C. R. Acad. Sci. Paris, Ser. I 354 (2016) 63–67

Contents lists available at ScienceDirect

C. R. Acad. Sci. Paris, Ser. I

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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 R T I C L E I N F O

Article history:
Received 25 May 2015
Accepted 13 October 2015
Available online 4 November 2015

Presented by the Editorial Board

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 sont 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

$$D(\nabla)\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -\mathrm{i}\partial_x v + \partial_y v \\ -\mathrm{i}\partial_x u - \partial_y u \end{pmatrix} = \omega \begin{pmatrix} u \\ v \end{pmatrix} - \delta P \begin{pmatrix} u \\ v \end{pmatrix} \quad \text{in} \quad \Pi \tag{1}$$

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

$$u(0, y) = 0,\ \ v(1, y) = 0 \quad \text{for} \quad y \in \mathbb{R} = (-\infty, +\infty). \tag{2}$$

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http://dx.doi.org/10.1016/j.crma.2015.10.007
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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 Π, 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^δ in the Lebesgue space $L^2(\Pi)^2$ having the domain $\mathcal{D}(A^\delta) = \{w = (u, v) \in L^2(\Pi)^2 : D(\nabla)w \in L^2(\Pi)^2,$ (2) is valid$\}$, independent of δ. 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

$$P(x, y) := P_\tau(x, y) = P_0(x, y) + \tau_1 P_1(x, y) + \cdots + \tau_{2(2N-1)} P_{2(2N-1)}(x, y), \quad \tau = (\tau_1, \ldots, \tau_{2(2N-1)}) \tag{3}$$

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

Since eigenvalues of A^δ 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 Π 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

$$w(x, y) = e^{-i\lambda y} W(x), \quad W = (U, V) \tag{4}$$

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

$$U(x) = a \sin(\kappa x), \quad V(x) = \varphi a i \sin(\kappa(x-1)) \tag{5}$$

where $\varphi = \mathrm{sign}(\sin\kappa)$ stands for sign of $\sin\kappa$, the values $\kappa > 0$ and λ are determined through the formulas

$$K(\kappa) := \kappa^{-2} \sin^2\kappa = \omega^{-2}, \ \lambda = \kappa \cot\kappa \quad \Rightarrow \quad \omega = \varphi\kappa \sec\kappa, \ (\lambda - 1)\partial_\kappa K(\kappa) \geq 0 \tag{6}$$

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

$$q_R(w, w) := \int_0^1 \left(v(x, R)\overline{u(x, R)} - u(x, R)\overline{v(x, R)} \right) dx = \pm i. \tag{7}$$

The Green formula for the Dirac operator shows that the symplectic (sesquilinear and anti-Hermitian) form $q_R(w, \mathcal{W})$ 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 $\mp\infty$ to $\pm\infty$.

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 $\partial_\kappa K(\kappa_n) = 0$, we have $\lambda_n = 1$, $\omega_n = |K(\kappa_n)|^{-1/2}$ and $\varphi_n = (-1)^n$. At the threshold $\omega = \omega_n$, in addition to the oscillatory wave $w_n^0(x, y)$, see (4)–(6), the problem (1), (2) at $\delta = 0$ gains the linear growing wave

$$w_n^1(x, y) = y w_n^0(x, y) + w_n'(x, y) = e^{iy}\left(y W_n^0(x) + W_n'(x) \right),$$

$$W_n'(x, y) = a_n \kappa_n^{-1} \left(\frac{i}{6} \kappa_n^{-2} W_n^0(x, y) - (i x \cos(\kappa x), \varphi_n (1 - x)\cos(\kappa(x-1))) \right). \tag{8}$$

Setting $a_n = \omega_0^{1/2}$ and $w^\pm(x, y) = w_n^1(x, y) \pm i\, w_n^0(x, y)$ yields the relation (7) for these functions, too.

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

$$\omega_N^\varepsilon = (\omega_N^{-1} + \varepsilon)^{-1} \quad \Rightarrow \quad \omega_N^\varepsilon = \omega_N(1 - \varepsilon\omega_N + O(\varepsilon^2)), \tag{9}$$

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

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