

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 $H > 1$.

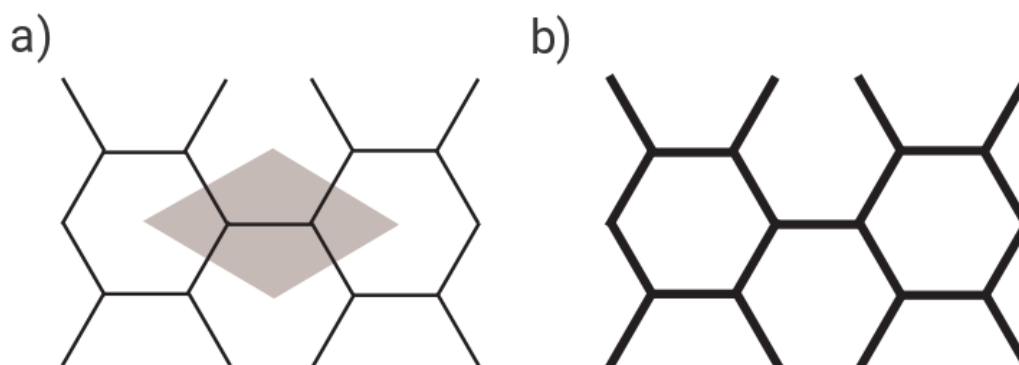


Fig. 1. The hexagonal graph G^0 and the fattened lattice G^h .

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 Σ_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 Σ_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 Σ_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 $L^2(Y_H^h)$.

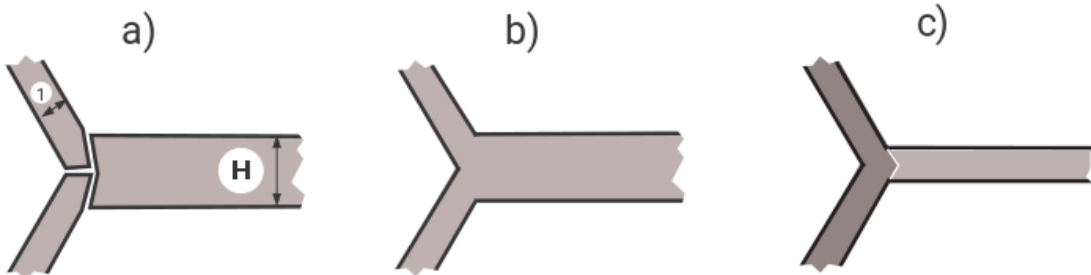


Fig. 3. The Y-shaped waveguide.

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

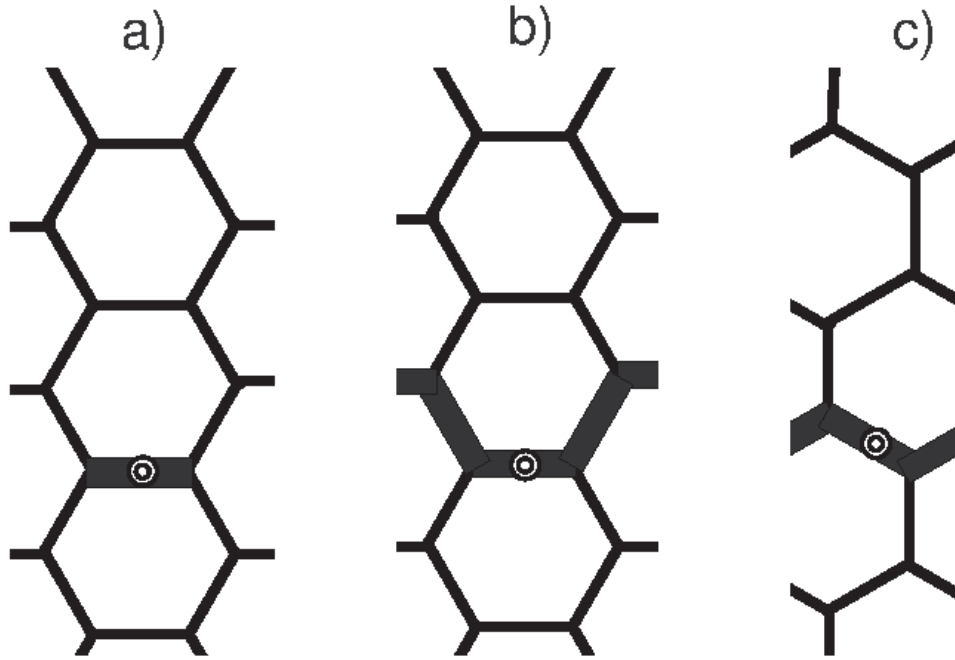


Fig. 4. The periodicity truss Π_H^h in the disconnected waveguide (a) and in the connected waveguide (b and c).

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 χ^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 β_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 χ^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

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

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