V. A. Kozlov, S. A. Nazarov, A. Orlof

TRAPPED MODES IN ARMCHAIR GRAPHENE NANORIBBONS

ABSTRACT. We study scattering on an ultra-low potential in armchair graphene nanoribbon. Using the continuous Dirac model and including a couple of artificial waves in the scattering process, described by an augumented scattering matrix, we derive a condition for the existence of a trapped mode. We consider the threshold energies, where multiplicity of the continuous spectrum changes and show that a trapped mode may appear for energies slightly less than a threshold and its multiplicity does not exceed one. For energies which are higher than a threshold, there are no trapped modes, provided that the potential is sufficiently small.

§1. INTRODUCTION

The very high quality of graphene samples [4, 15] allows us to consider the production of defects deliberately. There are two types of defects: short- and long-range. Vacancies and adatoms are classified as a short-range type and are modelled by Dirac-delta functions. On the other hand, electric or magnetic fields, interactions with the substrate, Coulomb charges, ripples and wrinkles can be considered as long-range disorder and modelled by smooth functions (a Gaussian for example). In the present study we assume that graphene is free of short-range defects and we consider only long-range defects described by an external potential.

We work within the continuous Dirac model, where electrons dynamics can be described by a system of 4 equations [3]

$$
\mathcal{D} \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} + \delta \mathcal{P} \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} = \omega \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix}, \tag{1}
$$

with

$$\mathcal{D} = \mathcal{D}(\partial_x, \partial_y) := \begin{pmatrix} 0 & i\partial_x + \partial_y & 0 & 0 \\ i\partial_x - \partial_y & 0 & 0 & 0 \\ 0 & 0 & 0 & -i\partial_x + \partial_y \\ 0 & 0 & -i\partial_x - \partial_y & 0 \end{pmatrix}, \quad (2)$$

where (x, y) are dimentionless cartesian coordinates (obtained by the change of coordinates $(x, y) \mapsto \frac{4}{3\sqrt{3}a_{CC}}(x, y)$ in the original problem [3], where $a_{CC} = 0.142$[nm] is a distance between nearest carbon atoms) and consequently ω is a dimensionless energy (where the original energy in [eV] can be recovered by the multiplication by $\frac{2t}{\sqrt{3}}$, where $t = 2.77$[eV] is nearest-neighbour hopping integral); the potential $\mathcal{P}$ is a dimensionless, real-valued function with a compact support and δ is a real-value small parameter.

In the discrete model graphene hexagonal lattice is described as a composition of two interpenetrating triangular lattices (called A and B). The consequence of this division is a two component wave function (ψ_A, ψ_B), where ψ_A (ψ_B) describes the electron on the sites of lattice A (B). In the discrete model there are two minima in the dispersion relation, called $\mathbf{K} = (0, -K)$ and $\mathbf{K}' = (0, K)$ valleys (with $K = \pi$ in our dimentionless formulation). Low energy approximation ($a_{CC} \to 0$), which enables the passage from discrete to continuous model, has to be done close to those minima separately, leading to the following form of the total wave functions [9]:

$$\psi_A(x, y) = e^{i\mathbf{K}\cdot(x,y)}u(x, y) - ie^{i\mathbf{K}'\cdot(x,y)}u'(x, y), \qquad (3)$$

$$\psi_B(x, y) = -ie^{i\mathbf{K}\cdot(x,y)}v(x, y) + e^{i\mathbf{K}'\cdot(x,y)}v'(x, y), \qquad (4)$$

with components (u, v) coming from the approximation close to $\mathbf{K}$ point and fulfilling the system of the two first equations in (1) and components (u', v') coming from the approximation close to $\mathbf{K}'$ point and fulfilling the system of the two last equations in (1). An armchair nanoribbon is modelled as a strip $\Pi = (0, L) \times \mathbb{R}$, $L > 0$, parallel to the x-axis. The wave function has to disappear on the nanoribbon edges, which in the armchair case contain sites from both sublattices A and B. Consequently it is required [2, 9]:

$$\psi_A(x, 0) = 0, \quad \psi_B(x, 0) = 0,$$
$$\psi_A(x, L) = 0, \quad \psi_B(x, L) = 0.$$

From (3) and (4), these boundary conditions transform to

$$u(x,0) - iu'(x,0) = 0, \quad -iv(x,0) + v'(x,0) = 0, \tag{5}$$

$$e^{-i2\pi L}u(x,L) - iu'(x,L) = 0, \quad -ie^{-i2\pi L}v(x,L) + v'(x,L) = 0. \tag{6}$$

These boundary conditions describe the mixing between valleys which is characteristic for armchair nanoribbons. For a detailed derivation of the continuous model see [9].

Our potential $\mathcal{P}$ is assumed to be of long-range type and can be described by a diagonal matrix with equal elements [1].

We introduce the energy thresholds

$$\omega_1 = \min_{j \in \mathbb{Z}} \left\{ \left| \pi + \frac{\pi j}{L} \right| : \left| \pi + \frac{\pi j}{L} \right| > 0 \right\},$$

and

$$\omega_{k+1} = \min_{j \in \mathbb{Z}} \left\{ \left| \pi + \frac{\pi j}{L} \right| : \left| \pi + \frac{\pi j}{L} \right| > \omega_k \right\}, \quad k = 1, 2, \ldots. \tag{7}$$

Note that

$$d_* \leqslant |\omega_{k+1} - \omega_k| \leqslant \frac{\pi}{L}, \quad d_* = \frac{\pi}{L} \min_{\substack{m \in \mathbb{Z} \\ 2L+m \neq 0}} |2L + m|. \tag{8}$$

The continuous spectrum of the problem (1), (5), (6) with $\mathcal{P} = 0$ depends on the nanoribbon width L and covers $(-\infty, \omega_1] \cup [\omega_1, +\infty)$. At the thresholds, the multiplicity of the continuous spectrum changes.

A trapped mode is defined as a vector eigenfunction (from L_2 space) that corresponds to an eigenvalue embedded in the continuous spectrum. The main result of the paper is the following theorem about the existence of trapped modes in armchair graphene nanoribbons for energies close to one of the thresholds that can be chosen arbitrary.

Theorem 1. *For every $N = 1, 2, \ldots$, there exists $\epsilon_N > 0$ such that for each $\epsilon \in (0, \epsilon_N)$ there exists $\delta \sim \sqrt{\epsilon}$ and a potential $\mathcal{P}$ with $\sup |\mathcal{P}| < 1$, such that the problem (1), (5), (6) has a trapped mode for $\omega = \omega_N - \epsilon$.*

The second result shows that trapped modes may appear only for energies slightly smaller than a threshold and that the spectrum far from the threshold is free of embedded eigenvalues, provided the potential is sufficiently small. Moreover their multiplicity does not exceed one.

Theorem 2. *There exist positive numbers ϵ_0 independent of N and δ_0, such that if*

(i) $\omega \in [\omega_N, \omega_N + \epsilon_0]$ *or* $|\omega - \omega_k| > \epsilon_0$, *for all* $k = 1, 2, \dots$ *and* $|\delta| < \delta_0$ *with* δ_0 *independent of* N *and* k, *then the problem* (1), (5), (6) *has no trapped modes;*

(ii) $\omega \in [\omega_N - \epsilon_0, \omega_N]$ *and* $|\delta| < \delta_0$ *with* δ_0 *which may depend on* N, *then the multiplicity of a trapped mode to probelm* (1), (5), (6) *does not exceed* 1.

To approach the problem, we follow the technique based on the augumented scattering matrix developed in [5, 10–12].

This is the second paper about trapped modes in graphene nanoribbons, that we consider. In the first one [7], we analysed the case of zigzag nanoribbon with a corresponding non-elliptic boundary value problem.

The paper is organised as follows. In Sec. 2 we analyse the Dirac equation without potential. For a fixed energy, we construct the bounded solutions (waves) in Sec. 2.3. Additionally, when the considered energy is close to a threshold (7), we construct the two unbounded solutions in Sec. 2.4. In Sec. 2.6, we introduce a symplectic form, used to define the direction of wave propagation in Sec. 2.7, 2.8. In Sec. 2.9, we give a solvability result for the non-homogenous problem.

In Sec. 3, we include a potential in the Dirac equation and consider a scattering problem using the augumented scattering matrix (Sec. 3.2). In Sec. 4.1, we give a necessary and sufficient condition for the existence of trapped modes from which, in Sec. 4.3, we extract an example potential that produces a trapped mode and prove Theorem 1. Finally in Sec. 4.3, we prove Theorem 2 about the multiplicity of trapped modes.

§2. The Dirac equation

2.1. Problem statement. First, we consider problem (1) without potential ($\mathcal{P} = 0$), i.e.

$$\mathcal{D} \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} = \omega \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix}, \tag{9}$$

with the boundary conditions (5), (6).

Our goal is to find solutions of at most exponential growth to the above problem; in particular, we need bounded solutions to describe the continuous spectrum of the operator corresponding to (9), (5), (6).

Let us introduce the space X_0 which contains (u, v, u', v'), such that each component belongs to $L^2(\Pi)$ and $(i\partial_x - \partial_y)u$, $(i\partial_x + \partial_y)v$, $(i\partial_x + \partial_y)u'$, $(-i\partial_x + \partial_y)v'$ are also in $L^2(\Pi)$; moreover the components fulfill the conditions (5), (6). The norm in X_0 is the usual L_2-norm for all the components and their derivatives described above. The operator $\mathcal{D}$ is self-adjoint in $(L^2(\Pi))^4$ with the domain X_0. One can verify that the problem (9), (5), (6) is elliptic. Another equivalent norm in X_0 is given by the following proposition.

Proposition 1. *It holds that*

$$\int_\Pi |\mathcal{D}(u, v, u', v')^\top|^2 dxdy = \int_\Pi \left(|\nabla u|^2 + |\nabla v|^2 + |\nabla u'|^2 + |\nabla v'|^2 \right) dxdy,$$

for $(u, v, u', v') \in X_0$.

Proof. Proof is presented in Appendix A. □

Due to the nanoribbon geometry we are looking for non-trivial exponential (or power exponential) solutions in x, namely

$$(u(x,y), v(x,y), u'(x,y), v'(x,y)) = e^{i\lambda x}(\mathcal{U}(y), \mathcal{V}(y), \mathcal{U}'(y), \mathcal{V}'(y)), \quad (10)$$

where a complex number λ is the longitudinal component of the wave vector parallel with the nanoribbon edge.

For $\omega = 0$ we have $(i\partial_x + \partial_y)v = (i\partial_x - \partial_y)u = (-i\partial_x + \partial_y)v' = (-i\partial_x - \partial_y)u' = 0$, therefore $u = u(x + iy)$, $v = v(-x + iy)$, $u' = u'(-x + iy)$, $v' = v'(x + iy)$, which together with the boundary conditions (5), (6) and the form (10) give solutions only for nanoribbons with a width L such that L is a natural number and $\lambda = 0$. These solutions are

$$(u, v, u', v') = (1, C, -i, iC), \quad C \in \mathbb{C}.$$

Now assume that $\omega \neq 0$, then (9) can be written as:

$$-\Delta u = \omega^2 u, \ v = \omega^{-1}(i\partial_x - \partial_y)u, \ -\Delta u' = \omega^2 u', \ v' = \omega^{-1}(-i\partial_x - \partial_y)u'. \ (11)$$

Then the insertion of (10) into (11) and (5), (6), gives

$$\begin{cases} -\mathcal{U}_{yy} = (\omega^2 - \lambda^2)\mathcal{U} \ , & -\mathcal{U}'_{yy} = (\omega^2 - \lambda^2)\mathcal{U}' \\ \mathcal{V} = \omega^{-1}(-\lambda\mathcal{U} - \mathcal{U}_y) \ , & \mathcal{V}' = \omega^{-1}(\lambda\mathcal{U}' - \mathcal{U}'_y), \\ \mathcal{U}(0) - i\mathcal{U}'(0) = 0 \ , & -i\mathcal{V}(0) + \mathcal{V}'(0) = 0 \\ e^{-i2\pi L}\mathcal{U}(L) - i\mathcal{U}'(L) = 0 \ , & -ie^{-i2\pi L}\mathcal{V}(L) + \mathcal{V}'(L) = 0. \end{cases} \quad (12)$$

If $\lambda^2 = \omega^2$, then problem (12) has a non-trivial solution only when L is a natural number. In this case

$$(u(x,y), v(x,y), u'(x,y), v'(x,y)) = e^{\pm i\omega x}(1, \mp 1, -i, \mp i) \qquad (13)$$

and there is no power exponential solution.

Now, consider the case $\lambda^2 \neq \omega^2$ ($\omega \neq 0$). If $\omega \neq \omega_N$, $N = 1, 2, \ldots$, then all the solutions of (9), (5), (6) have the form (10) with

$$\begin{aligned}
(\mathcal{U}(y), \mathcal{V}(y), \mathcal{U}'(y), \mathcal{V}'(y)) \\
= (e^{i\kappa y}, -\omega^{-1}(\lambda + i\kappa)e^{i\kappa y}, -ie^{-i\kappa y}, -i\omega^{-1}(\lambda + i\kappa)e^{-i\kappa y}), \quad (14)
\end{aligned}$$

where

$$\lambda = \pm\sqrt{\omega^2 - \kappa^2}, \quad \kappa = \pi + \frac{\pi j}{L}, \quad j = 0, \pm 1, \pm 2, \ldots. \qquad (15)$$

When $\omega = \omega_N$, $N = 1, 2, \ldots$ and $\lambda = 0$, we have two more solutions when $2L$ is not a natural number and they are

$$w_N^0(x,y) = (e^{i\kappa y}, -i\operatorname{sgn}(\kappa)e^{i\kappa y}, -ie^{-i\kappa y}, \operatorname{sgn}(\kappa)e^{-i\kappa y}), \qquad (16)$$

$$w_N^1(x,y) = xw_N^0(x,y) + |\kappa|^{-1}(0, ie^{i\kappa y}, 0, -e^{-i\kappa y}), \qquad (17)$$

with $\kappa = \pi + \frac{\pi m}{L}$, where m is defined through ω_N,

$$\omega_N = |\pi + \frac{\pi m}{L}| = \min_{j \in \mathbb{Z}}\left\{\left|\pi + \frac{\pi j}{L}\right| : \left|\pi + \frac{\pi j}{L}\right| > \omega_k\right\}, \quad k = 1, 2, \ldots, N-1.$$

It follows that κ is one of two ω_N or $-\omega_N$. Differently if $2L$ is a natural number, then we have four more solutions, two of the form (16) and (17) with $\kappa = \omega_N$ and two of the same form (16) and (17) but with $\kappa = -\omega_N$.

2.2. Symmetries. There are three symmetries in the system, let's denote them by T_1, T_2 and T_3. If $(u(x,y), v(x,y), u'(x,y), v'(x,y))$ is a solution to (9), (5), (6) then through symmetry transformations T_1, T_2 and T_3, there are three more solutions which respectively read

$$\begin{pmatrix} \overline{u}'(x,y) \\ \overline{v}'(x,y) \\ \overline{u}(x,y) \\ \overline{v}(x,y) \end{pmatrix}, \quad \begin{pmatrix} v(-x,y) \\ -u(-x,y) \\ -v'(-x,y) \\ u'(-x,y)) \end{pmatrix}, \quad \begin{pmatrix} e^{i2\pi L}\overline{u}(x, L-y) \\ -e^{i2\pi L}\overline{v}(x, L-y) \\ -\overline{u}'(x, L-y) \\ \overline{v}'(x, L-y) \end{pmatrix}.$$

Superpositions of those symmetries give eight solutions in total in this case. Moreover, if the nanoribbon width $2L$ is a natural number, then there is an additional symmetry T_4 giving the following solution

$$\begin{pmatrix} \overline{u}(-x,y) \\ \overline{v}(-x,y) \\ -\overline{u}'(-x,y) \\ -\overline{v}'(-x,y) \end{pmatrix},$$

and so there are 16 solutions in this case. In what follows we find solutions (u,v,u',v') for positive ω only. Then the solution for $-\omega$ is $(u,-v,u',-v')$.

2.3. Solutions with real wave number λ. In this paper we focus on the case when $2L$ is not a natural number (Figure 1 (a) and (b)).

Consider first the case when $\omega \in (\omega_{N-1}, \omega_N)$ for certain $N = 1, 2, \dots$ (we assume that $\omega_0 = 0$). We enumerate the real exponent in (15) as follows. Assuming that λ in (15) is real, we have that

$$-\omega < \pi + \frac{\pi j}{L} < \omega \ \text{ or } \ -L(1 + \frac{\omega}{\pi}) < j < L(\frac{\omega}{\pi} - 1). \tag{18}$$

According to the last inequality, we enumerate κ

$$-\omega < \kappa_1 < \kappa_2 < \dots < \kappa_M < \omega,$$

where $M = M(\omega) = N - 1$ is the number of indexes j satysfying (18). For any κ_j, $j = 1, 2, \dots, M$, there are two values of λ in (15) that define solutions (13), (14), let us denote them $\pm\lambda_j$ with $\lambda_j = \sqrt{\omega^2 - \kappa_j^2}$, $j = 1, 2, \dots, M$. We can introduce the notation for solutions (14)

$$w_j^{\pm}(x,y) = (u_j^{\pm}(x,y), v_j^{\pm}(x,y), u_j^{'\pm}(x,y), v_j^{'\pm}(x,y)) \tag{19}$$

$$= e^{\pm i\lambda_j x}(\mathcal{U}_j^{\pm}(y), \mathcal{V}_j^{\pm}(y), \mathcal{U}_j^{'\pm}(y), \mathcal{V}_j^{'\pm}(y)), \tag{20}$$

where

$$(\mathcal{U}_j^{\pm}(y), \mathcal{V}_j^{\pm}(y), \mathcal{U}_j^{'\pm}(y), \mathcal{V}_j^{'\pm}(y))$$
$$= (e^{i\kappa_j y}, -\omega^{-1}(\pm\lambda_j + i\kappa_j)e^{i\kappa_j y}, -ie^{-i\kappa_j y}, -i\omega^{-1}(\pm\lambda_j + i\kappa_j)e^{-i\kappa_j y}).$$

Now, consider the threshold case, that is $\omega = \omega_N$, $N = 1, 2, , 3, \dots$ and $\lambda = 0$. Then $\kappa^2 = \omega^2$. In the case $2L$ is not a natural number, there is only one value of j that satisfies one of the two relations

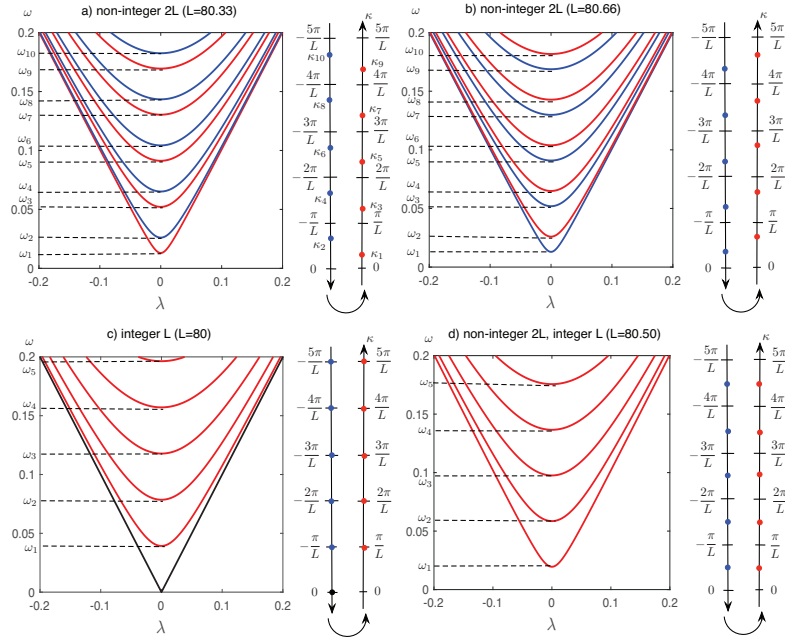$$\pi + \frac{\pi j}{L} = \pm\omega,$$

Figure 1. Dispersion relation: energy ω versus wave vector component λ for nanoribbons of different width L: (a) and (b) for non integer $2L$, (c) integer L, (d) integer $2L$ but non integer L. Threshold energies $\omega_1 < \omega_2 < \ldots$ and values of κ (blue and red dots) are indicated. The colors of the dots and curves correspond to the sign of the κ value, which when red is positive and when blue is negative.

using this value of j we define $\kappa_N = \pi + \frac{\pi j}{L}$, with the use of which we find two additional solutions to our problem (9), (5), (6)

$$w_N^0(x,y) = (e^{i\kappa_N y}, -i\operatorname{sgn}(\kappa_N)e^{i\kappa_N y}, -ie^{-i\kappa_N y}, \operatorname{sgn}(\kappa_N)e^{-i\kappa_N y}), \quad (21)$$

$$w_N^1(x,y) = xw_N^0(x,y) + \omega_N^{-1}(0, ie^{i\kappa_N y}, 0, -e^{-i\kappa_N y}). \quad (22)$$

Thus, the continuous spectrum depends on the nanoribbon width. For each $\omega \geqslant \omega_1$ there is a bounded solution to (9), (5), (6) of the form (10); additionally there are bounded solutions for $0 < \omega < \omega_1$ for L being a natural number. Hence the continuous spectrum for the Dirac operator

$\mathcal{D}$ is $(-\infty, -\omega_1] \cup [\omega_1, \infty)$ when L is not a natural number and $(-\infty, \infty)$ when L is a natural number. Note that ω_1 depends on L and is small for L close to a natural number.

2.4. Solutions with imaginary wave number λ. Consider the case when ω is close to the threshold ω_N. Introduce a small parameter ϵ and denote by ω_ϵ the energy $\omega_\epsilon = \omega_N - \epsilon$, $\epsilon > 0$. Then the root $\lambda = 0$ bifurcates into two imaginary roots $\pm \lambda_\epsilon = \pm \lambda_\epsilon(\epsilon)$, $\lambda_\epsilon > 0$, which can be found from the equation

$$\omega_\epsilon^2 = \omega_N^2 + \lambda_\epsilon^2.$$

They have the expansion

$$\lambda_\epsilon = i\sqrt{\epsilon}\sqrt{2\omega_N - \epsilon}), \tag{23}$$

so that $\overline{\lambda_\epsilon} = -\lambda_\epsilon$.

Now instead of two threshold solutions (21) and (22), we have two solutions of the form (10) with $\pm \lambda_\epsilon$

$$w_N^\pm(x,y) = e^{\pm i\lambda_\epsilon x}\left(e^{i\kappa_N y}, -\frac{\pm\lambda_\epsilon + i\kappa_N}{\omega_\epsilon}e^{i\kappa_N y}, -ie^{-i\kappa_N y}, -\frac{\pm i\lambda_\epsilon - \kappa_N}{\omega_\epsilon}e^{-i\kappa_N y}\right) \tag{24}$$

By (23), functions (24) can be written in terms of w_N^0, w_N^1 (see (16) and (17))

$$w_N^\pm(x,y) = w_N^0(x,y) \mp \sqrt{\epsilon}\sqrt{2\omega_N}w_N^1(x,y) + O(\epsilon).$$

The waves (24) are not analytic in ϵ but their linear combination

$$\mathbf{w}_N^{\epsilon+}(x,y) = \frac{w_N^+ + w_N^-}{2} = w_N^0 + O(\epsilon), \tag{25}$$

$$\mathbf{w}_N^{\epsilon-}(x,y) = \frac{w_N^+ - w_N^-}{2\lambda_\epsilon} = iw_N^1 + O(\epsilon), \tag{26}$$

are analytic with respect to ϵ for small $|\epsilon|$.

2.5. Proposition about the location of λ.

Proposition 2. *There is a constant $\epsilon_0 = \epsilon_0(L) > 0$ such that the following assertions are valid*

(1) For every ω_N there exist $\gamma_N = \gamma_N(L) > 0$ such that the strip $|\operatorname{Im}\lambda| \leqslant \gamma_N$ contains all the real and two imaginary values of λ described in Sec. 2.3 and Sec. 2.4 when $\omega \in [\omega_N - \epsilon_0, \omega_N)$.
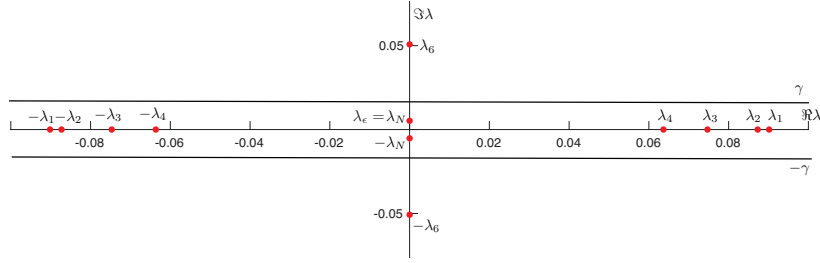
Figure 2. The values of λ are on the real and imaginary axis only. When the energy is close to one of the thresholds ω_N, it is possible to choose a strip $|\operatorname{Im}\lambda| \leqslant \gamma_N$ such that all real and only two imaginary values of λ are within the strip (indicated). For example when $L = 80.33$ and $\omega = \omega_5 - \epsilon$ ($\omega_5 = 0.0912$ and $\epsilon = 0.0001$), then all the possible values of λ are indicated with red dots, only real values are enumerated: $\pm\lambda_1, \pm\lambda_2, \ldots, \pm\lambda_4$ ($N = 5$) and the imaginary values of λ are indicated by $\pm\lambda_\epsilon$. For the sake of the proof of Proposition (2), we indicate λ_N ($\lambda_N = \lambda_5$ in our case and $\lambda_N = \lambda_\epsilon$ as ω is slightly less and close to the threshold) and $\lambda_{N+1} = \lambda_6$.

(2) *There exist $\gamma = \gamma(L) > 0$ such that the strip $|\operatorname{Im}\lambda| \leqslant \gamma$ contains the real values of λ described in Sec. 2.3 when $|\omega - \omega_k| > \epsilon_0$ with $k = 1, 2, \ldots$ or when $\omega \in [\omega_N, \omega_N + \epsilon_0]$.*

Proof. For the sake of the exposition, let us numerate κ_N and κ_{N+1} according to (15) so that $\kappa_N = \pi + \frac{\pi m}{L}$, where m is defined through ω_N

$$\omega_N = \left|\pi + \frac{\pi m}{L}\right| = \min_{j \in \mathbb{Z}}\left\{\left|\pi + \frac{\pi j}{L}\right| : \left|\pi + \frac{\pi j}{L}\right| > \omega_k\right\}, \quad k = 1, 2, \ldots, N-1.$$

It follows that κ_N is equal to ω_N or $-\omega_N$. Similarly $\kappa_{N+1} = \pi + \frac{\pi m}{L}$ with m defined through ω_{N+1},

$$\omega_{N+1} = \left|\pi + \frac{\pi m}{L}\right| = \min_{j \in \mathbb{Z}}\left\{\left|\pi + \frac{\pi j}{L}\right| : \left|\pi + \frac{\pi j}{L}\right| > \omega_k\right\}, \quad k = 1, 2, \ldots, N,$$

and so κ_{N+1} is equal to ω_{N+1} or $-\omega_{N+1}$. Consequently, we define $\lambda_m = \sqrt{\omega^2 - \kappa_m^2}$, $m = N, N+1$ (Fig. 2).

(1) Let us first estimate the difference $\operatorname{Im}\lambda_{N+1} - \operatorname{Im}\lambda_N$. Let ϵ_0 be a small positive number depending on L and being chosen later. We have

$$\operatorname{Im}\lambda_{N+1} - \operatorname{Im}\lambda_N = \sqrt{\omega_{N+1}^2 - \omega^2} - \sqrt{\omega_N^2 - \omega^2} = \frac{(\omega_{N+1}^2 - \omega_N^2)}{\sqrt{\omega_{N+1}^2 - \omega^2} + \sqrt{\omega_N^2 - \omega^2}}$$

$$\geqslant \frac{(\omega_{N+1} - \omega_N)(\omega_{N+1} + \omega_N)}{2\sqrt{\omega_{N+1}^2 - \omega^2}} \geqslant \frac{(\omega_{N+1} - \omega_N)\sqrt{\omega_{N+1} + \omega_N}}{2\sqrt{\omega_{N+1} - \omega_N + \epsilon_0}}.$$

Using estimate (8), we proceed as

$$\operatorname{Im}\lambda_{N+1} - \operatorname{Im}\lambda_N \geqslant \frac{\sqrt{d_*}\sqrt{2\omega_N}}{2\sqrt{1 + \frac{\epsilon_0}{\omega_{N+1} - \omega_N}}} \geqslant \frac{\sqrt{d_*}\sqrt{2\omega_N}}{2\sqrt{1 + \frac{\epsilon_0}{d_*}}}.$$

Now, γ_N exists only when $\operatorname{Im}\lambda_N$ is small enough. The upper bound on $\operatorname{Im}\lambda_N$ is

$$\operatorname{Im}\lambda_N = \sqrt{\omega_N^2 - \omega^2} \leqslant \sqrt{2\epsilon_0\omega_N}$$

and we consider it to be small when $\operatorname{Im}\lambda_N < \operatorname{Im}\lambda_{N+1} - \operatorname{Im}\lambda_N$ and ϵ_0 is chosen so that

$$\sqrt{\epsilon_0 2\omega_N} \leqslant \frac{d_*\sqrt{2\omega_N}}{2\sqrt{d_* + \epsilon_0}} \iff \sqrt{\epsilon_0} \leqslant \frac{d_*}{2\sqrt{d_* + \epsilon_0}}.$$

From the last inequality, we get that $\epsilon_0 \leqslant \frac{1+\sqrt{2}}{2}d_*$ and so ϵ_0 does not depend on N. The value of γ_N can be chosen as any between $\operatorname{Im}\lambda_N < \gamma_N < \operatorname{Im}\lambda_{N+1} - \operatorname{Im}\lambda_N$ (Figure 2).

(2) Consider first $|\omega - \omega_k| > \epsilon_0$ with $k = 1, 2, \ldots$. For $\operatorname{Im}\lambda_k \neq 0$, according to (15), we have

$$\operatorname{Im}\lambda_k = \sqrt{\omega_k^2 - \omega^2} \geqslant \sqrt{\epsilon_0}\sqrt{\omega_k + \omega} \geqslant \sqrt{\epsilon_0}\sqrt{\omega_1}.$$

Choosing $\gamma = \frac{1}{2}\sqrt{\epsilon_0\omega_1}$, we get that the strip contains only real values of λ.

If $\omega \in [\omega_N, \omega_N + \epsilon_0]$, then $\operatorname{Im}\lambda_N = 0$ and

$$\operatorname{Im}\lambda_{N+1} = \sqrt{\omega_{N+1}^2 - \omega^2} \geqslant \sqrt{\omega_{N+1} - \omega_N + \epsilon_0}\sqrt{\omega_{N+1} + \omega_N}$$

$$\geqslant \sqrt{d_* + \epsilon_0}\sqrt{\omega_2 + \omega_1} \geqslant \sqrt{\epsilon_0}\sqrt{\omega_1}.$$

Again, we can choose $\gamma = \frac{\sqrt{\epsilon_0\omega_1}}{2}$ so that the strip contains only real values of λ. $\qquad\square$

2.6. The symplectic form. For two solutions $w = (u, v, u', v')$ and $\tilde{w} = (\tilde{u}, \tilde{v}, \tilde{u}', \tilde{v}')$ of the problem (9), (5), (6), let us define the quantity

$$q_a(w, \tilde{w}) \tag{27}$$

$$= -i \int_0^L \overline{\tilde{u}}(a, y)v(a, y) + \overline{\tilde{v}}(a, y)u(a, y) - \overline{\tilde{u}}'(a, y)v'(a, y) - \overline{\tilde{v}}'(a, y)u'(a, y)dy.$$

Since

$$0 = \int_{\Pi_{a,b}} \begin{pmatrix} \overline{\tilde{u}} \\ \overline{\tilde{v}} \\ \overline{\tilde{u}'} \\ \overline{\tilde{v}'} \end{pmatrix} (\mathcal{D} - \omega \mathcal{I}) \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} dxdy - \int_{\Pi_{a,b}} \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} (\overline{\mathcal{D}} - \omega \mathcal{I}) \begin{pmatrix} \overline{\tilde{u}} \\ \overline{\tilde{v}} \\ \overline{\tilde{u}'} \\ \overline{\tilde{v}'} \end{pmatrix} dxdy$$

$$= -q_b(w, \tilde{w}) + q_a(w, \tilde{w}),$$

where $\Pi_{a,b} = (0, L) \times (a, b)$, $a < b$, we see that q_a does not depend on a and we use the notation q for this form.

The form q is symplectic because it is sesquilinear and anti-Hermitian.

2.7. Biorthogonality conditions when the wave vector λ is real. Here we discuss the biorthogonality conditions for the solutions to (9), (5), (6). Since we are interested mostly in the case when $\omega = \omega_\epsilon$, where $\omega_\epsilon = \omega_N - \epsilon$, we consider this case here. Using (27), we obtain the biorthogonality conditions for the oscillatory waves $w_j^{\pm}$ in (19):

$$q(w_j^\tau, w_k^\theta) = 0 \quad \text{if } (j, \tau) \neq (k, \theta) \quad \text{and } q(w_j^\tau, w_j^\tau) = \frac{4\tau i L \lambda_j}{\omega}.$$

Therefore

$$q(w_j^\tau, w_k^\theta) = \frac{4\tau i L \lambda_j}{\omega} \delta_{j,k} \delta_{\tau,\theta}, \tag{28}$$

for $j, k = 1, \ldots, N - 1$ and $\tau, \theta = \pm$. We put

$$\mathbf{w}_k^\tau = \frac{\sqrt{\omega}}{2\sqrt{L|\lambda_k|}} w_k^\tau, \quad k = 1, \ldots, N - 1, \quad \tau = \pm.$$

Then by (28), we have:

$$q(\mathbf{w}_j^\tau, \ \mathbf{w}_k^\theta) = \tau i \delta_{j,k} \delta_{\tau,\theta}. \tag{29}$$

and when $\omega = \omega_N$, then

$$q(w_N^0, w_N^0) = 0, \quad q(w_N^0, w_N^1) = -\frac{2L}{\omega_N}, \quad q(w_N^1, w_N^1) = 0. \tag{30}$$

2.8. Biorthogonality conditions when the wave vector λ is imaginary.

Let us check if the waves $\mathbf{w}_N^{\epsilon\pm}$ fulfil the orthogonality conditions. A direct evaluation gives

$$q(w_N^{\pm}, w_N^{\pm}) = 0, \quad q(w_N^-, w_N^+) = \frac{i4L}{\omega_\epsilon}\lambda_+, \quad q(w_N^+, w_N^-) = \frac{i4L}{\omega_\epsilon}\lambda_-.$$

Consequently

$$q(\mathbf{w}_N^{\epsilon+}, \mathbf{w}_N^{\epsilon+}) = 0, \quad q(\mathbf{w}_N^{\epsilon+}, \mathbf{w}_N^{\epsilon-}) = \frac{i2L}{\omega_\epsilon}, \quad q(\mathbf{w}_N^{\epsilon-}, \mathbf{w}_N^{\epsilon-}) = 0.$$

As waves $\mathbf{w}_N^{\epsilon+}$ and $\mathbf{w}_N^{\epsilon-}$ do not fulfil the biorthogonality conditions, we introduce their linear combinations

$$\mathbf{w}_N^{\pm} = \frac{\mathbf{w}_N^{\epsilon+} \pm \mathbf{w}_N^{\epsilon-}}{\mathcal{N}} = \frac{1}{2\mathcal{N}}\left(1 \pm \frac{1}{\lambda_\epsilon}\right)w_N^+ + \frac{1}{2\mathcal{N}}\left(1 \mp \frac{1}{\lambda_\epsilon}\right)w_N^-, \quad \mathcal{N} = 2\sqrt{\frac{L}{\omega_\epsilon}}. \quad (31)$$

Then the new waves (31) fulfill the condition

$$q(\mathbf{w}_N^\tau, \mathbf{w}_N^\theta) = \tau i \delta_{\tau,\theta}.$$

2.9. The non-homogeneous problem.

Consider the non-homogeneous problem

$$(i\partial_x + \partial_y)v - \omega u = g \quad \text{in } \Pi, \tag{32}$$

$$(i\partial_x - \partial_y)u - \omega v = h \quad \text{in } \Pi, \tag{33}$$

$$(-i\partial_x + \partial_y)v' - \omega u' = g' \quad \text{in } \Pi, \tag{34}$$

$$(-i\partial_x - \partial_y)u' - \omega v' = h' \quad \text{in } \Pi, \tag{35}$$

supplied with boundary conditions (5), (6).

In order to formulate the solvability results for this problem, we introduce some spaces. The space $L_\sigma^{\pm}(\Pi)$, $\sigma > 0$, consists of all functions g such that $e^{\pm\sigma x}g \in L^2(\Pi)$. Then the space $X_\sigma^{\pm}$ contains (u, v, u', v') such that $e^{\pm\sigma x}(u, v, u', v') \in X_0$. The norms in the above spaces are defined by $\|g; L_\sigma^{\pm}(\Pi)\| = \|e^{\pm\sigma x}g; L^2(\Pi)\|$ and $\|(u, v, u', v'); X_\sigma^{\pm}\| = \|e^{\pm\sigma x}(u, v, u', v'); X_0\|$ respectively.

Theorem 3. *Let $\omega > 0$ and let $\sigma > 0$ be such that the line $\operatorname{Im}\lambda = \pm\sigma$ contains no λ defined by (15). Then the operator*[1]

$$\mathcal{D} - \omega\mathcal{I} : X_\sigma^{\pm} \to L_\sigma^{\pm}(\Pi)$$

---

[1]For the simplicity of the notation, we write $L_\sigma^{\pm}(\Pi)$ for both spaces of functions and vectors. Here for example we write $L_\sigma^{\pm}(\Pi)$ instead of $L_\sigma^{\pm}(\Pi) \times L_\sigma^{\pm}(\Pi) \times L_\sigma^{\pm}(\Pi) \times L_\sigma^{\pm}(\Pi)$. This notation is applied to the other spaces introduced later as well.

is an isomorphism.

Proof. The following result is a consequence of ellipticity and it follows from Theorem 2.4.1 in [6]. To apply Theorem 2.4.1 in [6], we put that $l = 1$, $H_0 = L_2(0, L)^4$ and $H_1 = \{(\mathcal{U}, \mathcal{V}, \mathcal{U}', \mathcal{V}') \in H^1(0, L)^4 \colon \mathcal{U}(0) - i\mathcal{U}'(0) = 0,$ $-i\mathcal{V}(0) + \mathcal{V}'(0) = 0,\ e^{-i2\pi L}\mathcal{U}(L) - i\mathcal{U}'(L) = 0,\ -ie^{-i2\pi L}\mathcal{V}(L) + \mathcal{V}'(L) = 0\}$, then by Prop. 2.1, Condition I on p.27 and Condition II on p.28 in [6] are fulfilled and we can apply Theorem 2.4.1 in [6]. The assertion of this theorem can be obtained also from Theorem 1.1 in [14]. $\qquad\square$

In what follows we assume that the integer N defining a threshold ω_N is fixed. Then according to Proposition 2, there exist ϵ_0 and γ_N such that for $\omega = \omega_\epsilon$ with some small positive $\epsilon \in [0, \epsilon_0]$, the strip $|\operatorname{Im}\lambda| \leqslant \gamma_N$ contains only real wavenumbers $\pm\lambda_j$, $j = 1, \ldots, N-1$ and two imaginary $\pm\lambda_\epsilon$ and the corresponding wavefunctions are

$$\mathbf{w}_1^\pm, \mathbf{w}_2^\pm, \ldots, \mathbf{w}_{N-1}^\pm, \mathbf{w}_N^\pm.$$

All waves but last two are oscillatory. Those last waves are of exponential growth.

Theorem 4. *Let γ_N and ϵ_0 be the same positive numbers as in Proposition 2 and let also $(g, h, g', h') \in L_\gamma^+(\Pi) \cap L_\gamma^-(\Pi)$. Denote by $(u^\pm, v^\pm, u^{'\pm}, v^{'\pm}) \in X_\gamma^\pm$ the solution of problem* (32), (33), (34), (35) *with the boundary conditions* (5), (6), *which exist according to Theorem 3. Then*

$$(u^+, v^+) = (u^-, v^-) + \sum_{j=1}^N C_j^+ \mathbf{w}_j^+ + \sum_{j=1}^N C_j^- \mathbf{w}_j^-,$$

where

$$-iC_j^+ = \int_\Pi (g, h, g', h') \cdot \overline{\mathbf{w}_j^+} \, dxdy, \quad iC_j^- = \int_\Pi (g, h, g', h') \cdot \overline{\mathbf{w}_j^-} \, dxdy.$$

Proof. The functions $\mathbf{w}_j^\pm$ correspond to functions (2.11) and (2.12) on p.30 from [6], and so by Prop. 2.8.1 in [6] we obtain the claim in the theorem. $\qquad\square$

§3. The Dirac equation with potential

3.1. Problem statement. Here we examine the problem with a potential, prove its solvability result and asymptotic formulas for the solutions.

Consider the nanoribbon with a potential:

$$\mathcal{D} \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} + \delta \mathcal{P} \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} = \omega \begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix}, \tag{36}$$

with the boundary conditions (5), (6). Here, $\mathcal{D}$ is defined in (2), $\mathcal{P} = \mathcal{P}(x, y)$ is a bounded, continuous real-valued function with compact support in $\overline{\Pi}$ and δ is a small parameter. We assume in what follows that

$$\operatorname{supp}\mathcal{P} \subset [-R_0, R_0] \times [0, 1] \quad \text{and} \quad \sup_{(x,y) \in \Pi} |\mathcal{P}| \leqslant 1,$$

where R_0 is a fixed positive number.

We assume that N, γ, ϵ_0 are fixed and

$$\omega = \omega_\epsilon, \quad \text{where} \quad \omega_\epsilon = \omega_N - \epsilon,$$

with $\epsilon \in [0, \epsilon_0]$ according to 2(i).

Since the norm of the multiplication by $\delta\mathcal{P}$ operator in $L^2(\Pi)$ is less than δ we derive from Theorem 3 the following

Theorem 5. *The operator*

$$\mathcal{D} + (\delta\mathcal{P} - \omega_\epsilon)\mathcal{I} \; : \; X_\gamma^\pm \to L_\gamma^\pm(\Pi)$$

is an isomorphism for $|\delta| \leqslant \delta_0$, where δ_0 is a positive constant depending on the norm on the inverse operator $(\mathcal{D} - \omega_\epsilon I)^{-1} \; : \; L_\gamma^\pm(\Pi) \to L_\gamma^\pm(\Pi)$.

We introduce two new spaces for $\gamma > 0$

$$\mathcal{H}_\gamma^+ = \left\{ (u, v, u', v') \; : \; (u, v, u', v') \in X_\gamma^+ \cap X_\gamma^- \right\}$$

and

$$\mathcal{H}_\gamma^- = \left\{ (u, v, u', v') \; : \; (u, v, u', v') \in X_\gamma^+ \cup X_\gamma^- \right\}.$$

The norms in this spaces are defined by

$$\|(u, v, u', v'); \mathcal{H}_\gamma^\pm\|^2 = \int_\Pi e^{\pm 2\gamma|x|} \left(|u|^2 + |v|^2 + |u'|^2 + |v'|^2 + |\mathcal{D}(u, v, u', v')^t|^2 \right) dxdy.$$

Note that, $\mathcal{H}_0^+ = \mathcal{H}_0^- = X_0$, where X_0 was introduced in Sec. 2.1.

Let also $\mathcal{L}_\gamma^\pm$, $\gamma > 0$, be two weighted L^2-spaces in Π with the norms

$$\|(u, v, u', v'); \mathcal{L}_\gamma^\pm\|^2 = \int_\Pi e^{\pm 2\gamma|x|} \left(|u|^2 + |v|^2 + |u'|^2 + |v'|^2 \right) dxdy.$$

We define two operators acting in the introduced spaces

$$A_\gamma^\pm = A_\gamma^\pm(\epsilon, \delta) = \mathcal{D} + (\delta\mathcal{P} - \omega)\mathcal{I} \; : \; \mathcal{H}_\gamma^\pm \to \mathcal{L}_\gamma^\pm.$$

Some important properties of these operator are collected in the following

Theorem 6. *The operators $A_\gamma^\pm$ are Fredholm and* $\ker A_\gamma^+ = \{0\}$*,* $coker A_\gamma^- = \{0\}$*. Moreover*

$$\dim coker A_\gamma^+ = \dim \ker A_\gamma^- = 2N.$$

Proof. The proof repeats reasoning presented in the proof of Theorem 3.2 in [7]. □

In the next theorem and in what follows, we fix four smooth functions, $\chi_\pm = \chi_\pm(x)$ and $\eta_\pm = \eta_\pm(x)$ such that $\chi_+(x) = 1$, $\chi_-(x) = 0$ for $x > R_0$ and $\chi_+(x) = 0$, $\chi_-(x) = 1$ for $x < -R_0$. Then let $\eta_\pm(x) = 1$ for large positive $\pm x$, $\eta_\pm(x) = 0$ for large negative $\pm x$ and $\chi_\pm\eta_\pm = \chi_\pm$.

Let us derive an asymptotic formula for the solution to the perturbed problem (36), (5), (6).

Theorem 7. *Let $f \in \mathcal{L}_\gamma^+$ and let $w = (u, v, u', v') \in \mathcal{H}_\gamma^-$ be a solution to*

$$(\mathcal{D} + (\delta\mathcal{P} - \omega)\mathcal{I})w = f. \tag{37}$$

satisfying (5), (6). *Then*

$$w = \eta_+ \sum_{j=1}^N \sum_{\tau=\pm} C_j^\tau \mathbf{w}_j^\tau + \eta_- \sum_{j=1}^N \sum_{\tau=\pm} D_j^\tau \mathbf{w}_j^\tau + R,$$

where $R \in \mathcal{H}_\gamma^+$.

Proof. The proof is analogous to the proof of Theorem 3.3 in [7]. □

3.2. The augumented scattering matrix. The scattering matrix is our main tool for the identification of the trapped modes. Using the q-form, we define the incoming/outgoing waves. The scattering matrix is defined via coefficients in this combination of waves. It is important to point out that this matrix is often called augmented as it contains coefficients of the waves exponentially growing at infinity as well. Finally, by the end of the section we define a space with separated asymptotics and check that it produces a unique solution to the perturbed problem.

Let

$$Q_R(w, \tilde{w}) = q_R(w, \tilde{w}) - q_{-R}(w, \tilde{w}).$$

If $w = (u, v)$ and $\tilde{w} = (\tilde{u}, \tilde{v})$ are solutions to (36), (5), (6) for $|y| \geqslant R_0$, then using the Green's formula one can show that this form is independent of $R \geqslant R_0$. We introduce two sets of localized waves at $\pm\infty$ waves, which we call outgoing and incoming (for physical interpretation see Appendix B)

$$W_k^{\pm} = W_k^{\pm}(x, y; \epsilon) = \chi_{\pm}(y)\mathbf{w}_k^{\pm}(x, y) \tag{38}$$

and

$$V_k^{\mp} = V_k^{\mp}(x, y; \epsilon) = \chi_{\pm}(y)\mathbf{w}_k^{\mp}(x, y) \tag{39}$$

with $k = 1, \ldots, N$. The reason for introducing this sets of waves is the property

$$Q_R(W_k^{\tau}, W_j^{\theta}) = i\delta_{k,j}\delta_{\tau,\theta}, \quad Q_R(V_k^{\tau}, V_j^{\theta}) = -i\delta_{k,j}\delta_{\tau,\theta} \tag{40}$$

where for $j, k = 1, \ldots, N$. Moreover,

$$Q_R(W_k^{\tau}, V_j^{\theta}) = 0. \tag{41}$$

Thus the sign of the Q product separates waves W and V.

In the next lemma we give a description of the kernel of the operator A_{γ}^{-}, which is used in the definition of the scattering matrix.

Theorem 8. *There exists a basis in* $\ker A_{\gamma}^{-}$ *of the form*

$$z_k^{\tau} = V_k^{\tau} + \sum_{\theta=\pm} \sum_{j \in \mathcal{I}_{\kappa}} \mathbf{S}_{k\tau}^{j\theta} W_j^{\theta} + \tilde{z}_k^{\tau}, \tag{42}$$

where $\tilde{z}_k^{\tau} \in \mathcal{H}_{\gamma}^{+}$. *Moreover, the coefficients* $\mathbf{S}_{k\tau}^{j\theta} = \mathbf{S}_{k\tau}^{j\theta}(\epsilon, \delta)$ *are uniquely defined.*

Proof. The proof repeats the reasoning presented in the proof of Theorem 3.4 in [7]. □

The scattering matrix $\mathbf{S}$ is defined through the kernel of operator A_{γ}^{-} that is through the formula (42).

3.3. The block notation. An important role in the construction of a trapped mode, is played by a part of the scattering matrix defined within the block notation.

Let us write

$$\mathbf{W} = (\mathbf{W}_{\bullet}, \mathbf{W}_{\dagger}), \quad \mathbf{V} = (\mathbf{V}_{\bullet}, \mathbf{V}_{\dagger}),$$

where

$$\mathbf{W}_{\bullet} = (W_1^+, W_1^-, \ldots, W_{N-1}^+, W_{N-1}^-), \quad \mathbf{V}_{\bullet} = (V_1^+, V_1^-, \ldots, V_{N-1}^+, V_{N-1}^-),$$

and
$$\mathbf{W}_\dagger = (W_N^+, W_N^-), \quad \mathbf{V}_\dagger = (V_N^+, V_N^-).$$

Equation (42) in the vector form reads
$$\mathbf{z} = \mathbf{V} + \mathbf{S}\mathbf{W} + \mathbf{r} \tag{43}$$

with
$$\mathbf{z} = (\mathbf{z}_\bullet, \mathbf{z}_\dagger), \quad \mathbf{r} = (\mathbf{r}_\bullet, \mathbf{r}_\dagger),$$

and
$$\mathbf{z}_\bullet = (z_1^+, z_1^-, .., z_{N-1}^+, z_{N-1}^-) \in \mathcal{H}_\gamma^-, \quad \mathbf{r}_\bullet = (r_1^+, r_1^-, .., r_{N-1}^+, r_{N-1}^-) \in \mathcal{H}_\gamma^+, \tag{44}$$
$$\mathbf{z}_\dagger = (z_N^+, z_N^-) \in \mathcal{H}_\gamma^-, \quad \mathbf{r}_\dagger = (r_N^+, r_N^-) \in \mathcal{H}_\gamma^+.$$

Here both vectors $\mathbf{z}$ and r have $2N$ elements. The matrix $\mathbf{S} = \mathbf{S}(\epsilon, \delta)$ is written in the block form

$$\mathcal{S} = \begin{pmatrix} \mathbf{S}_{\bullet\bullet} & \mathbf{S}_{\bullet\dagger} \\ \mathbf{S}_{\dagger\bullet} & \mathbf{S}_{\dagger\dagger} \end{pmatrix}.$$

The symmetry transformations T_1, T_2, T_3 applied to waves (19), (31) gives

$$T_1 \mathbf{w}_j^\tau = i\mathbf{w}_j^{-\tau}, \quad T_3 \mathbf{w}_j^\tau = e^{i\kappa_j L}\mathbf{w}_j^{-\tau}, \quad j = 1, 2, \dots, N, \ \tau = \pm,$$

$$T_2 \mathbf{w}_j^\tau = -\frac{\tau\lambda_j + i\kappa_j}{\omega}\mathbf{w}_j^{-\tau}, \quad j = 1, 2, \dots, N-1, \ \tau = \pm$$

and

$$T_2 \mathbf{w}_N^+ = \frac{\lambda_\epsilon^2 - 1}{2\omega_\epsilon}\mathbf{w}_N^+ + \frac{-2i\kappa_N - 1 - \lambda_\epsilon^2}{2\omega_\epsilon}\mathbf{w}_N^-,$$

$$T_2 \mathbf{w}_N^- = \frac{-2i\kappa_N + 1 + \lambda_\epsilon^2}{2\omega_\epsilon}\mathbf{w}_N^+ + \frac{-\lambda_\epsilon^2 + 1}{2\omega_\epsilon}\mathbf{w}_N^-.$$

The symmetry T_1 leads to important properties of the matrix S, that are used later, in Sec. 4.2, namely

$$S_{k\tau}^{k\tau} = S_{k(-\tau)}^{k(-\tau)}, \quad S_{k\tau}^{j\theta} = S_{j(-\theta)}^{k(-\tau)}, \quad k, j = 1, \dots, N, \ k \neq j, \ \tau, \theta = \pm,$$

that is illustrated in colorful bullets in Figure 3. In the case $\mathcal{P}(x, y) = \mathcal{P}(x, L - y)$, the symmetry T_3 implies

$$S_{N\tau}^{j\theta} = 0 \quad \text{for} \quad N - j \text{ being an odd number}$$

and

$$S_{N-}^{k+} = S_{N+}^{k-}, \quad S_{k+}^{N-} = S_{k-}^{N+}.$$

The relations for symmetry T_2 require the assumption $\mathcal{P}(x, y) = \mathcal{P}(-x, y)$ and are more complicated. In our construction of a potential introducing

a trapped mode in Sec. 4.2, we use the symmetries T_1 and T_3 assuming $\mathcal{P}(x, y) = \mathcal{P}(x, L - y)$; however we do not require $\mathcal{P}(x, y) = \mathcal{P}(-x, y)$.

Relations (40) and (41) take the form

$$Q(\mathbf{W}, \mathbf{W}) = i\mathbb{I}\,, \quad Q(\mathbf{V}, \mathbf{V}) = -i\mathbb{I} \quad Q(\mathbf{W}, \mathbf{V}) = \mathbb{O}. \tag{45}$$

where $\mathbb{I}$ is the identity matrix and $\mathbb{O}$ is the null matrix of appropriate size.

3.4. Properties of the scattering matrix.

Proposition 3. *The scattering matrix* $\mathbf{S}$ *is unitary.*

Proof. From the Green's formula $Q(\mathbf{z}, \mathbf{z}) = 0$, that together with (45) gives

$$0 = Q(\mathbf{V} + \mathbf{SW}, \mathbf{V} + \mathbf{SW}) = Q(\mathbf{V}, \mathbf{V}) + Q(\mathbf{SW}, \mathbf{SW}) = -i\mathbb{I} + i\mathbf{SS}^*,$$

what furnishes the result. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Consider the non-homogeneous problem (37) with $f \in \mathcal{L}_\gamma^+(\Pi)$. This problem has a solution $w \in \mathcal{H}_\gamma^-$ which admits the asymptotic representation

$$w = \sum_{j=1}^{N} \sum_{\tau=\pm} C_{j\tau}^1 W_j^\tau + \sum_{j=1}^{N} \sum_{\tau=\pm} C_{j\tau}^2 V_j^\tau + R, \quad R \in \mathcal{H}_\gamma^+ \tag{46}$$

which is a rearrangement of the representation (47). This motivates the following definition of the space $\mathcal{H}_\gamma^{out}$ consisting of vector functions $w \in \mathcal{H}_\gamma^-$ which admits the asymptotic representation (46) with $C_{j\tau}^2 = 0$. The norm in this space is defined by

$$\|w; \mathcal{H}_\gamma^{\text{out}}\| = \left(\|R; \mathcal{H}_\gamma^+\|^2 + \sum_{j=1}^{N} \sum_{\tau=\pm} |C_{j\tau}^1|^2 \right)^{1/2}.$$

Now, we note that the kernel in Theorem 8 can be equivalently spanned by

$$Z_k^\tau = W_k^\tau + \sum_{\theta=\pm} \sum_{j=1}^{N} \tilde{\mathbf{S}}_{k\tau}^{j\theta} V_j^\theta + \tilde{Z}_k^\tau, \quad \tilde{Z}_k^\tau \in \mathcal{H}_\gamma^+,$$

where the incoming and outgoing waves were interchanged (compare with (42)) and $\tilde{S}$ is a scattering matrix corresponding to that exchange.

Theorem 9. *For any* $f \in \mathcal{L}_\gamma^+(\Pi)$, *problem* (37) *has a unique solution* $w \in \mathcal{H}_\gamma^{out}$ *and the following estimate holds*

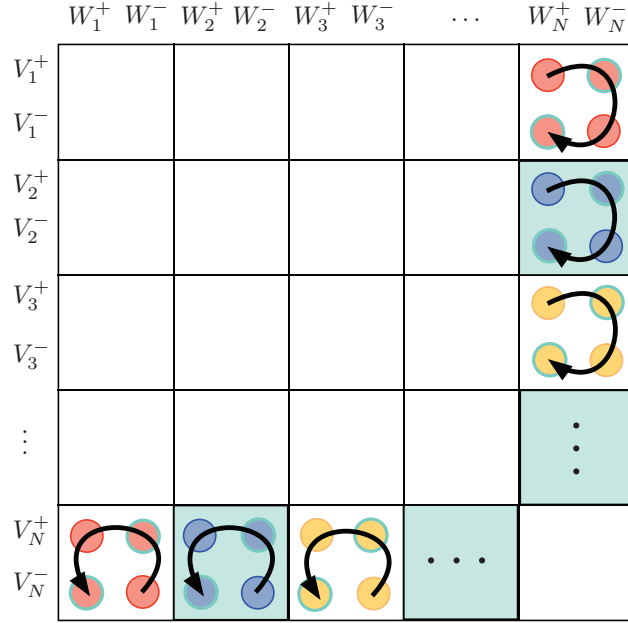$$\|w; \mathcal{H}_\gamma^{\text{out}}\| \leqslant c\|f; \mathcal{L}_\gamma^+(\Pi)\|,$$

Figure 3. Symmetries in the augumented scattering matrix S (only the part with $S_{\dagger\bullet}$ and $S_{\bullet\dagger}$ are considered). According to symmetry T_1, the left bottom square has permuted elements of the right top square: they are indicated in red and the permutation follows the arrows, that is the first element is placed by the beginnings of arrows and the last by the ends. Similar permutations for other squares are indicated in blue and yellow. From symmetry T_3 follows that all the elements in the green squares (every second square but not the right bottom square) are zero; moreover elements within square with red elements that have green borders are equal, similarly for blue and yellow elements.

where the constant c is independent of $\epsilon \in [0, \epsilon_N]$ and $|\delta| \leqslant \delta_0$. Moreover,

$$iC_{j\tau}^1 = \int_\Pi f \cdot \overline{Z_j^\tau} dx dy. \tag{47}$$

Proof. The proof is analogous to the proof of Theorem 3.5, presented in [7]. □

We represent $\mathbf{S}$ as

$$\mathbf{S} = \mathbb{I} + \mathbf{s}, \quad \text{or, equivalently,} \quad \mathbf{S}^{k\theta}_{j\tau} = \delta_{k,j}\delta_{\tau,\theta} + \mathbf{s}^{k\theta}_{j\tau}.$$

Theorem 10. *The scattering matrix $\mathbf{S}(\epsilon, \delta)$ depends analytically on small parameters $\epsilon \in [0, \epsilon_N]$ and $\delta \in [-\delta_0, \delta_0]$. Moreover,*

$$\mathbf{s}^{k\theta}_{j\tau} = i\delta \int\limits_\Pi \mathcal{P}\mathbf{w}^\tau_j \cdot \overline{\mathbf{w}^\theta_k} dxdy + O(\delta^2). \tag{48}$$

Proof. The proof follows the idea of the proof of Theorem 3.6 in [7]. □

§4. TRAPPED MODES

4.1. Necessary and sufficient conditions for the existence of trapped mode solutions. Let us first introduce a value d which is crucial for the formulation of the necessary and sufficient condition for the existence of trapped modes

$$d(\epsilon) = \frac{\lambda_\epsilon + 1}{\lambda_\epsilon - 1} = -1 - i2\sqrt{\epsilon}\sqrt{2\omega_N} + O(\epsilon), \quad |d| = 1. \tag{49}$$

Theorem 11. *Problem* (36) *with boundary conditions* (5), (6) *has a non-trivial solution in X_0 (a trapped mode), if and only if the following matrix is degenerate*

$$\mathbf{S}_{\dagger\dagger} + d(\varepsilon)\Upsilon, \quad \Upsilon = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Proof. A trapped mode $w \in X_0$, is a solution to (36) with boundary conditions (5), (6), so certainly $w \in \ker A_{-\gamma}$ and hence

$$w = a(\mathbf{V} + \mathbf{S}\mathbf{W} + \mathbf{r})^\top,$$

where $a = (a_\bullet, a_\dagger) \in \mathbb{C}^{2N}$ and $\mathbf{V}$, $\mathbf{W}$ and $\mathbf{r}$ are the vector functions from the representation of the kernel of $A_{-\gamma}$ in (43). Using the splitting of vectors and the scattering matrix in $\bullet$ and $\dagger$ components, we write the above relation as

$$w = a_\bullet(\mathbf{V}_\bullet + \mathbf{S}_{\bullet\bullet}\mathbf{W}_\bullet + \mathbf{S}_{\bullet\dagger}\mathbf{W}_\dagger + \mathbf{r}_\bullet)^T + a_\dagger(\mathbf{V}_\dagger + \mathbf{S}_{\dagger\dagger}\mathbf{W}_\dagger + \mathbf{S}_{\dagger\bullet}\mathbf{W}_\bullet + \mathbf{r}_\dagger)^\top.$$

The first term in the right-hand side contains waves oscillating at $\pm\infty$ and to guarantee the vanishing of this term we must require $a_\bullet = 0$. Since $\mathbf{r}$ vanishes at $\pm\infty$, a trapped mode $w \in X_0$ has a representation with

$$a_\dagger (\mathbf{V}_\dagger + \mathbf{S}_{\dagger\dagger}\mathbf{W}_\dagger + \mathbf{S}_{\dagger\bullet}\mathbf{W}_\bullet)^\top \text{ is vanishing at } \pm\infty. \tag{50}$$

From the representations (31) and (50), matching the coefficients for the increasing exponents at $\pm\infty$ we arrive at

$$\frac{a_1}{2\mathcal{N}}\frac{\lambda_\epsilon + 1}{\lambda_\epsilon} + (a_1, a_2)\mathbf{S}_{\dagger\dagger}\left(0, \frac{1}{2\mathcal{N}}\frac{\lambda_\epsilon - 1}{\lambda_\epsilon}\right)^\top = 0, \tag{51}$$

$$\frac{a_2}{2\mathcal{N}}\frac{\lambda_\epsilon + 1}{\lambda_\epsilon} + (a_1, a_2)\mathbf{S}_{\dagger\dagger}\left(\frac{1}{2\mathcal{N}}\frac{\lambda_\epsilon - 1}{\lambda_\epsilon}, 0\right)^\top = 0, \tag{52}$$

where $a_\dagger = (a_1, a_2)$. Using the definition of $d(\epsilon)$ in (49), we write equations (51) and (52) as

$$a_\dagger\left(\mathbf{S}_{\dagger\dagger} + d(\epsilon)\Upsilon\right) = 0. \tag{53}$$

Now, using the condition (53), the unitarity property of matrix $\mathbf{S}$ and $a_\bullet = 0$, we get

$$|a_\dagger|^2 = |a|^2 = |\mathbf{S}a|^2 = |a_\dagger\mathbf{S}_{\dagger\bullet}|^2 + |a_\dagger\mathbf{S}_{\dagger\dagger}|^2 = |a_\dagger\mathbf{S}_{\dagger\bullet}|^2 + |da_\dagger|^2.$$

Since $|d| = 1$, we have $a_\dagger\mathbf{S}_{\dagger\bullet} = 0$ and so w with asymptotic representation (50) does not contain any oscillatory waves and is vanishing at $\pm\infty$.
□

4.2. Proof of Theorem 1 . In this section, we construct an example potential, that produces a trapped mode. The potential is extracted from the asymptotic analysis of a set of conditions posed on the scattering matrix $\mathbf{S}$. The crucial condition concerns the augumented part of the scattering matrix $\mathbf{S}$ and arrives from Theorem 11

$$\det(\mathbf{S}_{\dagger\dagger} + d\Upsilon) = 0. \tag{54}$$

To distinguish between small and big elements in the asymptotic analysis, let us introduce the following notation

$$d(\epsilon) = -e^{i\sigma}, \quad \mathbf{S} = \mathbb{I} + \mathbf{s}, \quad \mathbf{s} =: i\delta s, \tag{55}$$

where

$$\sigma = \sqrt{\epsilon}2\sqrt{2\omega_N} + O(\epsilon^{3/2}), \tag{56}$$

from expansion (49). From (48), $\mathbf{s}$ is of order δ and hence s in (55) is of order 1. Now, we have three small parameters ϵ, σ and δ.

To resolve the condition (54), let us list the properties of the scattering matrix $\mathbf{S}$.

First of all, the symmetry T_1 is valid for any choice of potential $\mathcal{P}$, provided it is a real-valued function. This symmetry imposes the following relations on the elements of the matrix s:

$$s_{N\theta}^{j\tau} = s_{j(-\tau)}^{N(-\theta)}, \quad j = 1, \ldots, N-1, \ \ \tau, \theta = \pm, \tag{57}$$

$$s_{N+}^{N+} = s_{N-}^{N-}. \tag{58}$$

Those relations are illustrated in the sketch of the scattering matrix $\mathbf{S}$ in Figure 3.

Secondly, requiring the symmetry of the potential $\mathcal{P}(x, y) = \mathcal{P}(x, L-y)$, all the elements of the matrix $\mathbf{S}$ that are odd functions of y with respect to $\frac{L}{2}$ vanish. We identify those elements using the symmetry T_3 (Figure 3).

Taking into account the unitarity property of the matrix $\mathbf{S}$ and all the above listed properties, we seek for $\mathcal{P}$ and small $\delta > 0$ that satisfy the relations

$$s_{N+}^{j\tau} = 0, \quad s_{N-}^{N+} = 0 \tag{59}$$

with $\tau = \pm$, $j \in \mathcal{I}nd_S$, where

$$\mathcal{I}nd_S = \begin{cases} j = 1, 3, \ldots, N-1 & \text{when } N \text{ is even,} \\ j = 2, 4, \ldots, N-2 & \text{when } N \text{ is odd.} \end{cases}$$

This choice together with the unitarity property and symmetries (57), (58) yield

$$s_{N-}^{j\tau} = 0, \quad s_{j\tau}^{N+} = 0, \quad , s_{j\tau}^{N-} = 0, \quad s_{N+}^{N-} = 0,$$

with $\tau = \pm$, $j = 1, 2, \ldots, N-1$ and

$$|1 + i\delta s_{N+}^{N+}| = 1.$$

Thus condition (54) becomes

$$1 + i\delta s_{N+}^{N+} = \pm d,$$

that is equivalent to

$$\mathrm{Im}(1 + i\delta s_{N+}^{N+}) = \pm \,\mathrm{Im}\, d. \tag{60}$$

To solve this equation, we fix the last small parameter

$$\delta = \sin\sigma,$$

that according to the expansion (56) gives $\delta = \sqrt{\epsilon}C_d(1 + O(\epsilon))$ with $C_d = 2\sqrt{2\omega_N}$ and (60) becomes

$$\mathrm{Re}(s_{N+}^{N+}) = \pm 1,$$

In particular, we seek for the potential $\mathcal{P}$ so that

$$\mathrm{Re}(s_{N+}^{N+}) = 1, \tag{61}$$

together with (59).Let us use the asymptotic formula

$$s_{j\tau}^{k\theta}(\delta\mathcal{P}) = \int\limits_{\Pi} \mathcal{P}\mathbf{w}_j^\tau \cdot \overline{\mathbf{w}_k^\theta} dxdy + O(\delta) \tag{62}$$

with $j, k = 1, 2, \ldots, N$ and $\tau, \theta = \pm$ which follows from (48) and (55).

Getting together the set of conditions (59) and (61), we obtain the following system of $2(N+1)+3$ equations when N is even and of $2(N-1)+3$ equations, when N is odd

$$\mathrm{Re}\, s_{N+}^{j\tau}(\delta\mathcal{P}) = 0, \;\; \mathrm{Im}\, s_{N+}^{j\tau}(\delta\mathcal{P}) = 0, \;\; j \in \mathcal{I}nd_S, \;\; \tau = \pm, \tag{63}$$

$$\mathrm{Re}\, s_{N-}^{N+}(\delta\mathcal{P}) = 0, \;\; \mathrm{Im}\, s_{N-}^{N+}(\delta\mathcal{P}) = 0, \tag{64}$$

and

$$\mathrm{Re}\left(s_{N+}^{N+}(\delta\mathcal{P})\right) = 1. \tag{65}$$

To unite the notation, we introduce the set of indeces:

$$\mathcal{I}nd = \Big\{\alpha = (j, \tau, \Xi): \quad j \in \mathcal{I}nd_S; \tau = \{+, -\}; \Xi = \{\mathrm{Re, Im}\};$$

$$j = N; \tau = -; \Xi = \{\mathrm{Re, Im}\}; \quad j = N; \tau = +; \Xi = \mathrm{Re}\Big\}. \tag{66}$$

The indices with $j \in \mathcal{I}nd_S$ are related to equation (63), the indices with $j = N$, $\tau = +$ correspond to (64) and the last index $(N, +, \mathrm{Re})$ corresponds to (65).We are looking for the potential having the following from:

$$\mathcal{P}(x, y) = \Phi(x, y) + \sum_{\alpha \in \mathcal{I}nd} \eta^\alpha \Psi^\alpha(x, y)$$

where the functions $\Phi, \{\Psi^\alpha\}_{\alpha \in \mathcal{I}nd}$are continuous, real valued with compact support in $[-R_0, R_0] \times [0, 1]$. The functions are assumed to be fixed and are subject to a set of conditions that are presented later on in this section. The unknown coefficients $\{\eta^\alpha\}_{\alpha \in \mathcal{I}nd}$ can be chosen from the Banach Fixed Point Theorem. Using indices $\mathcal{I}nd$ (66) and the asymptotic form of the scattering matrix (62) we define

$$s_\alpha := \Xi s_{j\tau}^{N+}, \;\; \alpha \neq (N, +, \mathrm{Re}); \;\; s_\alpha := \mathrm{Re}(s_{N+}^{N+}), \;\; \alpha = (N, +, \mathrm{Re})$$

and

$$v_\alpha := \Xi\left(\mathbf{w}_j^\tau \cdot \overline{\mathbf{w}_N^+}\right), \quad \alpha \neq (N, +, \mathrm{Re}); \quad v_\alpha := \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^+}, \quad \alpha = (N, +, \mathrm{Re}).$$

This enables us to write equations (63), (64) and (65), first in the scalar form

$$s_\alpha\left(\delta(\Phi + \sum_{\beta \in \mathcal{I}nd} \eta^\beta \Psi^\beta)\right) = \int_\Pi \left(\Phi + \sum_{\beta \in \mathcal{I}nd} \eta^\beta \Psi^\beta\right) v_\alpha dx dy - \delta\mu_\alpha(\delta, \boldsymbol{\eta}) = 0,$$
$$\alpha \in \mathcal{I}nd,$$

and then combine to a matrix form

$$\mathcal{M}(\delta, \boldsymbol{\eta}) := \boldsymbol{\Phi} + \mathcal{A}\boldsymbol{\eta} - \delta\boldsymbol{\mu}(\delta, \boldsymbol{\eta}) = \delta_{(N, +, \mathrm{Re})}^\alpha, \tag{67}$$

with a vector function $\mathcal{M} = \{\mathcal{M}_\alpha\}_{\alpha \in \mathcal{I}nd}$, a vector $\boldsymbol{\Phi} = \{\Phi_\alpha\}_{\alpha \in \mathcal{I}nd}$ with the elements

$$\Phi_\alpha = \int_\Pi \Phi v_\alpha dx dy, \tag{68}$$

the matrix $\mathcal{A} = \{\mathcal{A}_\alpha^\beta\}_{\alpha, \beta \in \mathcal{I}nd}$ given by

$$\mathcal{A}_\alpha^\beta = \int_\Pi \Psi^\beta v_\alpha dx dy,$$

a vector $\boldsymbol{\eta} = \{\eta^\alpha\}_{\alpha \in \mathcal{I}nd}$ with real unknown coefficients and a vector function $\boldsymbol{\mu} = \{\mu_\alpha\}_{\alpha \in \mathcal{I}nd}$ that depends on δ and $\boldsymbol{\eta}$ analytically (analyticity follows form Theorem 10).

Our goal is to solve system (67) with respect to $\boldsymbol{\eta}$. We reach it in three steps. First, we eliminate the constant "1" on the right-hand side of (67), as $\delta_{(N, +, \mathrm{Re})}^\alpha = 1$ for $\alpha = (N, +, \mathrm{Re})$, by an appropriate choice of function Φ. Secondly, we choose the functions $\{\Psi^\alpha\}_{\alpha \in \mathcal{I}nd}$ in such a way that $\mathcal{A}$ is a unit and our system becomes nothing more than $\boldsymbol{\eta} = f(\boldsymbol{\eta})$ (with a certain small function f) and is solvable due to the Banach Fixed Point Theorem.

The choice of function Φ is the following

$$\Phi_\alpha = 0, \quad \alpha \neq (N, +, \mathrm{Re}); \quad \Phi_\alpha = 1, \quad \alpha = (N, +, \mathrm{Re}) \tag{69}$$

and it is possible due to the following lemma.

Lemma 1. *When $2L$ is not a natural number, then functions*

$$\mathrm{Re}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^\tau}, \; \mathrm{Im}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^\tau}, \; \mathrm{Re}\, \mathbf{w}_N^- \cdot \overline{\mathbf{w}_N^+}, \; \mathrm{Im}\, \mathbf{w}_N^- \cdot \overline{\mathbf{w}_N^+}, \; \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^+} \tag{70}$$

with $j \in \mathcal{I}nd_S$, $\tau = \pm$ are linearly independent.

Proof. We first note that functions (70) continuously depend on ϵ, so for the proof of linear independence, it is enough to consider the limit case $\epsilon = 0$. Using the expressions (19) for the oscillatory waves w_j^τ and the formulas (31) for the exponential waves $\mathbf{w}_N^+$ and $\mathbf{w}_N^-$ with their asymptotic behaviour (25), (26), we can write

$$\mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^\tau} = e^{-\tau i \lambda_j x} a_j(y)(C_1^{j\tau} + xC_3^{j\tau} + i(C_2^{j\tau} + xC_4^j)),$$

with $\tau = \pm$ and $j \in \mathcal{I}nd_S$ or separating real and imaginary parts

$$\mathrm{Re}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^\tau} = a_j(y)\Big((C_1^{j\tau} + xC_3^{j\tau}) \cos(\lambda_j x) + \tau(C_2^{j\tau} + xC_4^j)\sin(\lambda_j x)\Big), \quad (71)$$

$$\mathrm{Im}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^\tau} = a_j(y)\Big((C_2^{j\tau} + xC_4^j)\cos(\lambda_j x) - \tau(C_1^{j\tau} + xC_3^{j\tau})\sin(\lambda_j x)\Big), \quad (72)$$

and for the expoential waves

$$\mathrm{Re}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^-} = \frac{\omega_N}{L}\Big(-4x^2 + \frac{4\mathrm{sign}(\kappa_N)}{\omega_N}x - \frac{2}{\omega_N^2} + 4\Big), \qquad (73)$$

$$\mathrm{Im}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^-} = \frac{\omega_N}{L}\Big(8x - \frac{4\mathrm{sign}(\kappa_N)}{\omega_N}\Big), \qquad (74)$$

$$\mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^+} = \frac{\omega_N}{L}\Big(2x^2 - \frac{2\mathrm{sign}(\kappa_N)}{\omega_N}x + \frac{1}{\omega_N^2} + 2\Big), \qquad (75)$$

with

$$a_j(y) = \frac{\omega_N}{4L\lambda_j} \cos\Big((\kappa_N - \kappa_j)y\Big) = \frac{\omega_N}{4L\lambda_j} \cos(\frac{\pi}{L}(N-j)y) \qquad (76)$$

being an even function with respect to $\frac{L}{2}$, and constants

$$C_1^{j\tau} = 1 + \mathrm{sign}(\kappa_j)\frac{\kappa_j}{\omega} + \frac{\tau\lambda_j}{\omega^2}, \quad C_2^{j\tau} = \mathrm{sign}(\kappa_j)\frac{\tau\lambda_j}{\omega} - \frac{\kappa_j}{\omega},$$

$$C_3^{j\tau} = -\mathrm{sign}(\kappa_j)\frac{\tau\lambda_j}{\omega}, \quad C_4^j = 1 + \mathrm{sign}(\kappa_j)\frac{\kappa_j}{\omega}.$$

From the form (76), functions $\{a_j(y)\}_{j\in\mathcal{I}nd}$ are linearly independent. Still for a fixed j , functions $\mathrm{Re}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^+}$, $\mathrm{Re}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^-}$, $\mathrm{Im}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^+}$, $\mathrm{Im}\, \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_j^-}$ in (71) and (72) could be linearly dependent, as they are linear combinations of four types of functions $\cos(\lambda_j x)$, $x\cos(\lambda_j x)$, $\sin(\lambda_j x)$ and $x\sin(\lambda_j x)$. However this possiblity is ruled out as the determinant with the coefficients of the composite functions $\cos(\lambda_j x)$, $x\cos(\lambda_j x)$, $\sin(\lambda_j x)$

and $x \sin(\lambda_j x)$ is non-zero. It follows that (71) and (72) are linearly independent. Finally the functions (73), (74), (75) belong to $\{1, x, x^2\}$ and are linear independent as $\operatorname{Re} \mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^-} + 2\mathbf{w}_N^+ \cdot \overline{\mathbf{w}_N^+} = 8$. $\qquad\square$

By Lemma 1, all the functions v_α in (68) are linearly independent. It follows that it is possible to choose Φ so that (69) holds and equations (67) is

$$\mathcal{A}\boldsymbol{\eta} - \delta\boldsymbol{\mu}(\delta, \boldsymbol{\eta}) = 0. \tag{77}$$

Now we set matrix $\mathcal{A}$ to be unit, that is its elements fulfill the conditions

$$\mathcal{A}_\alpha^\beta = \delta_{\alpha,\beta}, \ \ \alpha, \beta \in \mathcal{I}nd. \tag{78}$$

Again using Lemma 1, it is possible to choose functions $\{\Psi^\alpha\}_{\alpha \in \mathcal{I}nd}$ so that the conditions (78) are fulfilled and (77) reads

$$\boldsymbol{\eta} = \delta\boldsymbol{\mu}(\delta, \boldsymbol{\eta}). \tag{79}$$

Now, as δ is small, the operator on the right hand side of equation (79) is a contraction operator, moreover $\boldsymbol{\mu}$ is analytic in δ and $\boldsymbol{\eta}$ so from Banach Fixed Point Theorem equation (79) is solvable for $\boldsymbol{\eta}$.

We have just shown that it is possible to choose functions Φ, $\{\Psi^\alpha\}_{\alpha \in \mathcal{I}nd}$ and tune parameters $\boldsymbol{\eta}$ in such a way that the potential $\mathcal{P}$ produces a trapped mode.

A numerical example of a potential (leading term Φ) that produces a trapped mode is

$$\mathcal{P}(x,y) \approx \Phi(x,y) = e^{-(\frac{y-0.67}{0.2})^2}(0.54e^{-(x+0.14)^2} - e^{-(x+0.32)^2} + 0.54e^{-(x+0.49)^2})$$

for a nanoribbon of width $L = 1.33$ ($\frac{L}{2} = 0.67$) and energy $\omega \approx \omega_2 = 1.57$.

4.3. Proof of Theorem. In this section, we present the proof to the theorem about the multiplicity of the Trapped modes. We show that (i) there are no trapped modes for energies that are slightly bigger than the thresholds or are far from the thresholds, (ii) the multiplicity of a trapped mode, for energies slightly less than a threshold, is no more than one.

Proof. (i) Assume the contrary: there exist a trapped mode solution, which belongs to X_0. According to the Theorem 7 and Proposition 2 (ii), λ in the strip $\{|\operatorname{Im} \lambda| \leqslant \gamma\}$, in the exponential factor of the solutions (10), (14),

$$w(x,y) = e^{i\lambda x}(\mathcal{U}(y), \mathcal{V}(y), \mathcal{U}'(y), \mathcal{V}'(y))$$

are real, it follows that $w \in \mathcal{H}_\gamma^+$. However according to the Theorem 5, the operator $\mathcal{D} + (\delta\mathcal{P} - \omega_\epsilon)\mathcal{I} : X_\gamma^\pm \to L_\gamma^\pm(\Pi)$ is an isomorphism, it follows that the only solution to $\left(\mathcal{D} + (\delta\mathcal{P} - \omega_\epsilon)\mathcal{I}\right)w = 0$ is $w = 0$.

(ii) There exists at least one trapped mode given in Sec. 1. Assume now, that we have two trapped modes $w_1 \neq w_2$. From Theorem 7 and Proposition 2 (i), which states that there are exactly two solutions $w(x,y) = e^{i\lambda x}(\mathcal{U}(y), \mathcal{V}(y), \mathcal{U}'(y), \mathcal{V}'(y))$ with complex λ in the strip $\{|\operatorname{Im}\lambda| \leqslant \gamma\}$, it follows that the trapped mode is of the form

$$w_j = C_j e^{i\lambda_\epsilon x}(\mathcal{U}_N^+(y), \mathcal{V}_N^+(y), \mathcal{U}_N^{'+}(y), \mathcal{V}_N^{'+}(y))$$
$$+ D_j e^{-\lambda_\epsilon x}(\mathcal{U}_N^-(y), \mathcal{V}_N^-(y), \mathcal{U}_N^{'-}(y), \mathcal{V}_N^{'-}(y)) + R_j,$$

with $j = 1, 2$ and $R_j \in \mathcal{H}_\gamma^+$. Consider the following linear combination of trapped modes ω_1 and ω_2

$$w_3 = w_1 - \frac{C_1}{C_2}w_2 = \left(D_1 - \frac{C_1}{C_2}D_2\right)e^{-i\lambda_\epsilon^- x}(\mathcal{U}_N^-(y), \mathcal{V}_N^-(y), \mathcal{U}_N^{'-}(y), \mathcal{V}_N^{'-}(y))$$
$$+ \left(R_1 - \frac{C_1}{C_2}R_2\right) \in X_\gamma^+,$$

however form Theorem 5 as the operator $\mathcal{D} + (\delta\mathcal{P} - \omega_\epsilon)\mathcal{I} : X_\gamma^+ \to L_\gamma^+(\Pi)$ is an isomorphism, it follows that $w_1 = \frac{C_1}{C_2}w_2$. □

APPENDIX §A. NORM

Proof. Let us consider only a part of $\int_\Pi |\mathcal{D}(u, v, u', v')^\top|^2 dx dy$, that contains elements with functions u and u', namely

$$\int_\Pi |(i\partial_x - \partial_y)u|^2 + |(-i\partial_x - \partial_y)u'|^2 dx dy$$

$$= \int_\Pi \left(|\nabla u|^2 + |\nabla u'|^2\right)dx dy + i\int_\Pi \left(\overline{u}_x u_y - \overline{u}_y u_x - \overline{u}'_x u'_y + \overline{u}'_y u'_x\right)dx dy.$$

We show that due to the boundary conditions (5) and (6)

$$\int_\Pi \left(\overline{u}_x u_y - \overline{u}_y u_x - \overline{u}'_x u'_y + \overline{u}'_y u'_x\right)dx dy = 0.$$

Using integration by parts, we get

$$\int\limits_{\Pi} \left(\overline{u}_x u_y - \overline{u}_y u_x - \overline{u}'_x u'_y + \overline{u}'_y u'_x \right) dxdy = \int\limits_{-\infty}^{+\infty} \overline{u}_x u - \overline{u} u_x - \overline{u}'_x u' + \overline{u}' u'_x \Big|_0^L dx$$

$$= \int\limits_{-\infty}^{+\infty} \Big(\overline{u}_x(x,L)\Big(u(x,L) - ie^{i2\pi L}u'(x,L)\Big) - u_x(x,L)\Big(\overline{u}(x,L) + ie^{-i2\pi L}\overline{u}'(x,L)\Big)$$

$$- \overline{u}_x(x,0)\Big(u(x,0) - iu'(x,0)\Big) + u_x(x,0)\Big(\overline{u}(x,0) + i\overline{u}'(x,0)\Big)\Big) dxdy = 0,$$

where the last two equalities are consequence of the boundary conditions (5) and (6). In a similar way, one can show that the remaining part of $\int_{\Pi} |\mathcal{D}(u,v,u',v')^\top|^2 dxdy$, that contains elements with functions v and v' is

$$\int\limits_{\Pi} \Big(|(i\partial_x + \partial_y)v|^2 + |(-i\partial_x + \partial_y)v'|^2 \Big) dxdy = \int\limits_{\Pi} \Big(|\nabla v|^2 + |\nabla v'|^2 \Big) dxdy,$$

consequently

$$\int\limits_{\Pi} |\mathcal{D}(u,v,u',v')^\top|^2 dxdy = \int\limits_{\Pi} \Big(|\nabla u|^2 + |\nabla u'|^2 + |\nabla v|^2 + |\nabla v'|^2 \Big) dxdy.$$

$$\square$$

Appendix §B. The Mandelstam radiation condition

Here we want to clarify the splitting of waves in two classes (outgoing/incoming) according to the appearance of the $\pm i$ in (29). To do this we use the Mandelstam radiation conditions which defines outgoing and incoming waves by the direction of the energy transfer [8, 13, 16].

Let us write the original system (1) in the form

$$\mathcal{D}\mathbf{w} = i\partial_t \mathbf{w}, \quad \mathbf{w} = e^{-i\omega t}w, \quad \mathbf{w} = (\mathbf{u}, \mathbf{v}, \mathbf{u}', \mathbf{v}'). \tag{80}$$

The energy flux through the boundary is defined as

$$-\frac{d}{dt} \int\limits_{\Omega} |\partial_t \mathbf{w}|^2 dxdy.$$

Using relations (80) and performing partial integration we get

$$-\frac{d}{dt}\int_{\Omega}|\partial_t \mathbf{w}|^2 dxdy = -|\omega|^2\int_{\Omega}\Big(\overline{\mathbf{w}}\partial_t\mathbf{w}+\mathbf{w}\partial_t\overline{\mathbf{w}}\Big)dxdy$$

$$=-|\omega|^2\int_{\Gamma}\Big(\overline{\mathbf{u}}\mathbf{v}+\overline{\mathbf{v}}\mathbf{u}-(\overline{\mathbf{u}}'\mathbf{v}'+\overline{\mathbf{v}}'\mathbf{u}'),-i(\overline{\mathbf{u}}\mathbf{v}-\overline{\mathbf{v}}\mathbf{u}+\overline{\mathbf{u}}'\mathbf{v}'-\overline{\mathbf{v}}'\mathbf{u}')\Big)\cdot(n_x,n_y)ds,$$

where Γ is the boundary of area Ω. Consider the energy flux through the cross-section, that is choose $(n_x,n_y)=(1,0)$, then the last formula is equal to

$$-\frac{d}{dt}\int_{\Omega}|\partial_t\mathbf{w}|^2 dxdy = -|\omega|^2\int_0^L\Big(\overline{u}v+\overline{v}u-(\overline{u}'v'+\overline{v}'u')\Big)dy = -i|\omega|^2 q(w,w),$$

where the last equality comes from the the definition of q-form (27). Accordingly the energy transfer along the nanoribbon is proportional to $-iq$, which is ± 1 for $q=\pm i$. It follows that the value of the q-form defines direction of wave propagation, namely $q=i$ describes waves propagating from from $-\infty$ to $+\infty$ and $q=-i$ those from $+\infty$ to $-\infty$. This leads to the definition of outgoing/incoming waves (38), (39) as those travelling to $\pm\infty$ and from $\pm\infty$.

REFERENCES

1. T. Ando, T. Nakanishi, *Impurity Scattering in Carbon Nanotubes – Absence of Back Scattering.* — J. Phys. Soc. Jpn. **67** (1998), 1704–1713.
2. L. Brey, H. A. Fertig, *Electronic states of graphene nanoribbons studied with the Dirac equation.* — Phys. Rev. **B** 73 (2006), 235411.
3. A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, *The electronic properties of graphene.* — Rev. Mod. Phys. **81** (2009), 109.
4. Q. Chen, L. Ma, J. Wang, *Making graphene nanoribbons: a theoretical exploration.* — WIREs Comput. Mol. Sci. **6**, No. 3 (2016), 243–254.
5. I. V. Kamotskii, S. A. Nazarov *An augmented scattering matrix and an exponentially decreasing solution of elliptic boundary-value problem in the domain with cylindrical outlets.* — Zap. Nauchn. Sem. POMI **264**, (2000) 66–82.
6. V. Kozlov, V. Maz'ya, *Differential equations with operator coefficients with applications to boundary value problems for partial differential equations.* Springer Monographs in Mathematics. Springer-Verlag, Berlin, 1999.
7. V. A. Kozlov, S. A. Nazarov, A. Orlof, *Trapped modes in zigzag graphene nanoribbons.* — Z. Angew. Math. Phys. **68**, no. 4 (2017), Art. 78, 31 pp.
8. L. I. Mandelstam, *Lectures on Optics, Relativity, and Quantum Mechanics.* 2, AN SSSR, M., 1947.

9. P. Marconcini, M. Macucci, *The k B· p method and its application to graphene, carbon nanotubes and graphene nanoribbons: the Dirac equation,* La Rivista del Nuovo Cimento **45**, No. 8–9 (2011), 489–584.

10. S. A. Nazarov, *Asymptotic expansions of eigenvalues in the continuous spectrum of a regularly perturbated quantum waveguide.* — Theoretical and Mathematical Physics **167**, No. 2 (2011), 239–262.

11. S. A. Nazarov, *Enforced stability of an eigenvalue in the continuous spectrum of a waveguide with an obstacle.* — Zh. Vychisl. Mat. i Mat. Fiz. **52**, No. 3 (2012), 521–538.

12. S. A. Nazarov, *Enforced stability of a simple eigenvalue in the continuous spectrum of a waveguide.* — Funct. Anal. Appl. **47**, No. 3 (2013), 195–209.

13. S. A. Nazarov, *Umov-Mandelstam radiation conditions in elastic periodic waveguides.* — SB MATH, **205**, No. 7 (2014), 953–982.

14. S. A. Nazarov, B. A. Plamenevsky, *Elliptic problems in domains with piecewise smooth boundaries.* Walter de Gruyter, Berlin, New York 1994.

15. K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, *Electric Field Effect in Atomically Thin Carbon Films.* — Science **306** (2004), 666.

16. I. I. Vorovich, V. A. Babeshko, *Dynamical mixed problems of elasticity theory for nonclassical domains.* Nauka, M., 1979, 320.

Mathematics and Applied Mathematics,
MAI, Linköping University,
SE-58183 Linköping, Sweden

E-mail: `vladimir.kozlov@liu.se`

St.Petersburg State University,
Peter the Great St. Petersburg Polytechnic University,
Institute of Problems of Mechanical Engineering RAS,
St.-Petersburg, Russia

E-mail: `srgnazarov@yahoo.co.uk`

Mathematics and Applied Mathematics,
MAI, Linköping University,
SE-58183 Linköping, Sweden

E-mail: `a.orlof@gmail.com`