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 $g^0(\tau)$, $\tau = (\tau_1, \tau_2)$, $\tau_j \in \mathbb{Z} = \{0, \pm 1, \pm 2, ..\}$, 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

$$-\Delta u_R^h(x) = \lambda_R^h u_R^h(x), \qquad x \in G_R^h, \qquad (1)$$
$$u_R^h(x) = 0, \qquad x \in \partial G_R^h, \qquad (2)$$

where λ_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 σ_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 σ^h of the problem (1), (2) in G^h consists of thin spectral bands separated

by the spectral gaps of width $O(1)$ as $h \to +0$. Such behavior is by no means attributed to the Pauling model which was employed in [4 - 6] and [1, 2] to imitate the Dirichlet problem, but has been rigorously justified [9, 10] only for the Neumann problem in G_R^h, i.e., for the differential equation (1) with the boundary condition

$$\partial_N u_R^h(x) = 0, \qquad\qquad x \in \partial G_R^h, \qquad\qquad\qquad (3)$$

where ∂_N stands for the normal derivative .

At the same time, as was mentioned in [8], see also [11], the transmission conditions may change at radii from a monotone unbounded sequence

$$R_* < R_1 < R_2 < \cdots < R_k < \cdots \longrightarrow +\infty. \qquad\qquad (4)$$

The main goal of our paper is to display all, highly-probable and hardly-probable, types of the limit ($h = 0$) transmission conditions at the vertices of the graph G^0 simulating the Dirichlet lattice G_R^h with $R = R_k$.
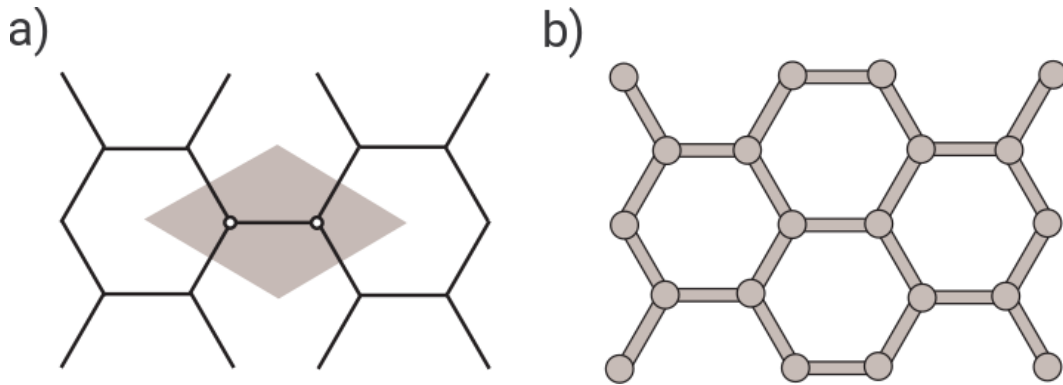

Fig. 1. a) Hexagonal one-dimensional structure G^0, b) the domain G_R^h.

2. The boundary layer phenomenon

Let $\mathcal{O}_l$ and $\mathcal{O}_r$ be vertices in the graph g^0 (marked with $\bigcirc$ in Fig. 1, a). Without the loss of generality we consider only the left vertex $\mathcal{O}_l$ and perform the coordinate change

$$x \mapsto \xi = (\xi_1, \xi_2) = h^{-1}(x - \mathcal{O}_l). \qquad\qquad\qquad (5)$$

Going over to the stretched coordinates ξ and setting $h = 0$ formally transform G_R^h into the domain $Y_R = Y \cup D_R$, where $D_R = \{\xi : |\xi| < R\}$ is a disk and Y a union of three pointed semi-infinite strips S^0 and $S^{\pm}$ of unit width, see Fig. 2a-c. We consider the spectral problem

$$-\Delta w(\xi) = \mu w(\xi), \qquad\qquad \xi \in Y_R, \qquad\qquad\qquad (6)$$
$$w(\xi) = 0, \qquad\qquad\qquad \xi \in \partial Y_R, \qquad\qquad\qquad (7)$$

whose continuous spectrum Σ_R^{co} coincides with the ray $[\mu_\dagger, +\infty)$ and the cutoff value $\mu_\dagger$ is π^2. We denote by

$$0 < M_1 < M_2 \le M_3 \le \cdots \le M_k \le \cdots \longrightarrow +\infty \qquad\qquad (8)$$

the unbounded monotone sequence of eigenvalues of the Dirichlet problem in the unit disk D_1. In (8) multiplicity of eigenvalues is counted in. The comparison principle [12] proves that, for a big R, the discrete spectrum $\Sigma_R^{di} \subset (0, \pi^2)$ of the problem (6), (7) contains isolated eigenvalues

$$\mu_R^k \le R^{-2} M_k < \pi^2$$

and, therefore, the total multiplicity $\#\Sigma_R^{di}$ of Σ_R^{di} grows unboundedly while the first (minimal) eigenvalue μ_R^1 becomes infinitesimal when $R \longrightarrow +\infty$. Notice that $\#\Sigma_R^{di}$ is a monotone increasing function of $R > 0$ and $\#\Sigma_R^{di} = 1$ for $R \in (0, R_*]$ owing to [8].

Eigenvalues in the discrete spectrum are stable under the variation of radius R and, hence, an increase of the multiplicity $\#\Sigma_R^{di}$, when the radius R grows, can occur only due to dropping of an eigenvalue down from the threshold of the continuous spectrum. In other words, the sequence (8) occurs such that the function

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

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

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

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

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

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

$$\mathcal{L}_R^{bo} = \mathcal{L}_R^{tr} \oplus \mathcal{L}_R^{st} \tag{10}$$

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 $d_R^{st} = \dim \mathcal{L}_R^{st}$.
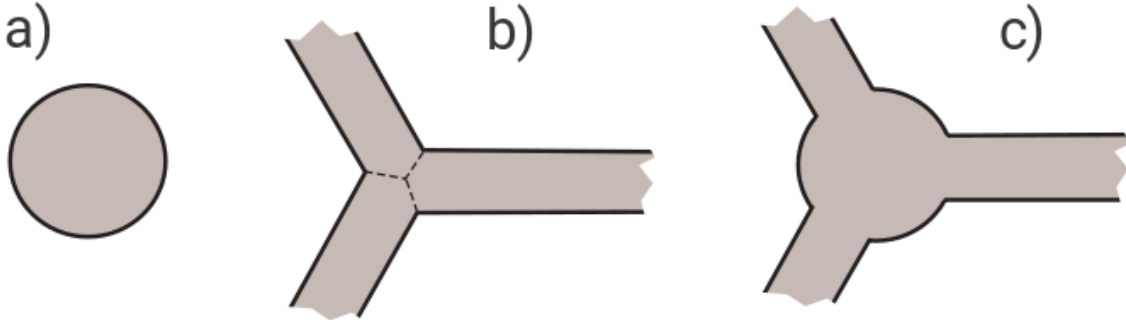

Fig. 2. a) The disk D_R, b) the union of three pointed semi-infinite strips Y and c) $Y_R = Y \cup D_R$.

3. The existence of threshold trapped modes

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

$$-\Delta v(\xi) = \beta v(\xi), \qquad \xi \in F_R, \tag{11}$$
$$v(\xi) = 0, \qquad \xi \in \Gamma_R, \tag{12}$$
$$v(\xi) = 0, \qquad \xi \in \Upsilon_0 \cup \Theta_R = \partial F_R \setminus \Gamma_R, \tag{13}$$

in the domain $F_R = \big\{\xi \in Y_R : 0 < \xi_2 < \sqrt{3}\,\xi_1\big\}$ (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 $\Upsilon_0 = \{\xi \in Y_R : \xi_1 > 0, \ \xi_2 = 0\}$ and $\Theta_R = \big\{\xi \in D_R : 0 < \xi_2 = \sqrt{3}\,\xi_1\big\}$.

Since the only outlet to infinity in F_R, is a strip of width ½, 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 $D_1^F = \big\{\xi \in D_1 : 0 < \xi_2 < \sqrt{3}\,\xi_1\big\}$. 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

such that β_R^k exists for $R > R_k^F$, but $\#\Sigma_R^{di}(F) < k$ for $R \in (0, R_k^F]$. Furthermore, the monotone continuous function
$$(R_k^F, +\infty) \ni R \mapsto \beta_R^k$$
satisfies the relations
$$\lim_{R \to R_k^F + 0} \beta_R^k = 4\pi^2, \qquad \lim_{R \to +\infty} \beta_R^k = 0$$
and, hence, takes the value π^2 at some point $R_k^{tr} > R_k^F$. Thus, we have found out the sequence
$$R_* < R_1^{tr} < R_2^{tr} < \cdots < R_k^{tr} < \cdots \longrightarrow +\infty \tag{14}$$
and the trapped modes $v_k^{tr}, k \in \mathbb{N}$, in the problem (11)-(13) with $\beta = \pi^2$ and $R = R_k^{tr}$.

Let us extend v_k^{tr} as an odd function over the positive semi-axis Y_0 with the Dirichlet conditions (13). This extension is still a smooth function which decays as $|\xi| \to \infty$ and satisfies the Dirichlet problem for the Helmholtz operator $\Delta + \pi^2$ in the doubled domain $\{\xi \in D_1 : 0 < |\xi_2| < \sqrt{3}\,\xi_1\}$. Repeating the extension procedure, we construct a trapped mode in $\mathcal{L}_{R_k^{tr}}^{tr}$ for each radius in (14).
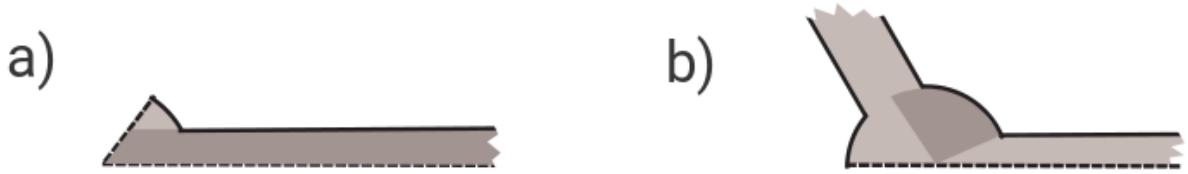

Fig. 3. a) The domain F_R, b) the upper half V_R of Y_R.

4. The case $d_R^{st} = 1$

In view of the symmetry of the domain Y_R any one-dimensional subspace $\mathcal{L}_R^{st}$ contains the solution (9) of the problem (6), (7) at $\mu = \pi^2$ with the coefficients $C_0 = C_\pm = 1$, i.e., with the coefficient string
$$(C_0, C_+, C_-) = E = (1,1,1). \tag{15}$$
To detect this solution, we again reduce the problem to the domain F_R in Fig. 3a, but impose the Neumann conditions
$$\partial_N v(\xi) = 0, \qquad \xi \in Y_0 \cup \Theta_R, \tag{16}$$
on the artificial boundary instead of (13). For a big R, the comparison principle [12] ensures the existence of eigenvalues
$$\beta_R^k \leq R^{-2} B_k < \pi^2 \tag{17}$$
in the discrete spectrum of the problem (11), (12), (16). In (17), $\{B_k\}_{k=1}^\infty$ is the eigenvalue sequence of the mixed boundary value problem in the disk sector D_1^F with the Dirichlet condition on the arc $\{\xi \in \partial D_1 : 0 < \xi_2 < \sqrt{3}\,\xi_1\}$ and the Neumann one on the rest of the boundary. Furthermore, the above-mentioned result [13] gives us the sequence
$$R_* < R_1^{bo} < R_2^{bo} < \cdots < R_k^{bo} < \cdots \longrightarrow +\infty \tag{18}$$
and a bounded solution v_R^{bo} of the problem (11), (12), (16) at $\beta = \pi^2$ for each $R = R_k^{bo}$. Unfortunately, this result does not provide an effective tool to distinguish between trapped modes and almost standing waves. However, it is quite unrealistic to assume that the threshold $\mu = \pi^2$ becomes an eigenvalue in the point spectrum for any radius in (18) and, therefore, one ought to expect an indication of a bounded solution in $\mathcal{L}_R^{st}$ by numerical experiments.

5. The case $d_R^{st} = 2$

Let $w \in \mathcal{L}_R^{st}$ be an almost standing wave in the waveguide Y_R (Fig. 2c). We set
$$w_\pm(\xi_1, \xi_2) = w(\xi_1, \xi_2) \pm w(\xi_1, -\xi_2) \tag{19}$$
and observe that the function $v = w_-$ satisfies the Dirichlet problem in the upper half $V_R = \{\xi \in Y_R : \xi_2 > 0\}$ of the waveguide Y_R, namely

$$-\Delta v(\xi) = \beta v(\xi), \qquad \xi \in V_R, \tag{20}$$
$$v(\xi) = 0, \qquad \xi \in V_R \backslash \Gamma_R, \tag{21}$$
$$v(\xi) = 0, \qquad \xi \in \Gamma_R. \tag{22}$$

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

$$E_- = (0,1,-1). \tag{23}$$

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

$$v^{\circlearrowright} = v^{\circlearrowleft\circlearrowleft} = -v - v^{\circlearrowleft}.$$

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 ½ 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°. Indeed, in cases 1°−4° we compose the solution w_0 with the string $(1,0,0)$ so that w_0 and $w_0^{\circlearrowleft}, w_0^{\circlearrowright}$ in $\mathcal{L}_R^{st}$ stay linear independent:

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

2°. $C_0 = 0, C = 1 \quad \Rightarrow \quad w_0 = \frac{1}{2}(v^{\circlearrowleft} + v^{\circlearrowright} - v)$;

3°. $C_0 = 1, C = -1 \quad \Rightarrow \quad w_0 = -\frac{1}{2}(v^{\circlearrowleft} + v^{\circlearrowright})$;

4°. $C_0 = 1, C \neq -1, -\frac{1}{2} \quad \Rightarrow \quad w_0 = \frac{1+C}{1+C-2C^2}\left(v - \frac{C}{1+C}(v^{\circlearrowleft} + v^{\circlearrowright})\right)$.

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

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

Hence, for 5°, 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

$$\partial_N w_0(\xi) = 0, \qquad \xi \in \Gamma_R. \tag{24}$$

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 $w_0^{\circlearrowleft}$ 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

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

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

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

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

$$-\Delta U_R^h(x; \theta) = \Lambda_R^h(\theta) U_R^h(x; \theta), \qquad x \in g_R^h, \tag{27}$$

$$U_R^h(x; \theta) = 0, \qquad x \in \partial g_R^h \backslash t^h, \tag{28}$$

with the quasi-periodicity conditions

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

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

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

$$0 < \Lambda_{R1}^h(\theta) \leq \Lambda_{R2}^h(\theta) \leq \Lambda_{R3}^h(\theta) \leq \cdots \leq \Lambda_{Rk}^h(\theta) \leq \cdots \longrightarrow +\infty, \tag{31}$$

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

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

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

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

Let $\mu_R^1, \dots, \mu_R^{m(R)} \in (0, \pi^2)$ be all eigenvalues in the discrete spectrum Σ_R^{di} of the problem (1), (2) and let $\mu_R^{m(R)+1} = \cdots = \mu_R^{m(R)+\kappa(R)} = \pi^2$ 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

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

This asymptotic formula means that the spectral bands $\varsigma_R^h(1), \dots, \varsigma_R^h(m(R) + \kappa(R))$ 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

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

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

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

$$-\partial_{z_\pm}^2 U_\pm^0(z_\pm; \theta) = \Lambda^0(\theta) U_0^0(z_0; \theta), \qquad z_\pm \in (-\frac{1}{2}, 0) \cup (0, \frac{1}{2}) \tag{37}$$

with the quasi-periodicity conditions

$$U^0_\pm(z_\pm;\theta)|_{z_\pm=\frac12} = e^{i\theta_\pm}U^0_\pm(z_\pm;\theta)|_{z_\pm=-\frac12}, \tag{38}$$

$$\partial_{z_\pm} U^0_\pm(z_\pm;\theta)|_{z_\pm=\frac12} = e^{i\theta_\pm}\partial_{z_\pm} U^0_\pm(z_\pm;\theta)|_{z_\pm=-\frac12}. \tag{39}$$

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

$$U^h_{R\alpha}(x;\theta) = U^0_\pm\big(z_\pm;\theta\big)\cos(\pi h^{-1}y_\alpha) + \cdots \tag{40}$$

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 $g^0_{l\pm}$, $g^0_{r\pm}$ 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 $(\partial g^h_R \cap \partial g^h)\backslash t^h$ are satisfied, too.

Near the nodes, the disks D^l_{hR} and D^r_{hR} centered at the points $\mathcal{O}_l$ and $\mathcal{O}_r$ with the local coordinates $z_0 = -\frac12$ and $z_0 = \frac12$, respectively, the geometry of the cell g^h_R 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

$$U^0_l = \big(U^0_0(-\tfrac12), U^0_{l+}(0), U^0_{l-}(0)\big), \qquad U^0_r = \big(U^0_0(+\tfrac12), U^0_{r-}(0), U^0_{r+}(0)\big), \tag{41}$$

$$\partial_z U^0_l = \big(\partial_{z_0} U^0_0(-\tfrac12), \partial_{z_+} U^0_{l+}(0), -\partial_{z_-} U^0_{l-}(0)\big),$$

$$\partial_z U^0_r = \big(\partial_{z_0} U^0_0(+\tfrac12), -\partial_{z_-} U^0_{r-}(0), \partial_{z_+} U^0_{r+}(0)\big). \tag{42}$$

Here, $U^0_{l\pm}$, $U^0_{r\pm}$ and U^0_0 are the restrictions of the function U^0 on the segments $g^0_{l\pm}$, $g^0_{r\pm}$ 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 $G^h_R = G^h$ 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

$$U^0_f = 0 \in \mathbb{C}^3, \quad f = l, r. \tag{43}$$

Since, by (43), the graph g^0 is divided into three independent segments with the Dirichlet conditions at the endpoints (notice that $g^0_{l\pm}$ and $g^0_{r\pm}$ 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 $\varsigma^h_R(k)$, $k > 1$, 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, $\dim \mathcal{L}^{st}_R = 0$. However, the total multiplicity $\#\Sigma^{di}_R$ 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 $\mathbb{L}^{st}_R \subset \mathbb{R}^3$ be a subspace of coefficient strings $C = (C_0, C_+, C_-)$ in the decomposition (9) of solutions in $\mathcal{L}^{st}_R$. We set $\mathbb{L}^{li}_R = \mathbb{R}^3 \ominus \mathbb{L}^{st}_R$ and observe that, for any $K \in \mathbb{L}^{li}_R$, the problem (6), (7) gets a solution in the form

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

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

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

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

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

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

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

$$U^h(x,\theta) \sim \Big(U_0^0(-\tfrac12;\theta) + (z_0 + \tfrac12)\partial_{z_0} U_0^0(-\tfrac12;\theta), U_{l+}^0(0;\theta) \tag{47}$$
$$+ \partial_{z_+} U_{l+}^0(0;\theta), U_{l-}^0(0;\theta) + z_-\, \partial_{z_-} U_{l-}^0(0;\theta) \Big)$$
$$= U_l^0(\theta) + h\zeta \partial_z U_l^0(\theta)$$

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

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

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°. $d_R^{st} = 0 \quad \Rightarrow \quad$ 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°. $d_R^{st} = 1 \quad \Rightarrow \quad$ the Kirchhoff conditions

$$U_f^0(\theta) = c_f(\theta)E, \qquad E \cdot \partial_z U_f^0(\theta) = 0, \ f = l, r. \tag{49}$$

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

$$U_0^0(-\tfrac12;\theta) = U_{l+}^0(0;\theta) = U_{l-}^0(0;\theta),$$

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,

$$\partial_{z_0} U_0^0(-\tfrac12;\theta) + \partial_{z_+} U_{l+}^0(0;\theta) - \partial_{z_-} U_{l-}^0(0;\theta) = 0.$$

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

$$E \cdot U_f^0(\theta) = 0, \qquad \partial_z U_f^0(\theta) = k_f(\theta)E, \ f = l, r. \tag{50}$$

In this case the strings (23) and $E_-^{\circlearrowleft} = (-1,0,1)$ 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:

$$U_0^0(-\tfrac12;\theta) + U_{l+}^0(0;\theta) + U_{l-}^0(0;\theta) = 0,$$
$$\partial_{z_0} U_0^0(-\tfrac12;\theta) = \partial_{z_+} U_{l+}^0(0;\theta) = -\partial_{z_-} U_{l-}^0(0;\theta).$$

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

$$\partial_z U_f^0(\theta) = 0, \qquad f = l, r, \tag{51}$$

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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