

# MULTIFARIOUS TRANSMISSION CONDITIONS IN THE GRAPH MODELS OF CARBON NANO-STRUCTURES

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**Abstract.** Considering a periodic carbon nano-structure of thin quantum waveguides, we list all possible transmission conditions at the vertices of the hexagonal graph in the one-dimensional model. We study the boundary layer phenomenon in the symmetric infinite tripod waveguide and outline an approach to evaluate almost standing waves, which determine the type of the transmission conditions.

## 1. Problem setting

The graph  $G^0$  in the plane  $\mathbb{R}^2$  forms a hexagonal one-dimensional structure in Fig. 1a, consisting of vertices and a set of unit straight segments, edges, where the angle between each couple among three edges emerging from a vertex is  $2\pi/3$ . Moreover,  $G^0$  can be 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 region  $\mathbb{P}$  which is shaded in Fig. 1a, and defined by the vectors  $e_{\pm} = (3/2, \pm\sqrt{3}/2)$ . We introduce the two-dimensional thin domain  $G^h = \{x = (x_1, x_2): \text{dist}(x, G^0) < h/2\}$  where  $h > 0$  is a small parameter. The domain  $G_R^h$ , our carbon nano-structure in Fig. 1b, is a union of  $G^h$  and an infinite family of disks  $D_{hR}$  of radius  $hR$  centered at vertices. Note that  $G_R^h = G^h$  for  $R \leq R_* = \sqrt{3}/3$ .

Interpreting  $G_R^h$  as a lattice of quantum waveguides, cf., [1, 2], we consider the spectral Dirichlet problem for the Laplace operator

$$-\Delta u_R^h(x) = \lambda_R^h u_R^h(x), \quad x \in G_R^h, \quad (1)$$

$$u_R^h(x) = 0, \quad x \in \partial G_R^h, \quad (2)$$

where  $\lambda_R^h$  is a spectral parameter. Since  $h \ll 1$ , a one-dimensional model on the graph  $G^0$  is suitable to describe asymptotically the spectrum  $\sigma_R^h$  of the problem (1), (2). The classical Pauling model [3] involving the Kirchhoff transmission conditions at the vertices has been employed in many studies, see, e.g., [4-6] as well as the review papers [1, 2]. In the informative paper [7] it was demonstrated that the type of the transmission conditions depends crucially on the boundary layer phenomenon in the vicinity of the nodes  $D_{hR}$  of the thin lattice  $G_R^h$ , see Section 2 below. The inspection [8] of this phenomenon in the primary lattice  $G^h$  substantiates that, according to [7], the valid transmission conditions at the vertices are nothing but the Dirichlet ones. This observation has an applicable consequence, namely the mid-frequency range of the spectrum  $\sigma^h$  of the problem (1), (2) in  $G^h$  consists of thin spectral bands separated



$R \mapsto \#\Sigma_R^{di}$

is constant inside intervals  $(R_n, R_{n+1})$  but has positive jumps at the radii  $R = R_n$  in (4). Finally, owing to an observation in [13], the problem (6), (7) in  $Y_R$  at the threshold  $\mu = \pi^2$  has a bounded solution.

By the Fourier method, any bounded solution  $w$  of the problem (6), (7) takes the form

$$w(\xi) = \sum_{\alpha=0,\pm} \chi_R(\zeta_\alpha) C_\alpha \cos(\pi\eta_\alpha) + \tilde{w}(\xi), \quad (9)$$

where  $\tilde{w}(\xi) = O(e^{-\sqrt{3}\pi|\xi|})$  is a remainder of exponential decay,  $C_\alpha \in \mathbb{R}$  are some coefficients,  $\chi_R$  is a smooth cut-off function,

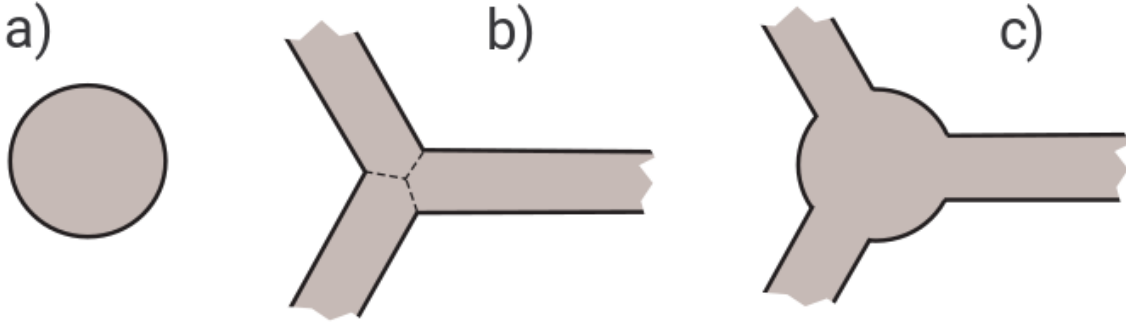
$$\chi_R(\zeta) = 0 \quad \text{for } \zeta < R \quad \text{and} \quad \chi_R(\zeta_\alpha) = 1 \quad \text{for } \zeta > 2R,$$

$(\eta_\alpha, \zeta_\alpha)$  is the local coordinate system such that  $S^\alpha \supset \{\xi: |\eta_\alpha| < \frac{1}{2}, \zeta_\alpha > 0\}$ . The subspace of all solutions (9) is denoted by  $\mathcal{L}_R^{bo}$  and admits the decomposition

$$\mathcal{L}_R^{bo} = \mathcal{L}_R^{tr} \oplus \mathcal{L}_R^{st} \quad (10)$$

Here the component  $\mathcal{L}_R^{tr}$  contains all trapped modes, i.e., the eigenfunctions of the problem (6), (7) corresponding to the eigenvalue  $\mu = \pi^2$  and having exponential decay ( $C_0 = C_\pm = 0$ ) while  $\mathcal{L}_R^{st}$  is a subspace of almost standing waves [14], i.e., bounded and sustained at infinity solutions (if  $|C_0|^2 + |C_+|^2 + |C_-|^2 = 0$  for  $w \in \mathcal{L}_R^{st}$ , then  $w(\xi) = 0$ ).

We will show in Section 8 that type of the transmission conditions in question is determined by the structure of the subspace  $\mathcal{L}_R^{st}$  in (10), more precisely by the dimension  $d_R^{st} = \dim \mathcal{L}_R^{st}$ .



**Fig. 2.** a) The disk  $D_R$ , b) the union of three pointed semi-infinite strips  $Y$  and c)  $Y_R = Y \cup D_R$ .

### 3. The existence of threshold trapped modes

Using the rich symmetry of the domain  $Y_R$  in Fig. 2c, we consider the spectral problem

$$-\Delta v(\xi) = \beta v(\xi), \quad \xi \in F_R, \quad (11)$$

$$v(\xi) = 0, \quad \xi \in \Gamma_R, \quad (12)$$

$$v(\xi) = 0, \quad \xi \in Y_0 \cup \Theta_R = \partial F_R \setminus \Gamma_R, \quad (13)$$

in the domain  $F_R = \{\xi \in Y_R: 0 < \xi_2 < \sqrt{3}\xi_1\}$  (Fig. 3a). Here,  $\Gamma_R = \partial Y_R \cap \partial F_R$  and the artificial straight boundaries (dotted lines in Fig. 3a) are given by  $Y_0 = \{\xi \in Y_R: \xi_1 > 0, \xi_2 = 0\}$  and  $\Theta_R = \{\xi \in D_R: 0 < \xi_2 = \sqrt{3}\xi_1\}$ .

Since the only outlet to infinity in  $F_R$  is a strip of width  $\frac{1}{2}$ , the continuous spectrum  $\Sigma_R^{co}(F)$  of the Dirichlet problem (11)-(13) is the ray  $[4\pi^2, +\infty)$ . The discrete spectrum  $\Sigma_R^{di}(F)$  is empty, see [15], when  $R \leq R_*$  since  $F_R$  becomes a tapered semi-strip shaded in Fig. 3a. At the same time, for a big  $R > R_*$ , the comparison principle [12] indicates the eigenvalues

$$\beta_R^k \leq R^{-2} B_k < 4\pi^2$$

in  $\Sigma_R^{di}(F)$  where  $\{B_k\}_{k=1}^\infty$  is the eigenvalue sequence of the Dirichlet problem in the disk sector  $D_1^F = \{\xi \in D_1: 0 < \xi_2 < \sqrt{3}\xi_1\}$ . These facts and the continuous dependence of the eigenvalues  $\beta_R^k \in \Sigma_R^{di}(F)$  on radius ensure that, for any  $k \in \mathbb{N} = \{1, 2, 3, \dots\}$ , one finds  $R_k^F$



$$-\Delta v(\xi) = \beta v(\xi), \quad \xi \in V_R, \quad (20)$$

$$v(\xi) = 0, \quad \xi \in V_R \setminus \Gamma_R, \quad (21)$$

$$v(\xi) = 0, \quad \xi \in \Gamma_R. \quad (22)$$

If the problem (20)-(22) at the threshold  $\beta = \pi^2$  has the almost standing wave  $v$  stabilizing in the outlet  $S^+$  to  $\cos(\pi\eta_+)$ , its odd extension over the Dirichlet semi-axis  $\Gamma_R = \{\xi \in Y_R: \xi_2 = 0\}$ , see (22), becomes the solution (9) of the problem (6), (7) in  $Y_R$  with the coefficient string  $E_- = (0, 1, -1)$ . (23)

Moreover, rotating the Cartesian coordinate system  $\xi = (\xi_1, \xi_2)$  counterclockwise by the angle  $2\pi/3$ , we obtain the solution  $v^\mathfrak{U}$  with the coefficient string  $E_-^\mathfrak{U} = (-1, 0, 1)$ . In the last formula and further,  $\mathfrak{U}$  and  $\mathfrak{V}$  denote cyclic counterclockwise and clockwise permutations, respectively. The functions  $v^\mathfrak{U}$  and  $v$  are linear independent but  $v^\mathfrak{V} = v^{\mathfrak{U}\mathfrak{U}} = -v - v^\mathfrak{U}$ .

Hence, we have marked a way to construct the subspace  $\mathcal{L}_R^{st}$  of dimension two provided  $w_+ = 0$  in (19).

The waveguide  $V_R$  has two outlets to infinity. However, only  $S^+$  generates the continuous spectrum  $\Sigma_R^{co}(V) = [\pi^2, +\infty)$  because, as in Section 2, the other semi-infinite strip has width  $1/2$  and both its lateral sides are supplied with the Dirichlet condition. We again refer to the comparison principle [12] and find out the eigenvalues (17) for a big  $R > R_*$  as well as the radius sequence (18) where  $\{B_k\}_{k=1}^\infty$  is the eigenvalue sequence of the Dirichlet problem in the disc sector  $D_1^V = \{\xi \in D_1: \sqrt{3}\xi_1 > -\xi_2, \xi_2 > 0\}$  (shaded in Fig. 3b).

The problem (20)-(22) with  $\beta = \pi^2$  and  $R = R_k^{bo}$  has a non-trivial bounded solution according to [13]. However, some of them turn into trapped modes due to the construction presented in Section 2. Thus to conclude with the existence of almost standing waves requires for numerical experiments.

## 6. The case $d_R^{st} = 3$

Assuming that the function  $v = w_+$  in (19) is nontrivial and has the coefficient string  $(C_0, C, C)$  with  $|C_0|^2 + 2|C|^2 \neq 0$ , we come across several situations and each of them provides  $d_R^{st} = 3$  with exception of  $5^\circ$ . Indeed, in cases  $1^\circ - 4^\circ$  we compose the solution  $w_0$  with the string  $(1, 0, 0)$  so that  $w_0$  and  $w_0^\mathfrak{U}, w_0^\mathfrak{V}$  in  $\mathcal{L}_R^{st}$  stay linear independent:

$$1^\circ. \quad C_0 = 1, C = 0 \quad \Rightarrow \quad w_0 = v;$$

$$2^\circ. \quad C_0 = 0, C = 1 \quad \Rightarrow \quad w_0 = \frac{1}{2}(v^\mathfrak{U} + v^\mathfrak{V} - v);$$

$$3^\circ. \quad C_0 = 1, C = -1 \quad \Rightarrow \quad w_0 = -\frac{1}{2}(v^\mathfrak{U} + v^\mathfrak{V});$$

$$4^\circ. \quad C_0 = 1, C \neq -1, -\frac{1}{2} \quad \Rightarrow \quad w_0 = \frac{1+C}{1+C-2C^2} \left( v - \frac{C}{1+C} (v^\mathfrak{U} + v^\mathfrak{V}) \right).$$

On the contrary, we create the almost standing wave  $v_0$  with the string (23) in the case

$$5^\circ. \quad C_0 = 1, C = -\frac{1}{2} \quad \Rightarrow \quad v_0 = \frac{2}{3}v + \frac{4}{3}v^\mathfrak{U}.$$

Hence, for  $5^\circ$ , we conclude  $d_R^{st} = 2$  provided the problem (6), (7) at  $\mu = \pi^2$  has no other almost standing wave.

The particular solution  $w_0$  satisfies the artificial boundary condition

$$\partial_N w_0(\xi) = 0, \quad \xi \in \Gamma_R. \quad (24)$$

At the same time, the continuous spectrum  $\Sigma_R^{co}(V) = [\pi^2, +\infty)$  of the problem (20), (21), (24) in the waveguide  $V_R$  with two outlets to infinity is relevant to both of them. Indeed, lateral sides of the narrowed strip  $S_{1/2}^0 = \{\xi: \xi_1 > R, \xi_2\}$  are supplied with different (Dirichlet in (21) and Neumann in (24)) boundary conditions which still support the standing wave  $\cos(\pi\zeta_0)$  at the threshold  $\beta = \pi^2$ . Furthermore, the problem gets two linear independent almost standing waves, namely the restrictions of  $w_0$  and  $w_0^\mathfrak{U}$  onto  $V_R$ . The latter is an exceptional situation: even in any complicated geometry there is no example yet of a waveguide providing  $\dim \mathcal{L}_R^{st} > 1$ , see

the papers [14, 16] for reasoning. We do not hope to find a radius  $R$  such that the almost standing wave  $w_0$  with the string  $(1,0,0)$  emerges in the simple symmetric tripod  $Y_R$ .

### 7. The spectral problem in the periodicity cell

The one-dimensional cell  $g^0 = G^0 \cap \mathbb{P}$  drawn in Fig. 1a, consists of five segments  $g_0^0 = \{z_0: z_0 \in (-\frac{1}{2}, \frac{1}{2})\}$  and

$$g_{l\pm}^0 = \{z_{\mp}: \pm z_{\mp} \in (0, \frac{1}{2})\}, \quad g_{r\pm}^0 = \{z_{\pm}: \pm z_{\pm} \in (0, \frac{1}{2})\}, \quad (25)$$

where  $z_0$  and  $z_{\pm}$  are the local longitudinal coordinates in  $g_0^0$  and  $g_{f\pm}^0$ ,  $f = l, r$ , respectively, while the transversal coordinates are denoted by  $y_{\alpha} \in (-h/2, h/2)$ . The symbols  $l$  and  $r$  stand for ‘‘left’’ and ‘‘right’’ as in Section 2. The two-dimensional periodicity cell  $g_R^h = G_R^h \cap \mathbb{P}$  has four truncation segments

$$t_{l\pm}^h = \{x \in \partial g_R^h: \pm z_{\mp} = \frac{1}{2}\}, \quad t_{r\pm}^h = \{x \in \partial g_R^h: \pm z_{\pm} = \frac{1}{2}\}. \quad (26)$$

Union of the sets (26) is denoted by  $t^h$ .

In the framework of the Floquet-Bloch-Gelfand theory, see e.g., [17, 18], the Gelfand transform with the dual variable  $\theta = (\theta_+, \theta_-) \in [-\pi, \pi]^2$  converts the problem (1), (2) in  $G_R^h$  into the spectral problem in the periodicity cell

$$-\Delta U_R^h(x; \theta) = \Lambda_R^h(\theta) U_R^h(x; \theta), \quad x \in g_R^h, \quad (27)$$

$$U_R^h(x; \theta) = 0, \quad x \in \partial g_R^h \setminus t^h, \quad (28)$$

with the quasi-periodicity conditions

$$U_R^h(x; \theta)|_{z_{\pm}=\frac{1}{2}} = e^{i\theta_{\pm}} U_R^h(x; \theta)|_{z_{\pm}=-\frac{1}{2}}, \quad (29)$$

$$\partial_{z_{\pm}} U_R^h(x; \theta)|_{z_{\pm}=\frac{1}{2}} = e^{i\theta_{\pm}} \partial_{z_{\pm}} U_R^h(x; \theta)|_{z_{\pm}=-\frac{1}{2}}. \quad (30)$$

The problem (27)-(30) has the discrete spectrum generating the eigenvalue sequence

$$0 < \Lambda_{R1}^h(\theta) \leq \Lambda_{R2}^h(\theta) \leq \Lambda_{R3}^h(\theta) \leq \dots \leq \Lambda_{Rk}^h(\theta) \leq \dots \rightarrow +\infty, \quad (31)$$

whose entries are continuous and  $2\pi$ -periodic in  $\theta$ . It is known, see e.g., [17, 18], that the spectrum  $\sigma_R^h$  of the problem (1), (2) possesses the band-gap structure

$$\sigma_R^h = \bigcup_{k \in \mathbb{N}} \zeta_R^h(k) \quad (32)$$

where  $\mathbb{N} = \{1, 2, 3, \dots\}$  and the spectral bands are determined by

$$\zeta_R^h(k) = \{ \Lambda_{Rk}^h(\theta): \theta \in [-\pi, \pi]^2 \}. \quad (33)$$

Let  $\mu_R^1, \dots, \mu_R^{m(R)} \in (0, \pi^2)$  be all eigenvalues in the discrete spectrum  $\Sigma_R^{di}$  of the problem (1), (2) and let  $\mu_R^{m(R)+1} = \dots = \mu_R^{m(R)+\kappa(R)} = \pi^2$  be an eigenvalue of multiplicity  $\kappa(R) \geq 0$ . In other words,  $m(R) = \#\Sigma_R^{di} > 0$  and  $\kappa(R) = \dim \mathcal{L}_R^{st} \geq 0$ . In [8], we have checked up that  $m(R) = 2$  and  $\kappa(R) = 0$  for  $R \in (0, R_*]$ , cf., Section 2.

According to the general result in [7], the eigenvalues  $\Lambda_{Rk}^h(\theta)$  with  $k = 1, \dots, m(R) + \kappa(R)$  take the asymptotic form

$$\Lambda_{Rk}^h(\theta) = h^{-2} \mu_k^h + O(e^{-\delta_k/h}), \quad \delta_k > 0. \quad (34)$$

This asymptotic formula means that the spectral bands  $\zeta_R^h(1), \dots, \zeta_R^h(m(R) + \kappa(R))$  have exponentially small length in  $h$  and the distance between the spectral bands is of order  $O(h^{-2})$ .

The other part of the spectrum (31) admits the asymptotic expansions

$$\Lambda_{Rm(R)+\kappa(R)+j}^h(\theta) = h^{-2} \pi^2 + \Lambda_j^0(\theta) + O(h), \quad (35)$$

where  $\{\Lambda_j^0(\theta)\}_{j=1}^{\infty}$  is the eigenvalue sequence of the one-dimensional model on the graph  $g^0$  involving the differential equations

$$-\partial_{z_0}^2 U_0^0(z_0; \theta) = \Lambda^0(\theta) U_0^0(z_0; \theta), \quad z_0 \in (-\frac{1}{2}, \frac{1}{2}), \quad (36)$$

$$-\partial_{z_{\pm}}^2 U_{\pm}^0(z_{\pm}; \theta) = \Lambda^0(\theta) U_{\pm}^0(z_{\pm}; \theta), \quad z_{\pm} \in (-\frac{1}{2}, 0) \cup (0, \frac{1}{2}) \quad (37)$$

with the quasi-periodicity conditions

$$U_{\pm}^0(z_{\pm}; \theta)|_{z_{\pm}=\frac{1}{2}} = e^{i\theta_{\pm}} U_{\pm}^0(z_{\pm}; \theta)|_{z_{\pm}=-\frac{1}{2}}, \quad (38)$$

$$\partial_{z_{\pm}} U_{\pm}^0(z_{\pm}; \theta)|_{z_{\pm}=\frac{1}{2}} = e^{i\theta_{\pm}} \partial_{z_{\pm}} U_{\pm}^0(z_{\pm}; \theta)|_{z_{\pm}=-\frac{1}{2}}. \quad (39)$$

These relations had appeared as a result of substituting the asymptotic ansätze (35) and

$$U_{R\alpha}^h(x; \theta) = U_{\pm}^0(z_{\pm}; \theta) \cos(\pi h^{-1} y_{\alpha}) + \dots \quad (40)$$

into the equation (27) and the conditions (28), (29). Here,  $y_0$  and  $y_{\pm}$  stand for the transversal coordinates in the thin rectangles  $g_0^0$  and  $g_{l\pm}^0$ ,  $g_{r\pm}^0$  in the periodicity cell  $g^0$ . Since  $\cos(\pi h^{-1} y_{\alpha})$  vanishes at  $y_{\alpha} = \pm h/2$ , the boundary conditions (28) on  $(\partial g_R^h \cap \partial g^h) \setminus t^h$  are satisfied, too.

Near the nodes, the disks  $D_{hR}^l$  and  $D_{hR}^r$  centered at the points  $\mathcal{O}_l$  and  $\mathcal{O}_r$  with the local coordinates  $z_0 = -\frac{1}{2}$  and  $z_0 = \frac{1}{2}$ , respectively, the geometry of the cell  $g_R^h$  changes crucially and the asymptotic ansatz (40) does not work. In the next section we will examine the boundary layer phenomenon which provides transmission conditions in the vicinity of the nodes. These conditions are necessary to close the problem and link the strings

$$U_l^0 = (U_0^0(-\frac{1}{2}), U_{l+}^0(0), U_{l-}^0(0)), \quad U_r^0 = (U_0^0(+\frac{1}{2}), U_{r-}^0(0), U_{r+}^0(0)), \quad (41)$$

$$\begin{aligned} \partial_z U_l^0 &= (\partial_{z_0} U_0^0(-\frac{1}{2}), \partial_{z_+} U_{l+}^0(0), -\partial_{z_-} U_{l-}^0(0)), \\ \partial_z U_r^0 &= (\partial_{z_0} U_0^0(+\frac{1}{2}), -\partial_{z_-} U_{r-}^0(0), \partial_{z_+} U_{r+}^0(0)). \end{aligned} \quad (42)$$

Here,  $U_{l\pm}^0$ ,  $U_{r\pm}^0$  and  $U_0^0$  are the restrictions of the function  $U^0$  on the segments  $g_{l\pm}^0$ ,  $g_{r\pm}^0$  and  $g_0^0$ , respectively. This function is not necessarily continuous at the vertices and with this reason the equations (37) are not valid at  $z_{\pm} = 0$ , i.e., at the points  $\mathcal{O}_l$  and  $\mathcal{O}_r$ .

In the paper [8], we have proved that the subspace (10) is trivial in the case  $G_R^h = G^h$  and the problem (6), (7) has the only eigenvalue  $\mu^1 \in (0, \pi^2)$  in the discrete spectrum. As a result, we concluded that the first two eigenvalues in (31) obey the asymptotic form (34). Moreover, the transmission conditions at the points  $\mathcal{O}_l$  and  $\mathcal{O}_r$  become the Dirichlet conditions

$$U_f^0 = 0 \in \mathbb{C}^3, \quad f = l, r. \quad (43)$$

Since, by (43), the graph  $g^0$  is divided into three independent segments with the Dirichlet conditions at the endpoints (notice that  $g_{l\pm}^0$  and  $g_{r\pm}^0$  are connected through the quasi-periodicity conditions (38), (39)), the problem (36)-(39), (43) gets the eigenvalues  $\pi^2 n^2$ ,  $n \in \mathbb{N}$ , each of multiplicity three. It should be emphasized that in this case the asymptotic formula (35) does not bring auxiliary information about the length of the bands  $\zeta_R^h(k)$ ,  $k > 1$ , but only about their position. In order to derive substantial asymptotics of the band length one may build a refined one-dimensional model, which takes lower-order asymptotic terms into account, cf., the study [11] of the Dirichlet ladder.

The same limit problem (36)-(39), (43) occurs for any radius  $R$  which differs from entries of the sequence (4) and, therefore,  $\dim \mathcal{L}_R^{st} = 0$ . However, the total multiplicity  $\#\Sigma_R^{di}$  grows unboundedly when  $R \rightarrow +\infty$ . In this way, the number of small bands (33) inside the interval  $(0, \pi^2)$  increases as well.

## 8. Derivation of the transmission conditions with the help of the method of matched asymptotic expansion

Let  $\mathbb{L}_R^{st} \subset \mathbb{R}^3$  be a subspace of coefficient strings  $C = (C_0, C_+, C_-)$  in the decomposition (9) of solutions in  $\mathcal{L}_R^{st}$ . We set  $\mathbb{L}_R^{li} = \mathbb{R}^3 \ominus \mathbb{L}_R^{st}$  and observe that, for any  $K \in \mathbb{L}_R^{li}$ , the problem (6), (7) gets a solution in the form

$$w^{li}(\xi; K) = \sum_{\alpha=0, \pm} \chi_R(\zeta_{\alpha})(K_{\alpha} \zeta_{\alpha} + \mathcal{P}_{\alpha}(K)) \cos(\pi \eta_{\alpha}) + \tilde{w}^{li}(\xi), \quad (44)$$

Here  $\mathcal{P}_{\alpha}(K)$ ,  $\alpha = 0, \pm$ , are some coefficients of no use in the present paper, however, these coefficients form a symmetric  $3 \times 3$ -matrix which is called the polarization matrix in the

waveguide  $Y_R$  and becomes the main ingredient of the refined model mentioned in Section 7. In the sequel we denote by  $w^{st}(\xi; C)$  the solution (9) from  $\mathcal{L}_R^{st}$ .

In the framework of the method of matched asymptotic expansions, cf., [19, 20] and [21; Ch. 2], we interpret (40) as the outer expansions and seek for the inner expansion near the left point  $\mathcal{O}_l$  (the right point  $\mathcal{O}_r$  is treated in the same way) in the form

$$U^h(x, \theta) \sim w^{st}(\xi; C(\theta)) + h w^{li}(\xi; K(\theta)). \quad (45)$$

Based on formulas (9) and (44), we rewrite the decomposition of (45) in the very condensed form

$$U^h(x, \theta) \sim (C_\alpha(\theta) + h\zeta K_\alpha(\theta) + h\mathcal{P}_\alpha(K(\theta)))_{\alpha=0,\pm} = C(\theta) + h\zeta K(\theta) + h\mathcal{P}(K(\theta)) \quad (46)$$

Here and in what follows, we skip in the notation lower-order terms, exponentially decaying remainders and cosines while presenting in each outlet  $S^\alpha$  only linear functions in  $\zeta_\alpha$  from (9) and (44).

In a similar way, we apply the Taylor formulas and transfigure the outer expansions near  $\mathcal{O}_l$  as follows:

$$\begin{aligned} U^h(x, \theta) \sim & \left( U_0^0(-1/2; \theta) + (z_0 + 1/2)\partial_{z_0} U_0^0(-1/2; \theta), U_{l+}^0(0; \theta) \right. \\ & \left. + \partial_{z_+} U_{l+}^0(0; \theta), U_{l-}^0(0; \theta) + z_- \partial_{z_-} U_{l-}^0(0; \theta) \right) \\ & = U_l^0(\theta) + h\zeta \partial_z U_l^0(\theta) \end{aligned} \quad (47)$$

where the notation (42) is recalled. Comparing (47) and (46) we readily derive the relations

$$U_l^0(\theta) = C(\theta) \in \mathbb{L}_R^{st}, \quad \partial_z U_l^0(\theta) = K(\theta) \in \mathbb{L}_R^{li}. \quad (48)$$

Now we have come into position to conclude all conceivable types of the transmission conditions in the vertices  $\mathcal{O}_l$  and  $\mathcal{O}_r$  of the graph  $g^0$ , that is the periodicity cell in the one-dimensional model of the hexagonal nano-structure  $G_R^h$ .

1°.  $d_R^{st} = 0 \Rightarrow$  the Dirichlet condition (43).

Since  $\mathbb{L}_R^{st} = \{0\}$  and  $\mathbb{L}_R^{li} = \mathbb{C}^3$ , we obtain the equality  $C(\theta) = 0$  which leads to (43). The string  $K(\theta)$  remains arbitrary.

2°.  $d_R^{st} = 1 \Rightarrow$  the Kirchhoff conditions

$$U_f^0(\theta) = c_f(\theta)E, \quad E \cdot \partial_z U_f^0(\theta) = 0, \quad f = l, r. \quad (49)$$

where the string  $E = (1, 1, 1)$  was introduced in (15),  $c_f(\theta) \in \mathbb{C}$  is unfixed complex number and the central dot stands for the scalar product. Indeed, we saw in Section 3 that any standing wave gets the coefficient string  $cE$  that leads to the first condition in (49). In other words, at the point  $\mathcal{O}_l$  we impose two conditions

$$U_0^0(-1/2; \theta) = U_{l+}^0(0; \theta) = U_{l-}^0(0; \theta),$$

so that the function  $U^0$  is continuous on the graph  $g^0$ . At the same time,  $\mathbb{L}_R^{li}$  becomes the subspace  $\mathbb{C}_\perp^3 = \{c \in \mathbb{C}^3 : E \cdot c = 0\}$  and produces the second condition in (49), that is,

$$\partial_{z_0} U_0^0(-1/2; \theta) + \partial_{z_+} U_{l+}^0(0; \theta) - \partial_{z_-} U_{l-}^0(0; \theta) = 0.$$

3°.  $d_R^{st} = 2 \Rightarrow$  the anti-Kirchhoff conditions

$$E \cdot U_f^0(\theta) = 0, \quad \partial_z U_f^0(\theta) = k_f(\theta)E, \quad f = l, r. \quad (50)$$

In this case the strings (23) and  $E^\perp = (-1, 0, 1)$  form a basis in  $\mathbb{C}_\perp^3 \ni C(\theta)$ . Hence,  $\mathbb{L}_R^{st} = \mathbb{C}_\perp^3$  while  $K(\theta) \in \mathbb{L}_R^{li}$  is nothing but  $k_f(\theta)E$ . It should be mentioned that the strings (41) and (42) interchange their roles played in (49) and, therefore, the conditions (50) with  $f = l$  read:

$$\begin{aligned} U_0^0(-1/2; \theta) + U_{l+}^0(0; \theta) + U_{l-}^0(0; \theta) &= 0, \\ \partial_{z_0} U_0^0(-1/2; \theta) = \partial_{z_+} U_{l+}^0(0; \theta) &= -\partial_{z_-} U_{l-}^0(0; \theta). \end{aligned}$$

4°.  $d_R^{st} = 3 \Rightarrow$  the Neumann conditions

$$\partial_z U_f^0(\theta) = 0, \quad f = l, r, \quad (51)$$

which follow from the equalities  $\mathbb{L}_R^{st} = \mathbb{C}^3$  and  $\mathbb{L}_R^{li} = \{0\}$  proved in Section 6.

The Dirichlet conditions (43) occur for any radius  $R$ , except for entries of the sequence (4). It has been explained that the Neumann condition (51) is hardly possible but the conditions



(49) and (50) are quite probable. However, the latter are not stable in the sense that any small perturbation of the critical radius  $R = R_k$  deletes the space  $\mathcal{L}_R^{st}$  of almost standing waves and returns the Dirichlet condition.

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