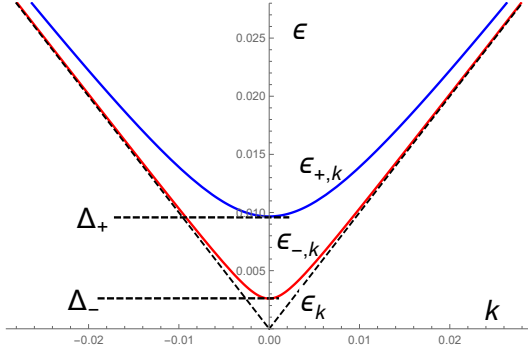


FIG. 9: SO splitting of the Dirac-like mode ε_k (dashed lines) into $\varepsilon_{\pm,k}$ at the choice of $\lambda = 5 \cdot 10^{-3}$ and $\Delta = 2.5 \cdot 10^{-4}$.

$$\Delta_{\pm} = \sqrt{\Delta^2 + \lambda^2 (2 \pm \sqrt{3})}, \quad (41)$$

are due to both SO types but their splitting is only due to the Rashba SO as shown in Fig. 9 for the choice of SO parameters $\Delta = 2.5 \cdot 10^{-4}$ [21] and $\lambda = 5 \cdot 10^{-3}$ [26], and they create the low-energy DOS singularities:

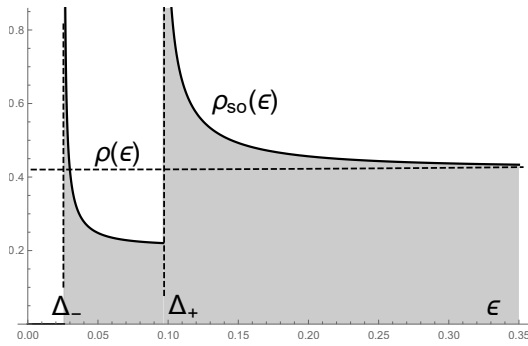


FIG. 10: Singularities of the low-energy DOS of 5-AGNR with split subbands at the same choice of SO parameters as in Fig. 9.

$$\rho_{so}(\varepsilon) = \frac{\varepsilon \rho_0}{2} \left[\frac{\theta(\varepsilon - \Delta_+)}{\sqrt{\varepsilon^2 - \Delta_+^2}} + \frac{\theta(\varepsilon - \Delta_-)}{\sqrt{\varepsilon^2 - \Delta_-^2}} \right], \quad (42)$$

as shown in Fig. 10.

Such DOS behavior, instead of its almost constancy at no account of SO (by Eq. 22), when used in Eq. 31 leads to the λ -dependence of the Fermi level given by the equation:

$$\sqrt{\varepsilon_F^2 - \Delta_+^2} + \sqrt{\varepsilon_F^2 - \Delta_-^2} \approx 2c/\rho_0. \quad (43)$$

Its numerical solution defines MIT to occur when λ reaches a certain critical value λ_{cr} as shown in Fig. 11.

Noting that for all relevant impurity concentrations $c > c_0$ we have $c/\rho_0 \gg \Delta$, the approximate solution of Eq. 43 for $\lambda \ll c/\rho(0)$ reads:

$$\varepsilon_F(\lambda) \approx \frac{c}{\rho_0} + \frac{\rho_0}{c} (\Delta^2 + 2\lambda^2). \quad (44)$$

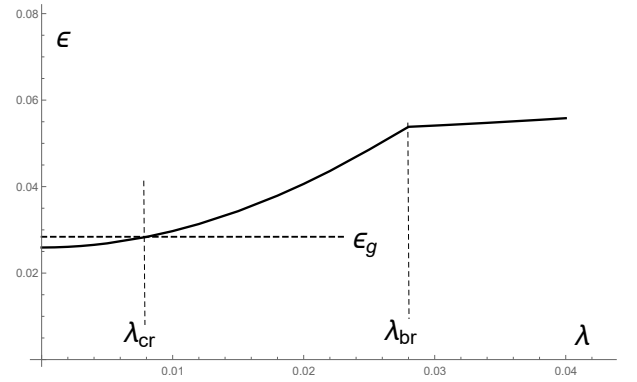


FIG. 11: Dependence of the Fermi level on Rashba SO coupling for 5-AGNR with Cu top impurities concentration fixed at $c = 0.011$, its crossing with the mobility edge ε_g at $\lambda = \lambda_{cr} \approx 0.0078$ indicates an SO-tuned MIT to occur.

This quadratic λ -dependence relates to filling of both $\varepsilon_{\pm,k}$ subbands by c charge carriers, it follows the lowest part of the numerical solution in Fig. 11. With further growing λ , a break of $\varepsilon_F(\lambda)$ occurs when it gets intercepted by the faster growing upper bandgap ε_+ at the break value $\lambda_{br} = c/(\sqrt{2}\sqrt{3}\rho_0)$. The next slower $\varepsilon_F(\lambda)$ growth at $\lambda > \lambda_{br}$ relates to filling of only the lower subband which is expressed as:

$$\varepsilon_F(\lambda) = \sqrt{(c/\rho_0)^2 + \Delta^2 + (2 - \sqrt{3})\lambda^2}. \quad (45)$$

Notably, for the considered case of Cu top impurities, both the impurity resonance ε_{res} and the mobility edge ε_g lie in the energy range $\varepsilon \gg \varepsilon_{\pm}$ where $\rho_{SO}(\varepsilon)$ already reaches its asymptote $\approx \rho(0)$, so the mobility gap structure stays practically insensitive to Rashba SO. Hence a possibility arises here for MIT to be realized by SO tuning of ε_F at fixed ε_g , unlike the above considered regimes with tuning of mobility edges at fixed Fermi level.

Notably, this tuning process can be realized in a combined way: a rough "tuning" of ε_F closeness to ε_g by a proper choice of impurity parameters ε_{res} , ω , c and also

by a strong structural contribution to the Rashba parameter λ , say, from a gold substrate atomic field [26], and then its fine tuning by an applied external field. Evidently, the expected MIT at such sub-meV energy scales would require a range of liquid He temperatures for its sufficient resolution.

VII. DISCUSSION

The obtained results demonstrate how the difference of electronic states in graphene nanoribbons defined by their edge orientations is reflected in their stability against impurity disorder. Physically, this opens the possibility for specific electronic phase transitions and for their controls by combining the disorder and external bias effects.

It is of interest to compare the above picture of 1D spectrum reconstruction under AM impurity disorder with the known such effects in 3D and 2D systems. This comparison can be done between the corresponding correlators, defined by the system dimensionality and low energy quasiparticles dispersion. For instance, such a correlator in 3D semiconductors (quadratic dispersion) [34], decays with distance r as: $\propto (\sin \sqrt{\epsilon}r)/(\sqrt{\epsilon}r)$, a similar behavior for 3D acoustic phonons (linear dispersion) [35] is found as: $\propto (\sin \epsilon r)/(\epsilon r)$, and it is modified to $\propto (\sin \epsilon r)/\sqrt{\epsilon r}$ in 2D graphene with linear Dirac dispersion [16]. All these systems admit both extended and localized quasiparticles based on impurity states [32]. But, unlike all those, a constancy or only a weak exponential decay of correlators are found for the present AGNR case

(see Eqs. A2, A6 below) which defines the complete localization of all the states near ϵ_{res} (as in Fig. 6a, unlike the 2D graphene case in Fig. 6b). Another AGNR specifics, the low-energy DOS constancy, defines a higher sensitivity of Fermi level to doping and so more possibilities for tuning of the system electronic properties.

The present study was limited to the simplest framework of tight-binding model for pure nanoribbons and simplest models for impurity perturbations on them. In principle, it can be extended to account for many other physical factors, as electron-electron Hubbard correlations, spin-ordering effects, phonon and spinon excitations, etc.

Also, the effects from passivating hydrogens, known to be commonly present at the edges of experimental nanoribbon samples [27–30], may influence the dynamics of host nanoribbon carriers. This factor can be naturally included into the above developed Hamiltonians and resulting GFs, to be possibly an object of future study. At least, an experimental check for the suggested effects, for instance, on carriers mobility and its collapse under definite external factors should be of considerable interest.

Acknowledgments

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Appendix A: Beyond the T-matrix

Validity of the above T-matrix solution should be yet verified in view of the effective 1D character of the relevant Dirac-like quasiparticles. It is known that generic 1D systems are unstable against any disorder, up to a full localization of all their eigen-states [31], and the IRM check with use of the simplest (single-impurity) T-matrix is not sufficient to detect this. Therefore the IRM results from Sec. III need a support by some T-matrix extensions known for many other disordered systems. There are two such possible extensions:

1) group expansions (GEs) in clusters of correlated impurity centers [32] and

2) self-consistent T-matrix approximation [33].

For GEs, their basic elements are the correlators, defined for different GE forms. The simplest form is that of non-renormalized GE, known to better apply for the energy ranges of localized states. Here the correlator for the considered Dirac-like quasiparticles is written as:

$$A_r(\varepsilon) = \frac{2T(\varepsilon)}{3\nu N} \sum_k e^{ikr} \left(\frac{1}{\varepsilon - \varepsilon_k} + \frac{1}{\varepsilon + \varepsilon_k} \right) \quad (\text{A1})$$

(taking into account equal contributions from $j = \nu$ and $j = 2\nu$ modes). Then, after integration in k by Eq. 20, the related integral has its long distance asymptotics at $r \gg 1$ as:

$$A_r(\varepsilon) = \frac{2T(\varepsilon)\varepsilon}{3\pi\nu} \int_{-\pi}^{\pi} \frac{e^{ikr} dk}{\varepsilon^2 - 4\sin^2 k/2} \approx \frac{2T(\varepsilon)\varepsilon}{3\nu} \sin \varepsilon r, \quad (\text{A2})$$

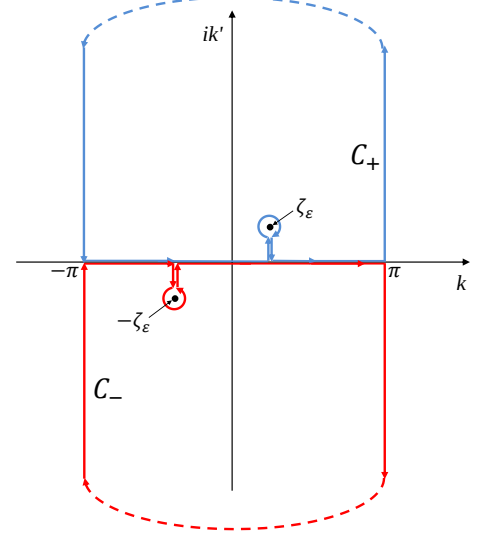


FIG. 12: Integration contours for calculation of the renormalized correlator $\tilde{A}_r(\varepsilon)$, Eq. A3: C_+ (blue lines) for $r > 0$ and C_- (red lines) for $r < 0$.

that is non-decaying. This contrasts with the decaying correlators in 3D and 2D systems and makes all the GE terms for the 1D-like system formally divergent. To avoid that problem, some alternative, renormalized GE forms (more adequate for conductive states) could be employed.

For instance, the first order renormalization for GE is obtained with the simple change, $\varepsilon \rightarrow \varepsilon - cT(\varepsilon)$ in the denominators of Eq. A1. Then the renormalized correlator $\tilde{A}_r(\varepsilon) = 2T(\varepsilon)[\varepsilon - cT(\varepsilon)]\tilde{I}_r(\varepsilon)/(3\nu)$, involves the integral:

$$\tilde{I}_r(\varepsilon) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{ikr} dk}{[\varepsilon - cT(\varepsilon)]^2 - 4\sin^2 k/2}. \quad (\text{A3})$$

This can be found analytically, passing to complex momentum: $k \rightarrow \zeta = k + ik'$ and extending integration to one of the closed contours shown in Fig. 8, depending on the 1D correlator direction. The forward direction, $r > 0$, relates to C_+ (blue lines) with the pole $\zeta_\varepsilon = 2\arcsin[\varepsilon - cT(\varepsilon)]/2$, and the backward direction, $r < 0$, does to C_- (red lines) with the pole $-\zeta_\varepsilon$.

The contour integral for the forward case:

$$\frac{1}{2\pi} \oint_{C_+} \frac{e^{i\zeta r}}{\varepsilon - cT(\varepsilon) - 2\sin \zeta/2} d\zeta, \quad (\text{A4})$$

presents a zero sum of three terms: $0 = I_r(\varepsilon) + R_r(\varepsilon) + V_r(\varepsilon)$. Here the residue term, $R_r(\varepsilon) = e^{i\zeta_\varepsilon r} / \cos(\zeta_\varepsilon/2)$, and the term from the semi-infinite vertical segments, $V_r(\varepsilon) \approx (2i \sin \pi r) / [(1 - \varepsilon)r]$, define the sought correlator

as:

$$\tilde{A}_r(\varepsilon) = \frac{2T(\varepsilon)[\varepsilon - cT(\varepsilon)]}{3f} \times \left[\frac{e^{i\zeta_\varepsilon r}}{\cos(\zeta_\varepsilon/2)} + 2i \frac{\sin \pi r}{(1 - \varepsilon)r} \right]. \quad (\text{A5})$$

For the low energy range, $|\varepsilon|, c|T(\varepsilon)| \ll 1$ and $\zeta_\varepsilon \approx \varepsilon - cT(\varepsilon)$, Eq. A5 simplifies to:

$$\tilde{A}_r(\varepsilon) \approx \frac{2T(\varepsilon)[\varepsilon - cT(\varepsilon)]}{3\nu} \times \left[e^{i[\varepsilon - c\text{Re } T(\varepsilon)]r} e^{-c|\text{Im } T(\varepsilon)r|} + 2i \frac{\sin \pi r}{r} \right]. \quad (\text{A6})$$

Here, unlike Eq. A2 both terms in the brackets are already decaying with r . For the backward case, integration over C_- gives the same result.

The relevant criterion for GE convergence, the smallness of the dominating contribution by impurity pair clusters into the quasiparticle self-energy compared to that by single impurities [32], is presented here in the form:

$$B_2(\varepsilon) \approx c \left| \int_0^\infty \tilde{A}_{-r}(\varepsilon) \tilde{A}_r(\varepsilon)^2 e^{-i(\varepsilon - c\text{Re } T(\varepsilon))r} dr \right| \ll 1. \quad (\text{A7})$$

Then the residue term in Eq. A6 with its slower expo-

ponential decay $\propto e^{-c|\text{Im } T(\varepsilon)r|}$ dominates in the r -integral and converts the above criterion into:

$$B_2(\varepsilon) \approx \frac{8}{81\nu^3} \left| \frac{T^3(\varepsilon)[\varepsilon - cT(\varepsilon)]^3}{\text{Im } T(\varepsilon)} \right| \ll 1. \quad (\text{A8})$$

The straightforward numerical check shows this criterion to surely hold for all the above considered impurity parameters (see an example in Fig. 13).

Also, the self-consistent extension of the T-matrix function:

$$T_{sc}(\varepsilon) = \frac{\omega^2}{2} \left\{ \varepsilon - \varepsilon_{res} - \frac{i\omega^2}{4\nu \sqrt{1 - \left[\frac{\varepsilon - cT_{sc}(\varepsilon)}{2} \right]^2}} \right\}, \quad (\text{A9})$$

practically coincides with its non-renormalized version $T(\varepsilon)$ by Eq. 25, due to the above noted smallness of $|\varepsilon - cT(\varepsilon)| \ll 1$, assured for all $|\varepsilon| \ll 1$.

Hence, the discussed T-matrix results for the quasiparticle spectra in disordered AGNRs and the related estimates for their mobility edges can be considered valid. We conclude that the inverse lifetime by the non-renormalized T-matrix in r.h.s. of Eq. 30 is the main factor for quasiparticle localization in AGNRs. So the results of Sec. III correctly determine the system observable characteristics.

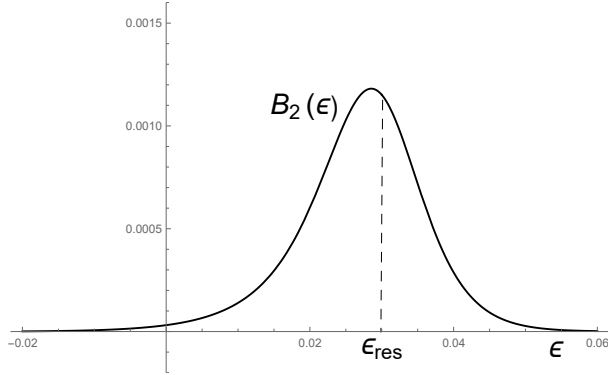


FIG. 13: Smallness of the relative contribution to GE by impurity pairs, $B_2(\varepsilon)$ by Eq. A8 (for Cu impurities with concentration $c = 0.05$ in 5-AGNR), assuring GE convergence for this system.