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Asymptotics of the spectrum of the Dirichlet Laplacian on a thin carbon nano-structure

Analyse asymptotique du spectre de l'opérateur laplacien de Dirichlet dans une fine nano-structure de carbone

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A B S T R A C T

For the honeycomb lattice of quantum waveguides, the limit passage is performed when the relative thickness h of ligaments tends to zero and the asymptotic structure of the spectrum of the Dirichlet Laplacian is described.

R É S U M É

Pour la structure en nid d'abeille du guide d'ondes quantique, on réalise un passage à la limite lorsque l'épaisseur relative h des liaisons tend vers zéro, et on décrit le comportement asymptotique du spectre de l'opérateur laplacien de Dirichlet.

1. Formulation of the spectral problem

The graph G^0 in Fig. 1a can be obtained as a union of the double-periodic family of shifts of the fundamental cell ω^0 entered into the parallelogram region $\lozenge$ defined by the vectors $\boldsymbol{e}_\pm = (3/2, \pm\sqrt{3}/2)$ and overshadowed in Fig. 1a. In the domain $G^h = \{x : \mathrm{dist}(x, G^0) < \frac{h}{2}\}$, that is the h-neighborhood of G^0, see Fig. 1b, we consider the spectral Dirichlet problem in the variational form

$$(\nabla u^h, \nabla v^h)_{G^h} = \lambda^h (u^h, v^h)_{G^h} \quad \forall v^h \in H^1_0(G^h)$$

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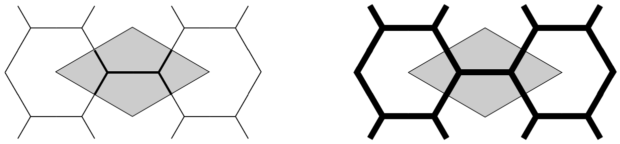

Fig. 1. The graph G^0 and h-neighborhood G^h where the width of the ligaments is h.

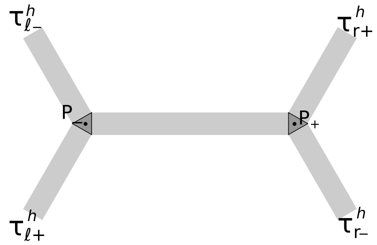

Fig. 2. The cell ω^h.

and study the asymptotics of its spectrum σ^h as $h \to +0$. Here, ∇ is the gradient, $(\,,\,)_{G^h}$ the scalar product in $L^2(G^h)$ and the Sobolev space $H^1_0(G^h)$ of functions vanishing at the boundary ∂G^h.

The Floquet–Bloch theory, cf. [1,2], provides the band-gap structure of the spectrum

$$\sigma^h = \bigcup_{n=1}^{\infty} B^h_n \text{ with the spectral bands } B^h_n = \left\{\Lambda^h_n(\theta) : \theta = (\theta_+, \theta_-) \in [-\pi, \pi]^2\right\} \subset \mathbb{R}_+ \tag{1}$$

defined by the eigenvalues $\{\Lambda^h_n(\theta)\}$ of the model problem on the periodicity cell $\omega^h = G^h \cap \lozenge$,

$$\left(\nabla U^h, \nabla V^h\right)_{\omega^h} = \Lambda^h\left(U^h, V^h\right)_{\omega^h} \quad \forall V^h \in H^1_0\left(\omega^h; \theta\right)$$

where $H^1_0(\omega^h; \theta)$ is a subspace of functions $V \in H^1(\omega^h)$ subject to the conditions

$$V(x) = 0, \quad x \in \partial\omega^h \setminus \partial\lozenge, \quad V \restriction \tau^h_{r\pm} = \mathrm{e}^{\mathrm{i}\theta_\pm} V \restriction \tau^h_{l\pm} \tag{2}$$

Here, $\tau^h_{p\pm}$ are the ends of the “legs” of ω^h indicated in Fig. 2 and supplied with the indices $p = l$ (left) and $p = r$ (right). Moreover, $\theta = (\theta_+, \theta_-)$ is the Floquet variable, which is not displayed explicitly as an argument for functions $U^h(x; \theta)$, $V^h(x; \theta)$, and $\Lambda^h(\theta)$ is a new notation for the spectral parameter. Clearly, the functions $[-\pi, \pi]^2 \ni \theta \mapsto \Lambda^h_n(\theta) \in (0, +\infty)$ are continuous and 2π-periodic in $\theta_\pm$.

2. The graph models

Since the groundbreaking experiment [3] of the extraction of carbon flakes, graphene, many publications focus on the examination of the spectrum of hexagonal lattices. In pioneering [4,5] and subsequent papers, the classical Pauling model [6] was accepted. Namely, they assume the asymptotic ansatz for the eigenvalues of the Dirichlet Laplacian to be

$$\lambda^h = h^{-2}\pi^2 + \beta + \mathcal{O}(h) \tag{3}$$

where β is the eigenvalue of the limit problem

$$\left(\partial_z u^0, \partial_z v^0\right)_{\omega^0} = \beta\left(u^0, v^0\right)_{\omega^0} \quad \forall v^0 \in H^1\left(\omega^0; \theta\right) \tag{4}$$

with the Kirchhoff transmission conditions at the interior nodes $P^\pm = (\pm 1/2, 0)$ and the quasi-periodicity conditions inherited from (2) at the exterior nodes. That is, functions in the subspace $H^1(\omega^0; \theta)$ are continuous at $P^\pm$. As a result, a quite intricate band-gap structure of the spectrum was described in [5].

The Kirchhoff conditions are rigorously justified in [7,8] (see also [9–11]) for the Neumann problem (where $h^{-2}\pi^2$ is omitted in (3)) while the Dirichlet problem does not retrieve a completed examination yet. An original approach developed in [7] (see also [12]) demonstrates that the limit conditions at $P^\pm$ depend on the boundary layer effects in the vicinity of nodes in a thin Dirichlet junction. For the quantum honeycomb lattice G^h, the boundary layer appears as solutions in the infinite waveguide $\mathbb{Y}$ in Fig. 3a, and its investigation is a principal issue of our note because variational methods useful in the Neumann case do not work in the Dirichlet one. However, Theorems 3.1 and 3.2 entail that, first, the asymptotic ansatz (3) is not suitable for the low-frequency range of the spectrum (1) and, second, the limit problem (4) involves the Dirichlet conditions

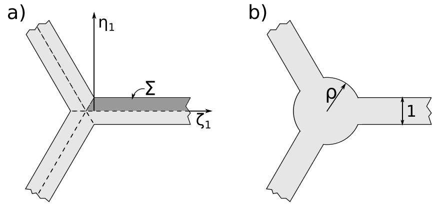

Fig. 3. The infinite waveguides $\mathbb{Y}$ and $\mathbb{Y}(\rho)$.

$$u^0\left(P^{\pm}\right)=0 \tag{5}$$

that divide the limit problem (4) into three independent problems for the operator $\partial_z^2+\beta$ on the interval $(-1/2,1/2)\ni z$ with the eigenvalues of multiplicity 3

$$\beta_m=\pi^2 m^2, \quad m=1,2,3,\ldots \tag{6}$$

In total, our asymptotic analysis shows that the spectrum σ^h consists of small bands and therefore has big gaps, cf. Theorems 4.1 and 4.2, but such structure differs significantly from that predicted in [5] on the basis of the Pauling model. It should be emphasized that the conditions (5) are related to the peculiar geometry in Fig. 3a, while for certain radii

$$1/\sqrt{3}<\rho_1<\rho_2<\ldots<\rho_q<\ldots\to+\infty \tag{7}$$

of the circular core in Fig. 3b, other limit conditions, in particular, the Kirchhoff ones, occur.

3. The Dirichlet problem in the infinite waveguide

Let $\mathbb{Y}$ be the triffid [13], Fig. 3a, that is a symmetric junction of three pointed unit semi-strips meeting at the angle $2\pi/3$ between their axes. The continuous spectrum of the Dirichlet problem

$$(\nabla w,\nabla v)_{\mathbb{Y}}=\mu\,(w,v)_{\mathbb{Y}} \quad \forall v\in H_0^1(\mathbb{Y}) \tag{8}$$

implies the ray $\left[\pi^2,+\infty\right)$, while its discrete spectrum has been examined in [14].

Theorem 3.1. *The problem (8) has only one eigenvalue μ_0 in the interval $\left(0,\pi^2\right)$ below the continuous spectrum. This eigenvalue is simple and the corresponding eigenfunction $w_0\in H_0^1(\mathbb{Y})$ is positive and symmetric with respect to the dotted lines in Fig. 3a, and decays at the rate $\mathcal{O}\left(\exp\left(-\sqrt{\pi^2-\mu_0}\,|\xi|\right)\right)$.*

The central result in this paper concerns the same Dirichlet problem, but at the threshold $\mu_\dagger=\pi^2$

$$-\Delta w(\xi)-\pi^2 w(\xi)=f(\xi),\ \xi\in\mathbb{Y}, \quad w(\xi)=0,\ \xi\in\partial\mathbb{Y} \tag{9}$$

Theorem 3.2. *The homogeneous ($f=0$) problem (9) has no bounded solutions, in particular, trapped modes in $H_0^1(\mathbb{Y})$ so that $\mu=\pi^2$ is not an eigenvalue in the point spectrum of the problem (8).*

Our proof of this most technical assertion is performed in several steps.

Lemma 3.3. *A bounded solution, if it exists, is unique up to a multiplicative constant.*

Proof. We dissect the triffid into three "legs" $\Pi^j=\left\{\xi:\zeta_j>0,\left|\eta_j\right|<1/2\right\}$, $j=1,2,3$, and the triangular "body" $\lhd$, where η_j,ζ_j are the local coordinates, see Fig. 3a. Let us assume that there exist two linearly independent bounded solutions w_1 and w_2. Since they cannot vanish everywhere in $\lhd$, cf. [15, Ch. 4], we may choose a non-trivial linear combination $w_\bullet=c_1 w_1+c_2 w_2$ such that

$$(w_\bullet,1)_{\lhd}=0 \tag{10}$$

By the Fourier method, the bounded solution $w_\bullet$ admits the representations

$$w_\bullet(\xi)=k_j\cos\left(\pi\eta_j\right)+\mathcal{O}\left(\exp\left(-\sqrt{3}\pi\zeta_j\right)\right), \quad \xi\in\Pi^j,\ k_j\in\mathbb{R},\ j=1,2,3 \tag{11}$$

In the truncated waveguide $\mathbb{Y}(R)=\left\{\xi\in\mathbb{Y}:\zeta_j<R,\ \ j=1,2,3\right\}$, the Green formula yields

$$\int_{\lhd} \left(|\nabla w_\bullet|^2 - \pi^2 |w_\bullet|^2\right) \mathrm{d}\xi + \sum_{j=1}^{3} \int_{\Pi^j(R)} \left(|\nabla w_\bullet|^2 - \pi^2 |w_\bullet|^2\right) \mathrm{d}\xi = \sum_{j=1}^{3} \int_{-1/2}^{1/2} \left(w_\bullet \partial_{\zeta_j} w_\bullet\right)_{|\zeta_j = R} \mathrm{d}\eta_j \tag{12}$$

The Poincaré inequality $\left\|\nabla w_\bullet; L^2(\lhd)\right\|^2 \geq \kappa_1 \left\|w_\bullet; L^2(\lhd)\right\|^2$ is valid due to the orthogonality condition (10) with the constant $\kappa_1 \geq 16\pi^2/9$ as the first positive eigenvalue of the Neumann problem in $\lhd$, cf. [16]. Moreover, the Poincaré inequality due to the Dirichlet condition assures that the integral over $\Pi_j(R)$ in (12) is non-negative. Because the right-hand side of (12) decays as $R \to +\infty$ but the left-hand side stays bigger than $7\pi^2/9 \left\|w_\bullet; L^2(\lhd)\right\|^2$, thus $w_\bullet \equiv 0$ in $\lhd$, which is impossible, see [15, Ch. 4]. □

Due to the uniqueness, a bounded solution $w_\bullet$ is symmetric with respect to three dotted lines in Fig. 3a. Hence, the restriction of $w_\bullet$ on the sharpened semi-strip $\Sigma = \left\{\xi = (\xi_1, \xi_2) \in \mathbb{Y} : \xi_2 \in \left(0, \frac{1}{2}\right), \sqrt{3}\xi_1 > \xi_2\right\}$ (overshadowed in Fig. 3a) satisfies the mixed boundary value problem at $\mu_\dagger = \pi^2$

$$-\Delta w(\xi) = \pi^2 w(\xi),\ \xi \in \Sigma, \qquad w(\xi) = 0,\ \xi \in \partial\Sigma \cap \partial\mathbb{Y}, \qquad \partial_\nu w(\xi) = 0,\ \xi \in \partial\Sigma \setminus \partial\mathbb{Y} \tag{13}$$

Clearly, the continuous spectrum of the problem (13) is still the ray $\left[\pi^2, +\infty\right)$ and the discrete spectrum consists of the only point $\mu = \mu_0$, cf. Theorem 3.1.

The next step deals with a perturbed problem in Σ, namely the integro-differential equation

$$-\Delta w^\varepsilon(\xi) - \varepsilon J\left(w^\varepsilon; \xi\right) = \mu^\varepsilon w^\varepsilon(\xi), \quad \xi \in \Sigma \tag{14}$$

with the boundary conditions from (13), a small parameter $\varepsilon > 0$, and the integral operator

$$J\left(w^\varepsilon; \xi\right) = \mathcal{J}\left(w^\varepsilon\right) \Psi(\xi),\ \mathcal{J}\left(w^\varepsilon\right) = \left(w^\varepsilon, \Psi\right)_\varsigma$$

where the kernel Ψ is a smooth function with a support in the triangle $\varsigma = \left\{\xi \in \Sigma : \xi_1 < 1/2\sqrt{3}\right\}$

Lemma 3.4. *For a small ε, the total multiplicity of the discrete spectrum of the problem (14), with the boundary conditions in (13), does not exceed* 1.

Proof. We assume the existence of two eigenvalues $\mu_1^\varepsilon, \mu_2^\varepsilon \in \left(0, \pi^2\right)$ and apply the max-min principle, see, e.g. [17, Thm. 10.2.2],

$$\mu_2^\varepsilon = \max_E \inf_{w^\varepsilon \in E \setminus \{0\}} \left\|w^\varepsilon; L^2(\Sigma)\right\|^{-2} \left(\left\|\nabla w^\varepsilon; L^2(\Sigma)\right\|^2 - \varepsilon \left|J(w^\varepsilon)\right|^2\right) \tag{15}$$

where E is any subspace of co-dimension 1 in the space $\left\{w^\varepsilon \in H^1(\Sigma) : w^\varepsilon = 0 \text{ on } \partial\Sigma \cap \partial\mathbb{Y}\right\}$. Let $E_\perp = \{w^\varepsilon \in H^1(\Sigma) : w^\varepsilon(\xi) = 0,\ \xi \in \partial\Sigma \cap \partial\mathbb{Y},\ \left(w^\varepsilon, 1\right)_\varsigma = 0\}$, while $\operatorname{codim} E_\perp = 1$. Using the Poincaré inequalities in $\Sigma \setminus \varsigma$ and ς in the same way as above and observing that $\left|\mathcal{J}\left(w^\varepsilon\right)\right| \leq c \left\|w^\varepsilon; L^2(\varsigma)\right\|$, we conclude that the Rayleigh quotient with $w^\varepsilon \in E_\perp$ in (15) is not smaller than π^2 and come across a contradiction. □

The last step relies upon an observation made in [18], although for a somewhat different problem, namely, if the perturbed problem (14) with boundary conditions (13) possesses a near-threshold eigenvalue

$$\mu_2^\varepsilon = \pi^2 - \tilde{\mu}_2^\varepsilon, \text{ where } \tilde{\mu}_2^\varepsilon > 0 \text{ and } \tilde{\mu}_2^\varepsilon = o(1) \text{ as } \varepsilon \to +0 \tag{16}$$

then the limit problem (13) at the threshold $\mu_\dagger = \pi^2$ has a bounded solution. We, in a sense, follow the reverse route. Assuming the existence of a bounded solution $w_\bullet$, we construct the eigenvalue (16) and detect a contradiction to Lemma 3.4 because the problem (14) with boundary conditions in (13) has an eigenvalue $\mu_1^\varepsilon = \mu_0 + \mathcal{O}(\varepsilon) \neq \mu_2^\varepsilon$, which is a small perturbation of the eigenvalue $\mu_0 \in \left(0, \pi^2\right)$ in Theorem 3.1.

To construct the eigenvalue (16), one may employ a standard approach, see, e.g. [19], based on the method of matched asymptotic expansions. In this way, assuming $k_\bullet := k_1 \neq 0$ in the representation (11) restricted on Σ, and imposing the normalization condition $(w_\bullet, \Psi)_\varsigma = 1$, yields the eigenvalue with $\tilde{\mu}_2^\varepsilon = 16k_\bullet^{-4}\varepsilon^2 + \mathcal{O}\left(\varepsilon^3\right)$. In the case $k_\bullet = 0$ when $w_\bullet$ is a trapped mode, the correction term in (16) takes the form $\tilde{\mu}_2^\varepsilon = \varepsilon \left\|w_\bullet; L^2(\Sigma)\right\|^{-2} + \mathcal{O}\left(\varepsilon^2\right)$. Theorem 3.2 is proved.

4. Asymptotics of the spectral bands

Our results on the problem (8) concretize the conclusions of the paper [7]. Asymptotics of the low-frequency range of the spectrum (1) inside $\left(0, h^{-2}\pi^2\right)$ is given by Theorem 4.1.

Theorem 4.1. *There exist* $\varepsilon_0, c_0 > 0$ *such that, for* $\varepsilon \in (0, \varepsilon_0)$ *and* μ_0 *from Theorem 3.1, we have*

$$B_1^h, B_2^h \subset \left(h^{-2}\mu_0 - c_0 \exp\left(-h^{-1}\sqrt{\pi^2 - \mu_0}\right), h^{-2}\mu_0 + c_0 \exp\left(-h^{-1}\sqrt{\pi^2 - \mu_0}\right)\right)$$

According to [7], the absence of bounded solutions concluded in Theorem 3.2 implies that the limit problem (4) on the graph ω^0 involves the Dirichlet conditions (5) and gets the eigenvalues (6). In this way, the middle-frequency range of the spectrum (1) is described by Theorem 4.2.

Theorem 4.2. *For* $m = 1, 2, 3, \ldots$, *there exists* $\varepsilon_m, c_m > 0$ *such that, for* $\varepsilon \in (0, \varepsilon_m)$, *three spectral bands* B_{3m+p}^h, $p = 0, 1, 2$, *lay inside the interval* $\left(h^{-2}\pi^2 + \pi^2 m^2 - c_m h, h^{-2}\pi^2 + \pi^2 m^2 + c_m h\right)$.

The comparison principle ensures that the total multiplicity of the discrete spectrum of the problem (8) in $\mathbb{Y}(\rho) = \mathbb{Y} \cup \{\xi : |\xi| < \rho\}$ grows indefinitely when $\rho \to +\infty$. Thus, the near-threshold eigenvalues (16) must appear in the spectrum of $\mathbb{Y}(\rho_q + \varepsilon)$ so that the above-mentioned result in [18] guarantees the existence of bounded solutions at $\mu_\dagger = \pi^2$ in the waveguide $\mathbb{Y}(\rho_q)$, Fig. 3b, for some radii in (7). Correspondingly, the procedure [7] gives rise to another, maybe, Kirchhoff transmission conditions at $P^\pm$, which however are unstable and enlarging a critical radius $\rho = \rho_q$ returns the Dirichlet conditions into the limit problem (4).

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