C. R. Mecanique 343 (2015) 360–364

Contents lists available at ScienceDirect

Comptes Rendus Mecanique

www.sciencedirect.com

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

Sergei A. Nazarov [a,b], Keijo Ruotsalainen [c], Pauliina Uusitalo [c,*]

[a] Saint-Petersburg State University, Universitetsky pr., 28, Peterhof, St. Petersburg, 198504, Russia
[b] Saint-Petersburg State Polytechnical University, Polytechnicheskaya ul., 29, St. Petersburg, 195251, Russia
[c] University of Oulu, Mathematics Division, P.O. Box 4500, 90014, Oulu, Finland

A R T I C L E I N F O

Article history:
Received 30 January 2015
Accepted 16 March 2015
Available online 7 April 2015

Keywords:
Spectrum
Dirichlet problem
Asymptotics
Quantum waveguide
Trapped modes and bounded solutions

Mots-clés :
Spectre
Opérateur laplacien de Dirichlet
Analyse asymptotique
Guides d'ondes quantiques
Modes piégés et solutions bornées

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 $\Diamond$ 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

$$(\nabla u^h, \nabla v^h)_{G^h} = \lambda^h (u^h, v^h)_{G^h} \quad \forall v^h \in H_0^1(G^h)$$

* Corresponding author.
E-mail addresses: srgnazarov@yahoo.co.uk (S.A. Nazarov), keijo.ruotsalainen@oulu.fi (K. Ruotsalainen), paulina.uusitalo@gmail.com (P. Uusitalo).

http://dx.doi.org/10.1016/j.crme.2015.03.001

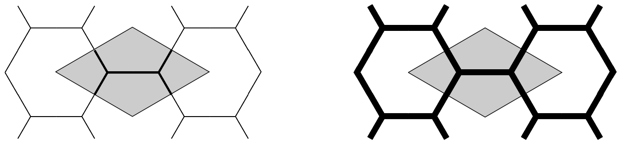

Fig. 1. The graph G^0 and h-neighborhood G^h where the width of the ligaments is h.

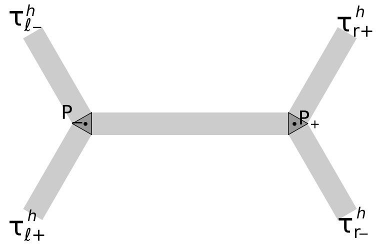

Fig. 2. The cell ω^h.

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 $\omega^h = G^h \cap \Diamond$,

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

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

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

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