Partial differential equations/Mathematical physics

Trapped modes supported by localized potentials in the zigzag graphene ribbon

Modes piégés supportés par des potentiels localisés dans des bandes de graphène en zigzag

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A B S T R A C T

Localized potentials in the Dirac equation for the electron dynamics in a zigzag graphene ribbon are constructed to support trapped modes while the corresponding eigenvalues are embedded into the continuous spectrum.

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R É S U M É

On construit des potentiels localisés pour les équations de Dirac décrivant le comportement des électrons dans une bande de graphène en zigzag, pour lesquels des modes piégés existent, tels que les valeurs propres correspondantes soient plongées dans le spectre continu.

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1. Statement of the problem

In the strip \( \Pi = \{(x, y) : x \in (0, d), y \in \mathbb{R}\} \) of width \( d > 0 \), reduced to 1 by rescaling, we consider the Dirac equation

\[
D(\nabla) \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -i\partial_x v + \partial_y v \\ -i\partial_y u - \partial_x u \end{pmatrix} = \omega \begin{pmatrix} u \\ v \end{pmatrix} - \delta P \begin{pmatrix} u \\ v \end{pmatrix} \quad \text{in} \quad \Pi
\]

perturbed by a compactly supported real-valued, continuous for simplicity, potential \( P \) and supplied with the boundary conditions:

\[
u(0, y) = 0, \quad v(1, y) = 0 \quad \text{for} \quad y \in \mathbb{R} = (-\infty, +\infty).
\]

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In (1), \( \delta > 0 \) is a small parameter. This boundary-value problem describes the electron dynamics within one of two valleys of the zigzag graphene ribbon \( \Pi \), see [2], while the other valley requires only the complex conjugation of the equations. The problem (1), (2) is associated with a self-adjoint operator \( A^\delta \) in the Lebesgue space \( L^2([\Pi]) \) having the domain \( \mathcal{D}(A^\delta) = \{ w = (u, v) \in L^2([\Pi]) : D(\nabla)w \in L^2([\Pi]^2) \} \) is valid, independent of \( \delta \). The spectrum \( \sigma(A^\delta) \) is continuous and covers the intact real axis \( \mathbb{R} \subset \mathbb{C} \). Our goal is to construct specific potentials

\[
P(x, y) := P_\tau(x, y) = P_0(x, y) + \tau_1 P_1(x, y) + \cdots + \tau_{2(2N-1)} P_{2(2N-1)}(x, y), \quad \tau = (\tau_1, \ldots, \tau_{2(2N-1)})
\]

that provide a non-empty point spectrum of \( A^\delta \) for a small \( \delta \). In other words, we detect eigenvalues of \( A^\delta \) and the corresponding eigenfunctions \( w \in \mathcal{D}(A^\delta) \) to the problem (1), (2) with the exponential decay as \( y \rightarrow -\infty \).

Since eigenvalues of \( A^\delta \) are embedded into the continuous spectrum, they possess the natural instability, namely a small perturbation of the potential may lead them out of the spectrum and turn into points of complex resonance, cf. [1,7]. This means that the appropriate structure [3] of the potential in (1) requires for “fine tuning” the free parameters \( \tau_1, \ldots, \tau_{2(2N-1)} \). Moreover, the absence of “profitable” symmetries in the Dirac operator does not allow us to employ any conventional trick, cf. [4] and [7], which by imposing artificial boundary conditions on the centerlines of the strip \( \Pi \) could simplify our task. We apply the approach [6], which is based on a criterion [5] for the existence of trapped modes, resorts to the notion [7,8] of enforced stability of embedded eigenvalues, and constructs an asymptotics of an artificial algebraic object, the augmented scattering matrix [5] involved in the criterion. Owing to the symmetry loss, the necessary technicalities become much more complicated than in acoustics, water waves, and quantum waveguides. Moreover, the whole boundary-value problem (1), (2) cannot be transformed into an elliptic one and arguments sustaining the obtained results diverge from the ones used previously in [3,6–8].

2. Incoming and outgoing waves and wave packets

We search for waves, that is bounded solutions of the unperturbed (\( \delta = 0 \)) problem (1), (2), in the form

\[
w(x, y) = e^{-i\omega y} W(x), \quad W = (U, V)
\]

with \( \lambda \in \mathbb{R} \). Assuming \( \omega > 1 \), we obtain

\[
U(x) = a \sin(k(x)), \quad V(x) = \psi \sin(k(x - 1))
\]

where \( \psi = \text{sign}(\sin(k)) \) stands for sign of \( \sin(k) \), the values \( \kappa > 0 \) and \( \lambda \) are determined through the formulas

\[
K(\kappa) := \kappa^{-2} \sin^2 k = \omega^{-2}, \quad \lambda = \kappa \cot k \quad \Rightarrow \quad \omega = \psi \kappa \sec k, \quad (\lambda - 1) \partial_k K(\kappa) \geq 0
\]

and, in view of the normalization factor \( a = \omega^{-1/2} |\lambda - 1|^{-1/2} \), the condition \( \mp \partial_k K(\kappa) > 0 \) assures that

\[
q_k(w, w) := \int_0^1 \left( v(x, R)u(x, R) - u(x, R)v(x, R) \right) \, dx = \pm i.
\]

The Green formula for the Dirac operator shows that the symplectic (sesquilinear and anti-Hermitian) form \( q_k(w, w) \) is independent of \( R \) for any wave (4). Furthermore, \( -iq(w, w) \) is proportional to the projection on the \( y \)-axis of the Poynting vector so that, according to the Mandelstam radiation principle, the sign \( \pm \) in (7) indicates that the wave \( w(x, y) \) propagates from \( +\infty \) to \( -\infty \).

Let \( \kappa_n \in (\pi n, \pi n + \pi) \) with \( n \in \{1, 2, \ldots\} \) be maximum points of the function \( K \), see Fig. 1. Since \( \partial_k K(\kappa_n) = 0 \), we have \( \lambda_n = 1, \omega_n = |K(\kappa_n)|^{-1/2} \) and \( \psi_n = (-1)^n \). At the threshold \( \omega = \omega_n \), in addition to the oscillatory wave \( w^0_{n}(x, y) \), see (4)–(6), the problem (1), (2) at \( \delta = 0 \) gains the linear growing wave

\[
w^0_n(x, y) = yw^0_n(x, y) + w'_n(x, y) = e^{iy} \left( yW^0_n(x) + W'_n(x) \right).
\]

\[
W'_n(x, y) = a_n\kappa_n^{-1} \left[ \frac{1}{6} \kappa_n^{-2} W^0_n(x, y) - (ix \cos(kx), \psi_n(1 - x) \cos(k(x - 1))) \right].
\]

Setting \( a_n = a_n^{1/2} \) and \( w^{\pm}(x, y) = w^0_n(x, y) \pm i w^0_n(x, y) \) yields the relation (7) for these functions, too.

We fix some \( N \in \{1, 2, \ldots\} \) and put

\[
\omega_N^\delta = (\omega_N^{-1} + \epsilon)^{-1} = \omega_N^0 = \omega_N(1 - \epsilon \omega_N + \Theta(\epsilon^2))
\]

where \( \epsilon > 0 \) is small. Let \( \kappa_0^\delta < \kappa_1^\delta < \kappa_1^- < \cdots < \kappa_{N-1}^\delta < \kappa_{N-1}^- \) be all positive roots of the equation \( K(k) = (\omega_k^\delta)^{-2} \), cf. (6) and the dotted line in Fig. 1. The superscript \( \psi = \pm \) in \( \kappa_0^{\psi} \) and the corresponding oscillating waves \( w_0^\psi, w_1^\psi, \ldots, w_{N-1}^\psi \) and \( w_{N-1}^\psi \), composing the row \( w^\psi \) of length \( 2N - 1 \), coincide with the sign on the right of (7) and simultaneously features out that the point \( (\kappa_n^{\psi}, K(\kappa_n^{\psi})) \) lays on the descending (\( \psi = - \)) or ascending (\( \psi = + \)) curve of the graph in Fig. 1.
Building the rows of outgoing and incoming waves

\[ w_{\text{out}}^i = (\chi + w_0^e, \chi - w_1^{e+}, \chi + w_1^{e-}, \ldots, \chi - w_{N-1}^{e+}, \chi + w_{N-1}^{e-}) , \]

\[ w_{\text{in}}^i = (\chi - w_0^e, \chi + w_1^{e-}, \chi - w_1^{e+}, \ldots, \chi + w_{N-1}^{e-}, \chi - w_{N-1}^{e+}) . \]

We localize them onto the waveguide branches \( \Pi \pm = \{(x, y) \in \Pi : \pm y > \ell \} \) by means of the smooth cut-off functions \( \chi_\pm \), while \( \chi_\pm(y) = 1 \) for \( \pm y > 2\ell \), \( \chi_\pm(y) = 0 \) for \( \pm y < \ell \) and \( \ell > 0 \) is fixed to ensure supp \( P \subset [0, 1] \times [-\ell, \ell] \). In view of the sign on the right of (7), all waves in (10) travel to infinity in \( \Pi \), but those in (11) do from infinity. A direct calculation furnishes the orthogonality and normalization conditions

\[ Q \left( w_{\text{out}}^i, w_{\text{out}}^{i'} \right) = i I_{\Pi} \quad Q \left( w_{\text{in}}^i, w_{\text{in}}^{i'} \right) = -i I_{\Pi} \quad Q \left( w_{\text{out}}^i, w_{\text{in}}^{i'} \right) = 0, \]

where \( I_{\Pi} \) and \( I_{\Pi} \) stand for the unit and null matrices of size \((2N - 1) \times (2N - 1)\) and the form \( Q = q_{R} - q_{R} \) takes both branches \( \Pi \pm \) of the waveguide \( \Pi \) into account. It should be emphasized that the problem (1), (2) has \( N \) outgoing and \( N \) incoming waves in the outlet \( \Pi_+ \). In \( \Pi_- \) these numbers becomes \( N - 1 \) and \( N \), respectively, so that both the rows (10) and (11) get the same length \( 2N - 1 \). For elliptic problems, the numbers of outgoing and incoming waves coincide in each cylindrical outlet to infinity.

The above definition also covers the threshold case \( \varepsilon = 0 \) after elongating the rows \( w_{\text{out}}^i \) and \( w_{\text{in}}^i \) with the couples \( w_{\text{out}}^{0} = (\chi + w_0^e, \chi - w_1^{e+}, \chi + w_1^{e-}, \ldots, \chi - w_{N-1}^{e+}, \chi + w_{N-1}^{e-}) \) of the linear waves.

In the next section we will define special packets \( w_{\text{out}}^{2N} \) and \( w_{\text{in}}^{2N} \) of exponential (Im\( \lambda \neq 0 \)) waves (4) at the frequency (9) and get the rows \( w_{\text{out}}^{2N} = (w_{\text{out}}^{0}, w_{\text{out}}^{2}) \) and \( w_{\text{in}}^{2N} = (w_{\text{in}}^{0}, w_{\text{in}}^{2}) \) of length \( 2N \) such that the relations (12) are verified with the subscript \( \dagger \) omitted and the matrices I, O of size \( 2N \times 2N \).

### 3. Scattering matrices

Considering the perturbed \( (\delta \neq 0) \) problem (1), (2) at the frequency (9), one observes that any incoming wave \( w_{\text{in}}^i \) in (11) scatters around the potential \( D_{\Pi} \) and gives rise to a solution \( \zeta_k^{\delta, \varepsilon} \) of the diffraction problem with the Mandelstam (energy) radiation conditions. The row \( \zeta_{\Pi}^{\delta, \varepsilon} \) of these solutions with \( k = 1, \ldots, 2N - 1 \), admits the asymptotic form \( \zeta_{\Pi}^{\delta, \varepsilon} = w_{\Pi}^{\delta, \varepsilon} + \zeta_{\Pi}^{\delta, \varepsilon} + \zeta_{\Pi}^{\delta, \varepsilon} \), where the remainder \( \zeta_{\Pi}^{\delta, \varepsilon}(x, y) \) gains the exponential decay as \( y \to \pm \infty \), namely \( e^{i(y)\zeta_{\Pi}^{\delta, \varepsilon}} \in D(A)^{2N-1} \) with a small exponent \( \beta > 0 \). The transmission and reflection coefficients \( s_{\text{in}}^{\delta, \varepsilon} \) assemble the scattering matrix \( \zeta_{\Pi}^{\delta, \varepsilon} \) of size \((2N - 1) \times (2N - 1)\) which, thanks to the bi-orthogonality conditions (12), is unitary.

At the threshold \( \omega_N \), we also can define a unitary scattering matrix \( \zeta_{\Pi}^{\delta, \varepsilon} \) of size \((2N + 1) \times (2N + 1)\) but we will not need it here. Instead, following [5], cf. [7,8], we spread the standard scattering matrix \( s_{\Pi}^{\delta, \varepsilon} \). Namely, since the problem (1), (2) with \( \delta = \varepsilon = 0 \) has just two polynomial in \( y \) solutions \( W_0^\delta(x, y) \), for a small \( \varepsilon > 0 \), there exist exactly two waves (4) with the frequency \( \omega_N^\varepsilon \) in (9), the complex exponents \( \lambda_{N+}^\varepsilon = 1 + O(\varepsilon^{1/2}) \), and a slow exponential growth at infinity. According to [5, Chap. 9], asymptotics of their ingredients have the form

\[ \lambda_{N+}^\varepsilon = 1 \pm i \varepsilon^{1/2} \theta_N + O(\varepsilon), \quad W_{N+}^\varepsilon = \alpha_N^r \left( W_N^0(x) \pm i \varepsilon^{1/2} \theta_N W_N^0(x) + O(\varepsilon) \right) \]

where \( W_N^0, W_N^0 \) are taken from (8) and \( \theta_N = \kappa_N(2\omega_N^0)^{1/2} \). Moreover, \( \lambda_{N+}^\varepsilon = \lambda_{N-}^\varepsilon \) and the waves \( w_{N \pm}^\varepsilon \) given by formula (4) with the attributes (13) and a proper normalization factor \( \alpha_N^r \) on \( e^{-1/4 (2\theta_N)}^{-1/2} + O(\varepsilon^{1/4}) \) compile the exponential wave packets \( w_{\text{out}}^{2N} = \chi_+(w_{N+}^0 + i w_{N-}^0), w_{\text{in}}^{2N} = \chi_+(w_{N+}^0 - i w_{N-}^0) \) and complete the rows \( w_{\text{out}}^{2N} = (w_{\text{out}}^0, w_{\text{out}}^2), w_{\text{in}}^{2N} = (w_{\text{in}}^0, w_{\text{in}}^2) \), see the end of Section 2. The relations (12) now without the subscript \( \dagger \) provide the solution row

\[ 2^{\delta, \varepsilon} = w_{\text{in}}^{\delta, \varepsilon} + w_{\text{out}}^{\delta, \varepsilon} + 2^{\delta, \varepsilon} \]

with a remainder of the exponential decay and a unitary \( 2N \times 2N \)-matrix \( S^{\delta, \varepsilon} \) called the augmented scattering matrix. Notice that the exponential packets have been introduced in the waveguide branch \( \Pi_+ \) only and, therefore, in the left branch \( \Pi_- \), the solutions (14) possess the slowly decaying term \( \chi_-(w_{N+}^0, K_{N+}^{\delta, \varepsilon}) \) with the coefficient row \( R^{\delta, \varepsilon} = (K_{0+}^{\delta, \varepsilon}, K_{1+}^{\delta, \varepsilon}, K_{2+}^{\delta, \varepsilon}, \ldots, K_{N-1+}^{\delta, \varepsilon}, K_{N+}^{\delta, \varepsilon}) \in \mathbb{C}^{2N} \).
4. The existence and uniqueness of trapped modes

The following assertion explains the very reason to introduce the augmented scattering matrix.

**Theorem 1.** The problem (1), (2) with the frequency (9) has a trapped mode \( w^{δ,ε} \in D(A^1) \) if and only if the right bottom entry \( S_{2N,2N}^{δ,ε} \) of the matrix \( S^{δ,ε} \) in (14) equals \(-1\).

This criterion and the next assertion can be verified in the same way as in [5,8] and [6], respectively, with certain modifications caused by the ellipticity lost.

**Theorem 2.** Let \( p = \max |P(x, y)| \). For any \( N \) and \( ρ > 0 \), there exist \( δ_N(ρ) > 0 \) such that in the case \( δ < p^{-1}δ_N(ρ) \) the segment \( (ω_{N−2} + ρ, ω_{N−1}) \) contains at most one eigenvalue of the problem (1), (2) while the segment \( (ω_{N−1}, ω_N − ρ) \) is always free of its point spectrum.

5. Constructing asymptotics

Applying the method of matched asymptotic expansions, cf. [10], in the interpretation [6,8], we will construct an embedded eigenvalue in the form

\[
ω = ω_N − ω^2_N \delta^2 (A − τ_0(δ)), \quad A > 0, \quad |τ_0(δ)| ≤ c_N δ
\]

(15)

by choosing proper ingredients \( P_k, τ_k = τ_k(δ) \) of the potential (3) and setting \( ε = δ^2 A + O(δ^3) \) in (9). Although the justification scheme is different due to the ellipticity loss, the asymptotic formalism remains the same as in [6,7]. For the last solution in the row (14), we accept the following inner expansion in a finite part of the strip \( Π \):

\[
Z_{2N}^{δ,ε}(x, y) = δ^{-1/2} \left( Z_{2N}^{0,0}(x, y) + δ^{1/2} Z_{2N}^r(x, y) + \ldots \right), \quad |y| \ll \infty,
\]

where ellipses substitute for higher-order terms. This expansion must be matched with two outer expansions in the waveguide branches \( Π_± \), which, according to the decomposition (14), turn into

\[
Z_{2N}^{δ,ε}(x, y) = w_{N}^{in}(x, y) + w_{N}^{out}(x, y) S_{2N,2N}^{δ,ε} + \left( w_{N}^{in}(x, y) S_{12,2N}^{δ,ε} \right)_+ + \ldots, \quad y \gg \ell,
\]

\[
Z_{2N}^{δ,ε}(x, y) = K^{δ,ε} w_{N}(x, y) + \left( w_{N}^{in}(x, y) S_{12,2N}^{δ,ε} \right)_− + \ldots, \quad -y \gg \ell,
\]

where the operation \([ \ldots ]_\pm \) extracts a linear combination of waves which are supplied with the sigh \( ± \) in the row (10). Furthermore, accepting the asymptotic ansätze

\[
S_{2N,2N}^{δ,ε} = S_{2N,2N}^{0,0} + δ S_{2N,2N}^{δ,ε}, \quad S_{12,2N}^{δ,ε} = δ \left( S_{12,2N}^{0,0} + δ S_{12,2N}^{δ,ε} \right), \quad |S_{2N,2N}^{δ,ε}| + |S_{12,2N}^{δ,ε}| \leq C δ
\]

(16)

for the fragments (a scalar and a column in \( C^{2N−1} \)) of the last column in the matrix \( S^{δ,ε} \), we use the representation formulas (13) and perform the matching procedure at the level \( δ^{-1} \) to conclude that

\[
Z_{2N}^{0,0}(x, y) = K^{0,0} w_{N}(x, y), \quad K^{0,0} = 1 + i(1 + i) S_{2N,2N}^{0,0}.
\]

At the same time, the correction term \( Z_{2N}^r \) satisfies the inhomogeneous Dirac equations

\[
D(∇)Z_{2N}^r(x, y) − ω_N Z_{2N}^r(x, y) = −P(τ; x, y) Z_{2N}^{0,0}(x, y), \quad (x, y) ∈ Π,
\]

with the homogeneous boundary conditions of type (2). The general solution \( Z_{2N}^r = w_N^0 c_1 + w_N^0 c_0 + w_N^1 c_1 + Z_{2N}^* \) of this problem gets a linear growth at infinity; here, \( c_1 \in C^{2N−1} \) and \( c_0, c_1 \) are arbitrary and a particular solution can be chosen such that

\[
Z_{2N}^* = iK^{0,0} w_{N}^{out} J_τ(w_{N}^{0}, w_{N}^{0}) + 2K^{0,0} w_{N}^{1} J_{τ}(w_{N}^{0}, w_{N}^{0}) − 2K^{0,0} w_{N}^{0} J_{τ}(w_{N}^{0}, w_{N}^{1}) + Z_{2N},
\]

(17)

\[
J_{τ}(w_{N}^{0}, ∇) = \int_{Π} P_{τ}(x, y) w_{N}^{0}(x, y) ∇(x, y) d x d y.
\]

(18)

Formulas for coefficients in (17) are derived by means of the symplectic form \( Q \). Applying the matching procedure again and comparing the coefficients of the waves \( w_{N}^{1} \) and \( w_{N}^{0} \), we finally obtain the relations

\[
S_{2N,2N}^{0,0} = (1 + B_T^2)^{−2} (2B_T + i(B_T^2 − 1)), \quad S_{12,2N}^{0,0} = 2B_T^2 (1 + B_T^2)^{−2} (B_T + 1 + i(1 − B_T)) J_{τ}(w_{N}^{0}, w_{N}^{1}),
\]

\[
B_T = 1 − 2Δ^{−1/2} φ_{N}^{−1} J_{τ}(w_{N}^{0}, w_{N}^{0}).
\]

(19)
Note that \( s_{2N,2N}^{0,0} = -1 \) for \( B_T = -1 \) and thus we have computed the main correction term in (15):

\[
\Lambda = \theta^{-2}_N J_\tau (w_N^0, w_N^0)^2 \quad \text{provided} \quad J_0(w_N^0, w_N^0) > 0.
\]

(20)

6. Detecting embedded eigenvalues and the corresponding trapped modes

Following the scheme in [6,8] we impose the following conditions on the ingredients of the potential (3):

\[
J_0(w_N^0, w_N^0) > 0, \quad J_0(w_N^0, w_N^0) = 0 \in \mathbb{C}^{2N-1}, \quad \int_{\mathbb{D}} P_j(x, y) z_k(x, y) \, dx \, dy = \delta_{j,k}
\]

(21)

where \( J_0 \) is defined by (18) with \( \tau = 0 \), \( \delta_{j,k} \) is the Kronecker symbol, \( j, k = 1, \ldots, 4N - 2 \), and the functions \( z_k \) compose the row \( (\text{Re}(w_N^0), \text{Im}(w_N^0)) \) of length \( 4N - 2 \). These conditions can be satisfied by choosing \( P_1, \ldots, P_{4N-2} \) because the functions \( z_1, \ldots, z_{4N-2} \) are linear independent. Then we insert representations (16), (19) and (21) into the equations \( \text{Im} S_{2N,2N}^3 = 0 \) and \( S_{1,2N}^4 = 0 \in \mathbb{C}^{2N-1} \), which are obviously equivalent to the criterion in Theorem 1 and convert them into the abstract equation

\[
(\tau_0, \tau) = \delta T_N^{\delta,\tau} (\tau_0, \tau) \quad \text{in} \quad \mathbb{R}^{4N-1}
\]

(22)

with the contraction operator in the ball \( \mathbb{B}_R \subset \mathbb{R}^{4N-1} \) of a small radius \( R > 0 \). Solving the equation (22) by means of the Banach contraction principle yields the main conclusion in this note.

**Theorem 3.** Let us fix \( N \in \{1, 2, \ldots\} \) and let \( P_0, P_1, \ldots, P_{4N-2} \) fulfill the conditions (21). There exists \( \delta_N(P) > 0 \) such that, for any \( \delta \in (0, \delta_N(P)) \), we find out the coefficient column \( \tau = \tau(\delta) \) in (3), \( |\tau(\delta)| \leq R_N \delta \) and simultaneously the eigenvalue (15), (20) of the problem (1), (2) with the potential \( \delta P_T \).

Owing to Theorem 2, Theorem 3 describes all eigenvalues around the threshold \( \omega_N \).

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**References**