

# LOCALIZED WAVES IN CARBON NANO-STRUCTURES WITH CONNECTED AND DISCONNECTED OPEN WAVEGUIDES

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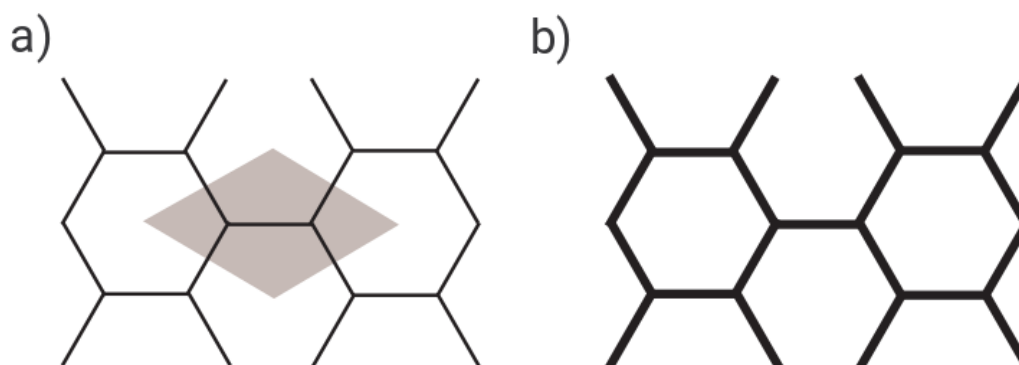
**Abstract.** A hexagonal lattice of quantum waveguides is considered with thickening or thinning of ligaments, which form open waveguides in the periodic nano-structure. Propagation of localized waves along the open connected and disconnected waveguides is studied and nodes in the lattice are indicated that support trapped modes with the exponential decay in all directions.

## 1. Problem setting

The graph  $G^0$  in the plane  $\mathbb{R}^2$  (see Fig. 1a) for a hexagonal one dimensional structure consisting of vertices and unit straight segments, edges, is expressed as a union of the shifts  $g^0(\tau)$ ,  $\tau = (\tau_1, \tau_2)$ ,  $\tau_j \in \mathbb{Z} = \{0, \pm 1, \pm 2, \dots\}$ , of the fundamental cell  $g^0$  entered into the parallelogram  $\mathbb{P}$  (shaded in Fig. 1a) defined by the vectors  $e_{\pm} = (3/2, \pm\sqrt{3}/2)$ . Angles between each three edges emerging from a vertex are  $2\pi/3$ . We consider two types of the “fat” structures in Fig. 1b, and 2a and b,

$$G^h = \{x = (x_1, x_2) : \text{dist}(x, G^0) < h/2\}, \quad G_H^h = (G^h \setminus L_1^h) \cup L_H^h, \quad (1)$$

where  $L_H^h$  is an open waveguide, either connected or disconnected. To obtain  $L_H^h$ , one chooses a subgraph  $L^0$  in  $G^0$  which can be a path as in Fig. 2a, or disruptive as in Fig. 2b. Then,  $L_H^h$  is a tubular  $hH$ -neighborhood of  $L^0$ . In the case  $H < 1$ , we observe thinning of ligaments in  $L_1^h \subset G^h$  and thickening while  $H > 1$ .



**Fig. 1.** The hexagonal graph  $G^0$  and the fattened lattice  $G^h$ .



## 2. The discrete spectrum of infinite tripod waveguides

Let us consider the Dirichlet problem

$$-\Delta w^H(\xi) = \mu^H w^H(\xi), \quad \xi \in Y_H^1, \quad (4)$$

$$w^H(\xi) = 0, \quad \xi \in \partial Y_H^1. \quad (5)$$

The infinite waveguide  $Y_H^h$  is composed from three pointed semi-strips, see Fig. 3a. The horizontal strip  $S_H^0$  is of width  $H$  and the tilted ones  $S_h^\pm$  of width  $h$ . Mid-lines of  $S_H^0$  and  $S_h^\pm$  meet each other at the coordinate origin  $\xi = 0$  and the angles between them are  $2\pi/3$ . The junction  $Y_H^1$ , in particular with  $H = 1$ , is obtained from  $G_H^h$  by the coordinate dilation

$$x \mapsto \xi = h^{-1}(x - \mathcal{O}) \quad (6)$$

and the formal passage to  $h = 0$ ; here,  $\mathcal{O}$  is a vertex of the graph  $G^0$ .

The continuous spectrum  $\Sigma_H^{co}$  of the problem (4), (5) is the semi-axis  $[\mu_+(1, H), +\infty)$  with the cut-off value  $\mu_+(1, H) = \pi^2 \min\{1, H^{-2}\}$ . It was verified in [7] that the discrete spectrum  $\Sigma_1^{di}$  consists of the only point  $\mu_1^1 \in (0, \pi^2)$ . It is also known, see e.g. [17], that the V-shaped waveguide shaded in Fig. 3c has a non-empty discrete spectrum in  $(0, \pi^2)$  and, hence the comparison principle [12, Theorem 10.2.2] assures the existence of an eigenvalue in  $\Sigma_H^{di}$  for  $H < 1$ . The same principle proves that the total multiplicity  $\#\Sigma_H^{di}$  is one because  $\#\Sigma_H^{di} \leq \#\Sigma_1^{di} = 1$  for  $H < 1$ .

The case  $H > 1$  is slightly more complicated because the growth of  $H$  leads to a decrease of the cut-off value  $\mu_+(1, H)$  in the waveguide  $Y_H^1$ . However, in the same way as in [19] it is possible to find  $H_* > 1$  such that  $\#\Sigma_H^{di} = 1$  when

$$H \in (0, H_*) \quad (7)$$

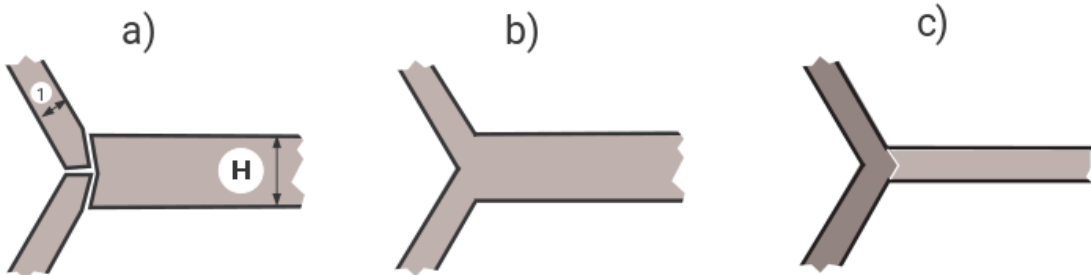
The discrete spectrum is empty for  $H \geq H_*$ . In what follows we vary the width  $H$  within the interval (7) and denote the corresponding isolated eigenvalue by  $\mu_H^1 \in (0, \mu_+(1, H))$ .

**Remark.** A result in [20] demonstrates that the problem (4), (5) in the waveguide  $Y_{H_*}^1$  with the critical width  $H_*$  has a bounded solution at the threshold spectral parameter  $\mu = \mu_+(1, H_*)$ . As was shown, see [7] and [11] for hexagonal lattices, this peculiar feature of the tripod causes a change of transmission conditions at the vertices of the graph  $G^0$  modeling the lattice.

The coordinate change  $\xi \mapsto H^{-1} \xi$  reveals the only point  $\mu_H^H = H^{-2} \mu_1^1$  in the discrete spectrum of the waveguide  $Y_H^H$  composed of three congruent tapered strips of width  $H \neq 1$ . The same transformation converts  $Y_1^H$  into  $Y_{1/H}^1$  and, thus,  $\mu_H^H = H^{-2} \mu_{1/H}^1$ . To keep the conclusion on the single eigenvalue we assume in this case that  $H \in (H_*^{-1}, +\infty)$ . The eigenfunction  $W_H^h$  of the problem (4), (5) in  $Y_H^h$  corresponding to the above-mentioned eigenvalue  $\mu_H^h \in (0, \mu_+(h, H))$  has the exponential decay at infinity

$$W_H^h(\xi) = \mathcal{O}\left(e^{-\delta_H^h |\xi|}\right), \quad \delta_H^h = \sqrt{\pi^2 - (\mu_H^h)^2} > 0. \quad (8)$$

We normalize this function in Lebesgue space  $L^2(Y_H^h)$ .



**Fig. 3.** The Y-shaped waveguide.



in the infinite vertical truss  $\Pi_H^h = \left\{x: |x_1| < \frac{3}{2}, (x_1 - 3N, x_2) \in G_{H+}^h\right\}$  (this domain is independent of  $N \in \mathbb{N}$  and enters the shaded strip in Fig. 2b with the quasi-periodicity conditions at the truncation sets  $T_{H\pm}^h = \left\{x: x_1 = \pm \frac{3}{2}, (x_1 - 3N, x_2) \in G_{H+}^h\right\}$ )

$$U(x; \vartheta)|_{T_{H-}^h} = e^{i3\vartheta} U(x; \vartheta)|_{T_{H+}^h}, \quad (20)$$

$$\frac{\partial U}{\partial x_1}(x; \vartheta)|_{T_{H-}^h} = e^{i3\vartheta} \frac{\partial U}{\partial x_1}(x; \vartheta)|_{T_{H+}^h}. \quad (21)$$

Here,  $\Lambda(\vartheta)$  is a new notation for the spectral parameter.

The variational form of the problem (18)-(21) reads

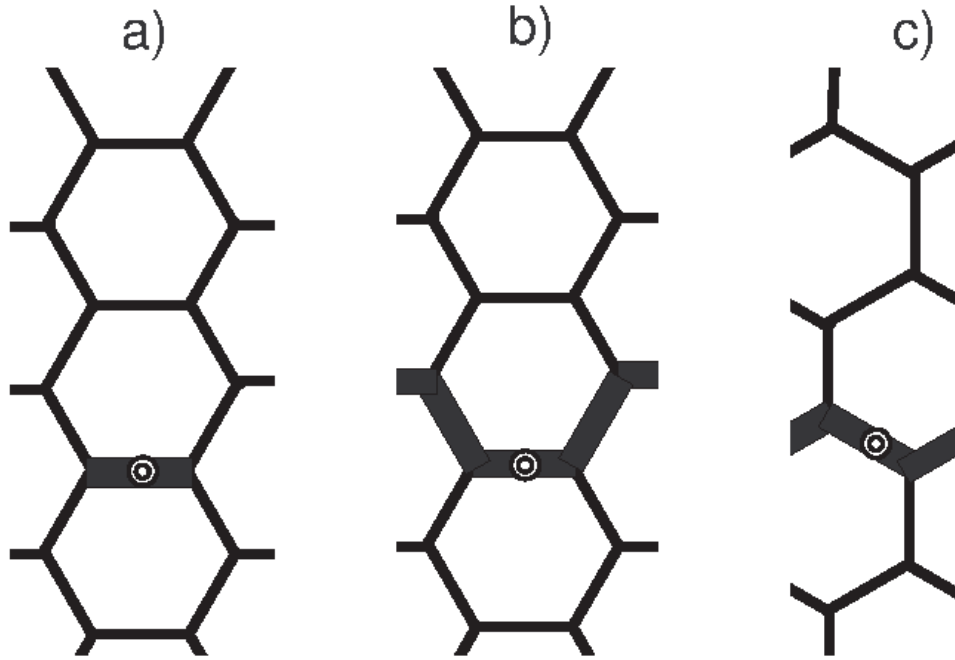
$$(\nabla U, \nabla V)_{\Pi_H^h} = \Lambda(\vartheta)(U, V)_{\Pi_H^h} \quad \forall V \in H_{0\vartheta}^1(\Pi_H^h) \quad (22)$$

and gives rise [12; §10] to a positive definite self-adjoint operator  $A_H^h(\vartheta)$  in the Lebesgue space  $L^2(\Pi_H^h)$ . In (22),  $H_{0\vartheta}^1(\Pi_H^h)$  is the Sobolev space of functions verifying the Dirichlet condition (19) and the stable quasi-periodicity condition (20). According to [24], [25; §3] and [17], the essential spectrum  $\Sigma_{H,es}^h(\vartheta)$  of the operator  $A_H^h(\vartheta)$ , that is of the problem (22) or (18)-(21), includes the set

$$\bigcup_{n \in \mathbb{N}} \{\Lambda_n^h(3\vartheta, \theta_-): \theta_- \in [-\pi, \pi]\} \quad (23)$$

constructed from eigenvalues (14) but also may get the discrete spectrum  $\Sigma_{H,di}^h(\vartheta)$  below  $\Sigma_{H,es}^h(\vartheta)$  or inside spectral gaps in (23).

The truss  $\Pi_H^h$  has two nodes with center points  $\mathcal{O}^\pm = (\pm \frac{1}{2}, 0)$ , see Fig. 4a.



**Fig. 4.** The periodicity truss  $\Pi_H^h$  in the disconnected waveguide (a) and in the connected waveguide (b and c).

By the coordinate dilation (6), these nodes turn into the infinite tripod waveguide  $Y_H^1$  and its mirror reflection. The number  $h^{-2}\mu_H^1$  and the functions  $W_{H\pm}^h(x) = \chi^h(x - \mathcal{O}^\pm)w_H^1(\xi^\pm)$  with an appropriate cut-off function  $\chi^h$ , see Section 6, are perfect approximations for the eigenvalue  $\Lambda_\pm^h(\vartheta)$  and the eigenfunction  $U_\pm^h(x; \vartheta)$  of the problem (18)-(21). According to (8), the couple  $\{h^{-2}\mu_H^1, W_{H\pm}^h\}$  leaves the exponentially small discrepancy in  $h$  in the differential equation (18) and satisfies the relations (19)-(21) in full. In Section 6 we will demonstrate that this evidence provides the approximation estimates



outlets of equal width  $H$ . The eigenvalue in the discrete spectrum of  $Y_H^H$  satisfies the relations  $H^{-2}\mu_1^1 = \mu_H^H < \mu_1^H < \mu_1^1$  for  $H \in (1, H_*)$ ,

$$(29)$$

$H^{-2}\mu_1^1 = \mu_H^H > \mu_1^H > \mu_1^1$  for  $H \in (H_*^{-1}, 1)$ .

$$(30)$$

Thus, in the case (29) the point  $h^{-2}\mu_H^H$  stays below the essential spectrum of the lattice  $G_H^h$  but in the case (30) it belongs to the spectral gap between the bands  $\beta_3^h$  and  $B_H^h$ ,  $\mathbb{B}_H^h$  described above.

Let us outline the standard scheme to prove the existence of an eigenvalue  $\Lambda_{H^\odot}^h$  in the discrete spectrum of the problem (2), (3). The Hilbert space  $\mathcal{H}_H^h = H_0^1(G_H^h)$  consisting of functions in the Sobolev space  $H^1(G_H^h)$  which enjoy the Dirichlet condition (3), is equipped with the scalar product

$$\langle u_H^h, v_H^h \rangle = (\nabla u_H^h, \nabla v_H^h)_{G_H^h} + h^{-2}(u_H^h, v_H^h)_{G_H^h}, \quad (31)$$

where  $\nabla = \text{grad}$  and  $(\cdot, \cdot)_{G_H^h}$  is the natural scalar product in the Lebesgue space  $L^2(G_H^h)$ . Instead of the unbounded operator  $A_H^h$  in Section 1, the identity

$$\langle \mathcal{A}_H^h u_H^h, v_H^h \rangle = (u_H^h, v_H^h)_{G_H^h} \quad \forall u_H^h, v_H^h \in \mathcal{H}_H^h \quad (32)$$

gives us the positive definite symmetric and continuous, therefore, self-adjoint operator  $\mathcal{A}_H^h$  in  $\mathcal{H}_H^h$ .

By the definitions (31) and (32), the variational formulation

$$(\nabla u_H^h, \nabla v_H^h)_{G_H^h} = \lambda_H^h (u_H^h, v_H^h)_{G_H^h} \quad \forall v_H^h \in \mathcal{H}_H^h \quad (33)$$

of the problem (2), (3) becomes the abstract equation  $\mathcal{A}_H^h u_H^h = \kappa_H^h u_H^h$  in  $\mathcal{H}_H^h$  with a new spectral parameter

$$\kappa_H^h = (h^{-2} + \lambda_H^h)^{-1}. \quad (34)$$

The norm of  $\mathcal{A}_H^h$  is smaller than one and, hence, its spectrum  $\mathcal{S}_H^h$  belongs to  $[0, 1]$ . The relations (29) and (30) demonstrate that a  $Ch^2$ -neighborhood of the point

$$\mathcal{K}_H^h = h^2(1 + \mu_H^H)^{-1} \quad (35)$$

is free of the essential spectrum  $\mathcal{S}_H^{h,es}$  of  $\mathcal{A}_H^h$ . However, the well-known formula, see e.g. [12; §6.1],

$$\text{dist}(\mathcal{K}_H^h, \mathcal{S}_H^h) = \left\| (\mathcal{A}_H^h - \mathcal{K}_H^h)^{-1}; \mathcal{H}_H^h \rightarrow \mathcal{H}_H^h \right\|^{-1}$$

shows that, under the condition

$$\left\| \mathcal{A}_H^h u_H^h - \mathcal{K}_H^h u_H^h; \mathcal{H}_H^h \right\| \leq Ch^{3/2} e^{-\delta/h} \|u_H^h; \mathcal{H}_H^h\|, \quad \delta > 0, \quad (36)$$

there exists an eigenvalue  $\kappa_{H^\odot}^h$  of  $\mathcal{A}_H^h$  such that

$$\left| \kappa_{H^\odot}^h - \mathcal{K}_H^h \right| \leq ch^{3/2} e^{-\delta/h} \implies \left| \lambda_{H^\odot}^h - h^{-2}\mu_1^1 \right| < ch^{-5/2} e^{-\delta/h}. \quad (37)$$

The last estimate follows from (35).

Let us build a function  $u_H^h$  which satisfies (36), namely

$$u_H^h(x) = \chi^h(x) w_H^H(h^{-1}x), \quad (38)$$

where  $\chi^h$  is a smooth cutoff function,

$$\chi^h(x) = 1 \text{ for } |x| < 1 - 4h, \chi^h(x) = 0 \text{ for } |x| > 1 - 2h. \quad (39)$$

We easily derive the estimate

$$\|u_H^h; \mathcal{H}_H^h\|^2 \geq 2h(1 + \mu_H^H), \quad (40)$$

where formulas  $\|w_H^H; L^2(Y_H^H)\| = 1$  and  $\text{mes}_2 \text{supp}(\chi^h) \geq 2h$  were taken into account. Furthermore, using a definition of the norm in Hilbert space, we derive

$$\begin{aligned} \left\| \mathcal{A}_H^h u_H^h - \mathcal{K}_H^h u_H^h; \mathcal{H}_H^h \right\| &= \sup |\langle \mathcal{A}_H^h u_H^h - \mathcal{K}_H^h u_H^h, v_H^h \rangle| = \\ &= h^2(1 + \mu_H^H)^{-1} \sup \left| (\nabla u_H^h, \nabla v_H^h)_{G_H^h} - h^{-2}\mu_H^H (u_H^h, v_H^h)_{G_H^h} \right| = \\ &= h^2(1 + \mu_H^H)^{-1} \sup \left| (\Delta u_H^h + h^{-2}\mu_H^H u_H^h, v_H^h)_{G_H^h} \right|. \end{aligned} \quad (41)$$





## **Acknowledgements**

*This research was supported by Russian Science Foundation (Grant 14-29-00199).*

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