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A mathematical basis for the graphene

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Abstract
We present a new basis of representation for the graphene honeycomb structure that facilitates the solution of the eigenvalue problem by reducing it to one dimension. We define spaces in these geometrical basis that allow us to solve the Hamiltonian in the edges of the lattice. We conclude that it is enough to analyze a one-dimensional problem in a set of coupled ordinary second-order differential equations to obtain the behavior of the solutions in the whole graphene structure.

Keywords Periodic solutions · Stability · General spectral theory · Spectral theory and eigenvalue problems · Graphene · Honeycomb structure

Mathematics Subject Classification 34L05 · 82D80 · 34B60 · 34B45 · 47A10 · 34D20

1 Introduction

Graphene is a novel material with carbon atoms arranged in a honeycomb lattice. In the past years, it has caught the attention of the scientific community for its unique electronic properties (Alexander 1983; Avron et al. 1988; De Gennes 1981; Harris 2002; Katsnelson 2007; Kuchment and Post 2007; Saito et al. 1998). The behavior of the electrons in the lattice can be captured by solving the Hamilton equations of the system as an spectral,

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or eigenvalues, problem $\mathcal{H}\Psi \equiv \lambda\Psi$. However, a complete analytical solution stands as a mathematical challenge.

We present a new basis of representation for the graphene honeycomb structure G that facilitates the solution of the eigenvalue problem by reducing it to one dimension. For this, we define two spaces in the geometrical basis G, $L^2(G)$ and $H^2(G)$, that allow us to solve the Hamiltonian in the edges of G as $\mathcal{H} : H^2(G) \subset L^2(G) \to L^2(G)$.

The paper is organized as follows. As part of this introduction, in Sect. 1.1, we show a survey of the previous results and in Sect. 1.2 we define the basis of the graphene as a set of edges L_q of G such that every eigenfunction Ψ can be extended to all G from the values of Ψ in each edge L_q. We also explicitly show the canonical basis of the system and some of its properties are presented. In Sect. 2, we present the proofs of the principal results exposed in Sect. 1.2. Finally, in Sect. 3, we analyze bases with support in the half-plane, i.e., we seek for solutions of $\mathcal{H}\Psi \equiv \lambda\Psi$ such that $\Psi \in L^2(G)$ has a compact support.

1.1 Survey of the previous results

The mathematical definition of the problem has been set in previous works (Conca et al. 2019). However, here we summarize theorems and definitions necessaries to present our current results.

1.1.1 Floquet theory

Let us consider the Hill's equation defined in Eastham (1973) as

$$-\Psi''(x) + V(x)\Psi(x) = \lambda\Psi(x). \tag{1}$$

Here, the function V is real, piecewise-continuous and 1-periodic. We know that equation (1) has a basis of two linearly independent solutions $\varphi_1(\cdot;\lambda)$ and $\varphi_2(\cdot;\lambda)$, functions of the parameter λ, that satisfy

$$\varphi_1(0;\lambda) = 1,\ \varphi_1'(0;\lambda) = 0,\ \varphi_2(0;\lambda) = 0,\ \varphi_2'(0;\lambda) = 1. \tag{2}$$

It is clear that any solution Ψ of (1) can be written as a linear combination:

$$\Psi(x) = \Psi(0)\varphi_1(x;\lambda) + \Psi'(0)\varphi_2(x;\lambda). \tag{3}$$

The *discriminant* of (1) is given by

$$\mathcal{D}(\lambda) = \varphi_1(1;\lambda) + \varphi_2'(1;\lambda).$$

If the function V satisfies the symmetry relation $V(1-x) = V(x)$, then

$$\varphi_2'(1;\lambda) = \varphi_1(1;\lambda), \tag{4}$$

implying

$$\mathcal{D} = 2\varphi_1(1;\lambda). \tag{5}$$

1.1.2 The graphene

The graphene is a substance made of pure carbon, where the atoms follow a regular hexagon pattern. This atoms are mathematically described by a set of vertices $\mathcal{V} \subseteq \mathbb{R}^2$ as Fig. 1 shows.

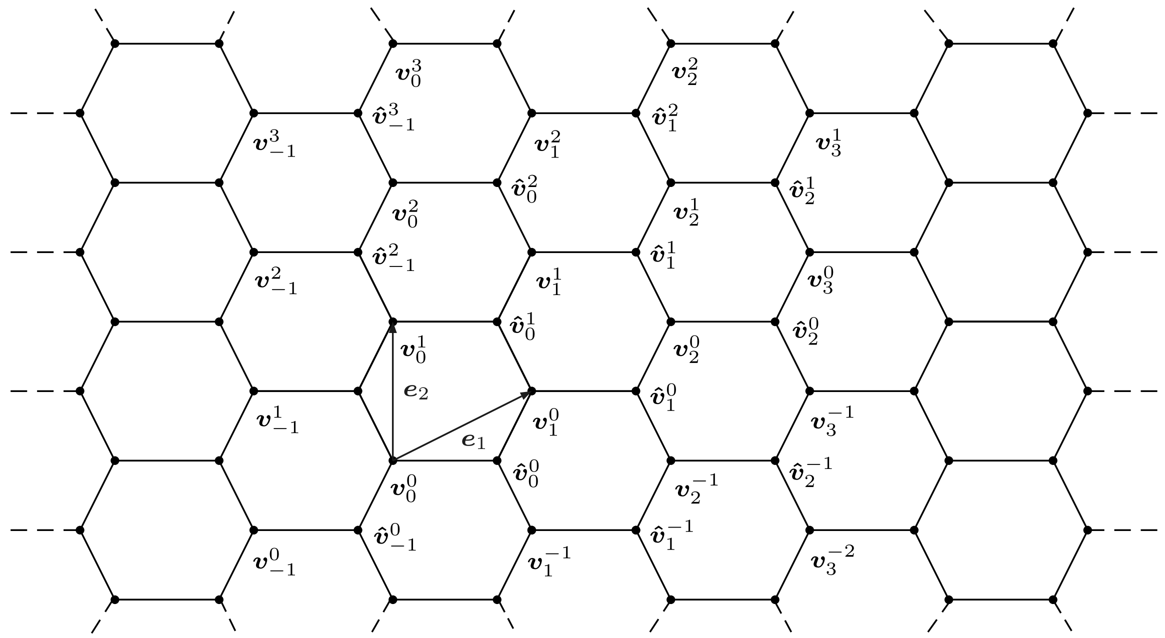

Fig. 1 Vertices $\boldsymbol{v}_i^j$ and $\hat{\boldsymbol{v}}_i^j$ representing the graphene G

More precisely, let us introduce the vectors

$$\boldsymbol{e}_1 = \left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right) \qquad \text{y} \qquad \boldsymbol{e}_2 = \left(0, \sqrt{3}\right). \tag{6}$$

Then, the set of vertices $\mathcal{V}$ is defined by

$$\mathcal{V} = \left\{\boldsymbol{v}_i^j, \hat{\boldsymbol{v}}_i^j : i, j \in \mathbb{Z}\right\}, \tag{7}$$

where the family of vertices $(\boldsymbol{v}_i^j)_{i,j\in\mathbb{Z}}$ and $(\hat{\boldsymbol{v}}_i^j)_{i,j\in\mathbb{Z}}$ are defined by the relations:

$$\boldsymbol{v}_i^j = i\boldsymbol{e}_1 + j\boldsymbol{e}_2 \tag{8}$$

$$\hat{\boldsymbol{v}}_i^j = \boldsymbol{v}_i^j + (1, 0). \tag{9}$$

As Fig. 1 shows, these vertices are connected by a set of edges $\mathcal{A}$ defined by

$$\mathcal{A} = \left\{a_E^{i,j}, a_N^{i,j}, a_S^{i,j} : a_E^{i,j} = [\boldsymbol{v}_i^j, \hat{\boldsymbol{v}}_i^j], a_N^{i,j} = [\boldsymbol{v}_i^j, \hat{\boldsymbol{v}}_{i-1}^j], a_S^{i,j} = [\boldsymbol{v}_i^j, \hat{\boldsymbol{v}}_{i-1}^{j+1}], i, j \in \mathbb{Z}\right\}, \tag{10}$$

as it is displayed in Fig. 2. These set of edges and vertices constitute an hexagonal grid.

Using this notation, the structure of the graphene is represented by a non-oriented graph G determined by the set of vertices and edges previously defined, i.e.,

$$G = (\mathcal{V}, \mathcal{A}).$$

We notice that each edge of the graphene is bijective to the segment $[0, 1] \subseteq \mathbb{R}$. In fact, to visualize this bijection, we consider the parameterization $\boldsymbol{\sigma}$, oriented from $\boldsymbol{v}$ to $\boldsymbol{w}$, defined by:

$$\begin{aligned} \boldsymbol{\sigma} &: [0, 1] \times \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}^2 \\ &(t; \boldsymbol{v}, \boldsymbol{w}) \mapsto \boldsymbol{\sigma}(t; \boldsymbol{v}, \boldsymbol{w}) = \boldsymbol{v} + t(\boldsymbol{w} - \boldsymbol{v}). \end{aligned} \tag{11}$$

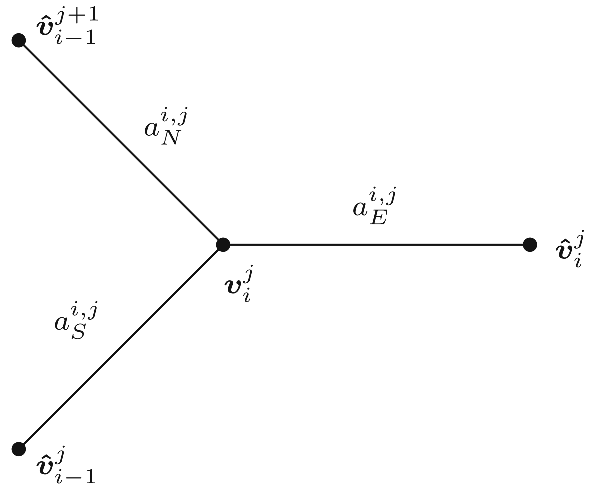

Fig. 2 Edges $a_E^{i,j}$, $a_N^{i,j}$ and $a_S^{i,j}$, and their respective vertices

Thus, each edge $[\boldsymbol{v}_1, \boldsymbol{v}_2] \in \mathcal{A}$ can be written as $\boldsymbol{\sigma}([0,1]; \boldsymbol{v}_1, \boldsymbol{v}_2)$. The inverse function is such that

$$\mathbf{x} \in [\boldsymbol{v}_1, \boldsymbol{v}_2] \mapsto \boldsymbol{\sigma}^{-1}(\mathbf{x}; \boldsymbol{v}_1, \boldsymbol{v}_2) = \frac{\| \mathbf{x} - \boldsymbol{v}_1 \|}{\| \boldsymbol{v}_2 - \boldsymbol{v}_1 \|}. \tag{12}$$

Using the parametrization (11), whose inverse is (12), for each edge $[\boldsymbol{v}_1, \boldsymbol{v}_2] \in \mathcal{A}$ we can define the space $L^2(\boldsymbol{v}_1, \boldsymbol{v}_2)$ as follows:

$$L^2(\boldsymbol{v}_1, \boldsymbol{v}_2) = \left\{ \widetilde{\Psi} \circ \boldsymbol{\sigma}^{-1}(\cdot; \boldsymbol{v}_1, \boldsymbol{v}_2) : \widetilde{\Psi} \in L^2(0,1) \right\},$$

endowed with the norm $\|\widetilde{\Psi} \circ \boldsymbol{\sigma}^{-1}(\cdot; \boldsymbol{v}_1, \boldsymbol{v}_2)\|_{L^2(\boldsymbol{v}_1, \boldsymbol{v}_2)} = \|\widetilde{\Psi}\|_{L^2(0,1)}$. Then, we can define $L^2(\mathcal{A})$ as:

$$L^2(\mathcal{A}) = \left\{ (\Psi_a)_{a \in \mathcal{A}} \in \bigotimes_{a \in \mathcal{A}} L^2(a) : \sum_{a \in \mathcal{A}} \|\Psi_a\|^2_{L^2(a)} < \infty \right\}. \tag{13}$$

This space can be also called $L^2(G)$.

Similarly, for each edge $[\boldsymbol{v}_1, \boldsymbol{v}_2] \in \mathcal{A}$ we can define the Sobolev space $H^2(\boldsymbol{v}_1, \boldsymbol{v}_2)$ by:

$$H^2(\boldsymbol{v}_1, \boldsymbol{v}_2) = \left\{ \widetilde{\Psi} \circ \boldsymbol{\sigma}^{-1}(\cdot; \boldsymbol{v}_1, \boldsymbol{v}_2) : \widetilde{\Psi} \in H^2(0,1) \right\},$$

endowed the norm $\|\widetilde{\Psi} \circ \boldsymbol{\sigma}^{-1}(\cdot; \boldsymbol{v}_1, \boldsymbol{v}_2)\|_{H^2(\boldsymbol{v}_1, \boldsymbol{v}_2)} = \|\widetilde{\Psi}\|_{H^2(0,1)}$. Thus, the Sobolev space $H^2(G)$ is defined as the subset of functions $(\Psi_a)_{a \in \mathcal{A}} \in \bigotimes_{a \in \mathcal{A}} H^2(a)$ which satisfy the three following conditions:

$$\sum_{a \in \mathcal{A}} \|\Psi_a\|^2_{H^2(a)} < \infty, \tag{14}$$

$$\forall \boldsymbol{v} \in \mathcal{V}, \forall a_1, a_2 \in \mathcal{A} \; [\boldsymbol{v} \in a_1 \cap a_2 \Rightarrow \Psi_{a_1}(\boldsymbol{v}) = \Psi_{a_2}(\boldsymbol{v})], \tag{15}$$

$$\forall \boldsymbol{v} \in \mathcal{V} \quad \sum_{\substack{\boldsymbol{v}_2 \in \mathcal{V} \\ [\boldsymbol{v}, \boldsymbol{v}_2] \in \mathcal{A}}} D\Psi_{[\boldsymbol{v}, \boldsymbol{v}_2]}(\boldsymbol{v}; \boldsymbol{v}_2 - \boldsymbol{v}) = 0, \tag{16}$$

where we have denoted by $D\Psi_{[\boldsymbol{v}, \boldsymbol{v}_2]}(\boldsymbol{v}; \boldsymbol{v}_2 - \boldsymbol{v})$ the directional derivative of the function $\Psi_{[\boldsymbol{v}, \boldsymbol{v}_2]}$ at the point $\boldsymbol{v}$ in the direction $[\boldsymbol{v}_2 - \boldsymbol{v}]$. These conditions are usually called Neumann conditions of the graphene or Kirchhoff conditions. The first condition, (15), corresponds to the continuity condition on each vertex going from one edge to the other. The second condition, (16), states that the sum of the outward fluxes from the vertex $\boldsymbol{v}$ must be zero.

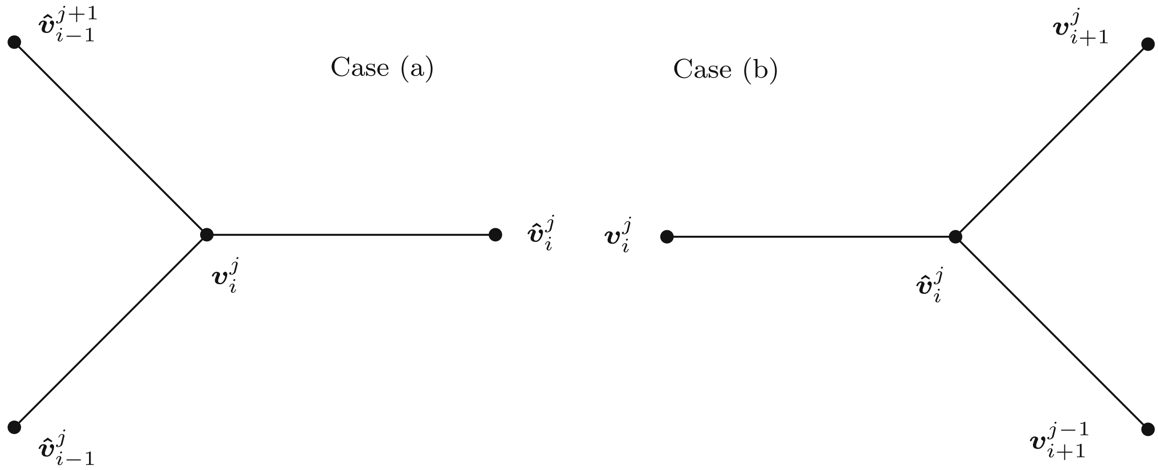

Fig. 3 Adjacent edges to the vertices of type $\hat{\boldsymbol{v}}_i^j$ (Case (a)) and type $\boldsymbol{v}_i^j$ (Case (b))

1.1.3 The Hamiltonian of graphene

Let us now define the Hamiltonian of graphene in $L^2(G)$. Let $V(t)$ be a function in $L^2(0, 1)$ such that

$$V(t) = V(1-t). \tag{17}$$

The *Hamiltonian of graphene* $\mathcal{H} : \mathcal{D}(\mathcal{H}) \subset L^2(G) \to L^2(G)$ is the operator, with domain $\mathcal{D}(\mathcal{H}) = H^2(G)$, that maps $\Psi = (\Psi_a)_{a\in\mathcal{A}} \in H^2(G)$ to $\mathcal{H}\Psi \in L^2(G)$, $\mathcal{H}\Psi = ((\mathcal{H}\Psi)_a)_{a\in A}$, such that

$$(\mathcal{H}\Psi)_a(\mathbf{x}) = \left(-\widetilde{\Psi}_a'' + V\widetilde{\Psi}_a\right) \circ \boldsymbol{\sigma}^{-1}(\mathbf{x}; a), \tag{18}$$

where, for each edge $a \in \mathcal{A}$, $\widetilde{\Psi}_a = \Psi_a \circ \boldsymbol{\sigma}(\cdot; a) \in H^2(0, 1)$.

The goal of this section is to study the spectrum of the operator $\mathcal{H}$, characterizing the functions Ψ which are bounded or unbounded solutions. To do this, we seek for non-zero functions $\Psi = (\Psi_a)_{a\in\mathcal{A}}$ satisfying (15)–(16) and the following differential equations

$$-\widetilde{\Psi}_a''(t) + V(t)\widetilde{\Psi}_a(t) = \lambda\widetilde{\Psi}_a(t), \quad \forall a \in \mathcal{A}, \forall t \in (0, 1), \tag{19}$$

where $\lambda \in \mathbb{R}$ is a parameter.

1.1.4 Kirchhoff's conditions

In this section, we will properly characterize the functions $\Psi = (\Psi_a)_{a\in\mathcal{A}}$ that satisfy Kirchhoff's conditions (15)–(16). First of all, we notice that each vertex $\boldsymbol{v} \in \mathcal{V}$ has exactly three adjacent edges, as Fig. 3 shows. Hence, continuity and flux conditions will be explicitly written at the vertices of type $\boldsymbol{v}_i^j$ and $\hat{\boldsymbol{v}}_i^j$ of $\mathcal{V}$, where $i, j \in \mathbb{Z}$ (see definition (7)).

The main result in this section will be splited into two theorems separating the cases $\varphi_2(1; \lambda) \neq 0$ and $\varphi_2(1; \lambda) = 0$, where $\varphi_2(\cdot; \lambda)$ is the function defined in (2). This separation is important because in the second case λ is included in the Dirichlet case. The first Theorem completely characterizes the functions that satisfy the flux and continuity conditions stated in (15)–(16).

Theorem 1 *If $\varphi_2(1;\lambda) \neq 0$, then every function $\Psi = (\Psi_a)_{a\in\mathcal{A}}$ satisfying* (19)*, also satisfies* (15)–(16) *if and only if, for each $i, j \in \mathbb{Z}$, it holds*

$$-3\varphi_1(1;\lambda)\Psi(\boldsymbol{v}_i^j) + \Psi(\hat{\boldsymbol{v}}_i^j) + \Psi(\hat{\boldsymbol{v}}_{i-1}^j) + \Psi(\hat{\boldsymbol{v}}_{i-1}^{j+1}) = 0, \tag{20}$$

$$-3\varphi_1(1;\lambda)\Psi(\hat{\boldsymbol{v}}_i^j) + \Psi(\boldsymbol{v}_i^j) + \Psi(\boldsymbol{v}_{i+1}^j) + \Psi(\boldsymbol{v}_{i+1}^{j-1}) = 0, \tag{21}$$

where $\varphi_1(\cdot;\lambda)$ and $\varphi_1(\cdot;\lambda)$ are the functions described in (2)*.*

Theorem 2 *If $\varphi_2(1;\lambda) = 0$, every function $\Psi = (\Psi_a)_{a\in\mathcal{A}}$ satisfying* (19)*, also satisfies the* (15)–(16) *if and only if the following conditions hold:*

(1) *There exists $k_\Psi \in \mathbb{R}$, depending on Ψ, such that*

$$\Psi(\boldsymbol{v}_i^j) = k_\Psi \quad y \quad \Psi(\hat{\boldsymbol{v}}_i^j) = k_\Psi\varphi_1(1;\lambda), \quad \forall i, j \in \mathbb{Z}. \tag{22}$$

(2) *If on each edge $a \in \mathcal{A}$ the functions Ψ_a can be written as*

$$\widetilde{\Psi}_a(t) = \widetilde{\Psi}_a(0)\varphi_1(t;\lambda) + c_a\varphi_2(t;\lambda), \tag{23}$$

where the parameterization t is chosen such that the edge goes from left to right, then the constants $(c_a)_{a\in\mathcal{A}}$ satisfy the relations:

$$2k_\Psi\varphi_1'(1;\lambda) + c_{[\hat{\boldsymbol{v}}_{i-1}^{j+1},\boldsymbol{v}_i^j]} + c_{[\hat{\boldsymbol{v}}_{i-1}^j,\boldsymbol{v}_i^j]} = c_{[\boldsymbol{v}_i^j,\hat{\boldsymbol{v}}_i^j]}\varphi_1(1;\lambda), \quad \forall i, j \in \mathbb{Z}, \tag{24}$$

$$k_\Psi\varphi_1'(1;\lambda) + c_{[\boldsymbol{v}_i^j,\hat{\boldsymbol{v}}_i^j]}\varphi_1(1;\lambda) = c_{[\hat{\boldsymbol{v}}_i^j,\boldsymbol{v}_{i+1}^j]} + c_{[\hat{\boldsymbol{v}}_i^j,\hat{\boldsymbol{v}}_{i+1}^{j-1}]}, \quad \forall i, j \in \mathbb{Z}. \tag{25}$$

1.2 Presentation of new results

The goal of this article is to study in more detail the structure of the function space $\Psi = (\Psi_a)_{a\in\mathcal{A}}$ that satisfies the Kirchhoff conditions (15)–(16) and the equations (19). Onwards we will consider these types of functions, and a parameter λ such that $\varphi_2(1;\lambda) \neq 0$, where $\varphi_2(\cdot;\lambda)$ is the function described in (2), and therefore, the conclusions in Theorem 1 hold true.

In the hexagonal grid G, we call *profile* L_q, $q \in \mathbb{Z}$, to the following set of vertices (see Fig. 4):

$$L_q = \left\{\boldsymbol{v}_{2k}^{q-k}, \hat{\boldsymbol{v}}_{2k}^{q-k}, \boldsymbol{v}_{2k+1}^{q-k}, \hat{\boldsymbol{v}}_{2k+1}^{q-k} : k \in \mathbb{Z}\right\}. \tag{26}$$

Thus, all the vertices of G belong to one of these sets, i.e,

$$\mathcal{V} = \bigcup_{q\in\mathbb{Z}} L_q.$$

The profile L_q consists of four generating vertices periodically repeated with period $2\boldsymbol{e}_1 - \boldsymbol{e}_2$. That is, for all $k \in \mathbb{N}$,

$$\boldsymbol{v}_{2k}^{q-k} = \boldsymbol{v}_0^q + k(2\boldsymbol{e}_1 - \boldsymbol{e}_2) \tag{27}$$

$$\hat{\boldsymbol{v}}_{2k}^{q-k} = \hat{\boldsymbol{v}}_0^q + k(2\boldsymbol{e}_1 - \boldsymbol{e}_2) \tag{28}$$

$$\boldsymbol{v}_{2k+1}^{q-k} = \boldsymbol{v}_1^q + k(2\boldsymbol{e}_1 - \boldsymbol{e}_2) \tag{29}$$

$$\hat{\boldsymbol{v}}_{2k+1}^{q-k} = \hat{\boldsymbol{v}}_1^q + k(2\boldsymbol{e}_1 - \boldsymbol{e}_2). \tag{30}$$

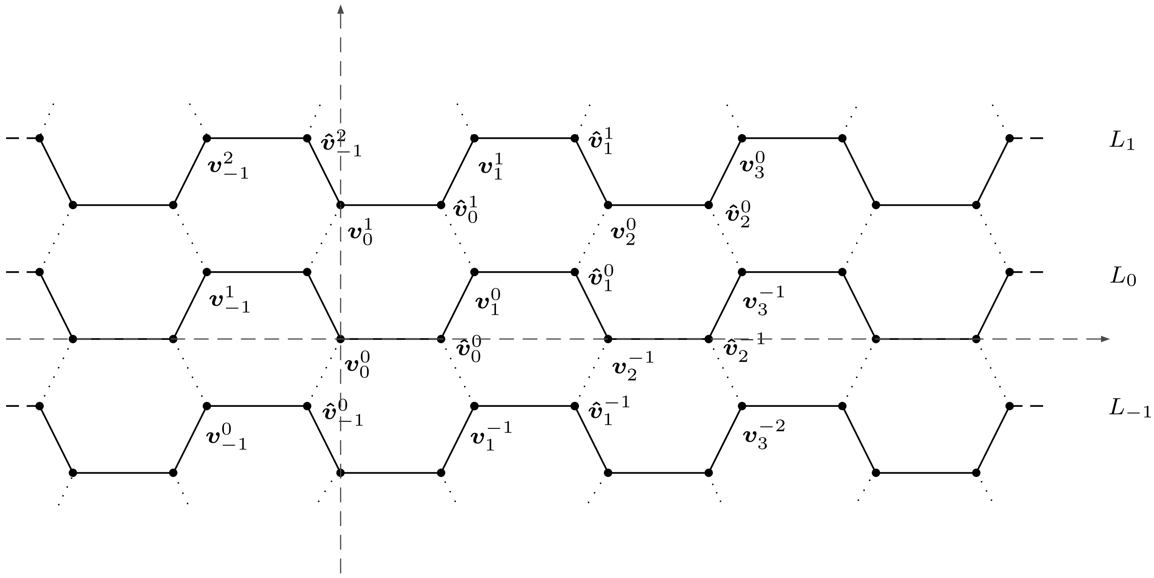

Fig. 4 Set L_q, $q \in \{-1, 0, 1\} \subset \mathbb{Z}$ and its respective edges

Proposition 1 *Let $\Psi \in L^2(G)$ such that $\mathcal{H}\Psi \equiv \lambda\Psi$. If the values of Ψ at the vertices of L_q are known, then the value of Ψ at every node and edge of G can be determined using the following recursive relations:*

$$\begin{pmatrix} \Psi\left(\hat{\boldsymbol{v}}_{2(k-1)+1}^{(q+1)-(k-1)}\right) \\ \Psi\left(\boldsymbol{v}_{2k}^{(q+1)-k}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2k}^{(q+1)-k}\right) \\ \Psi\left(\boldsymbol{v}_{2k+1}^{(q+1)-k}\right) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Psi\left(\boldsymbol{v}_{2(k-1)+1}^{q-(k-1)}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2(k-1)+1}^{q-(k-1)}\right) \\ \Psi\left(\boldsymbol{v}_{2k}^{q-k}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2k}^{q-k}\right) \\ \Psi\left(\boldsymbol{v}_{2k+1}^{q-k}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2k+1}^{q-k}\right) \end{pmatrix} \tag{31}$$

$$\begin{pmatrix} \Psi\left(\hat{\boldsymbol{v}}_{2(k-1)}^{(q-1)-k}\right) \\ \Psi\left(\boldsymbol{v}_{2(k-1)+1}^{(q-1)-k}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2(k-1)+1}^{(q-1)-(k+1)}\right) \\ \Psi\left(\boldsymbol{v}_{2k}^{(q-1)-(k+1)}\right) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Psi\left(\boldsymbol{v}_{2(k-1)}^{q-k}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2(k-1)}^{q-k}\right) \\ \Psi\left(\boldsymbol{v}_{2(k-1)+1}^{q-k}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2(k-1)+1}^{q-k}\right) \\ \Psi\left(\boldsymbol{v}_{2k}^{q-(k+1)}\right) \\ \Psi\left(\hat{\boldsymbol{v}}_{2k}^{q-(k+1)}\right) \end{pmatrix}, \tag{32}$$

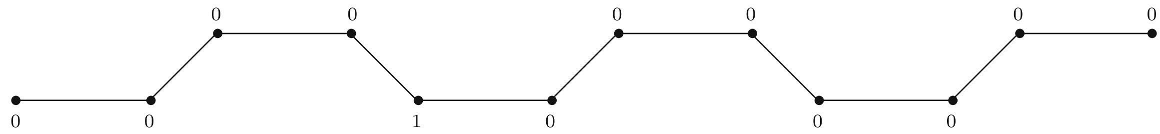

Fig. 5 Function $\Phi_{1,k}$ in some vertices of L_0, including the vertex $\boldsymbol{v}_{2k}^{-k}$ where is equal to one

with

$$\mathcal{M} = \begin{pmatrix} s & s^2-1 & s & 1 & s & 1 \\ -1 & -s & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & -s & -1 \\ 1 & s & 1 & s & s^2-1 & s \end{pmatrix}. \tag{33}$$

and

$$s = -3\varphi_1(1; \lambda),$$

where $\varphi_1(\cdot; \lambda)$ *defined* (2).

Corollary 1 *If* $\Psi \in L^2(G)$ *is such that* $\mathcal{H}\Psi \equiv \lambda\Psi$ *and* $\Psi = 0$ *at each vertex of* L_q*, for some fix* $q \in \mathbb{Z}$*, then* $\Psi \equiv 0$.

Remark 1 We say that the profile L_q is a basis for the graphene G, because every function Ψ defined on G can be generated from the values of Ψ at each node of L_q.

Remark 2 Since all profiles L_q can be chosen as a basis for graphene, without loss of generality we explicitly defined the basis function for $q = 0$. Using the one-dimensional structure of L_0, it is known that an arbitrary function in this profile can be generated by introducing a canonical basis. This basis is composed by functions, whose values on each vertex of L_0 are equal to zero, except in one of them where the value becomes one. The L_0 vertices are defined in (26), from four core vertices and the observed periodicity on (27)–(30). We denote the canonical basis functions in L_0 by $\Phi_{1,k}$, $\Phi_{2,k}$, $\Phi_{3,k}$, $\Phi_{4,k}$, $k \in \mathbb{Z}$, such that

$$\Phi_{1,k}(\boldsymbol{v}) = 0 \quad \forall \boldsymbol{v} \in L_0 \backslash \{\boldsymbol{v}_{2k}^{-k}\}, \quad \Phi_{1,k}(\boldsymbol{v}_{2k}^{-k}) = 1, \tag{34}$$

$$\Phi_{2,k}(\boldsymbol{v}) = 0 \quad \forall \boldsymbol{v} \in L_0 \backslash \{\hat{\boldsymbol{v}}_{2k}^{-k}\}, \quad \Phi_{2,k}(\hat{\boldsymbol{v}}_{2k}^{-k}) = 1, \tag{35}$$

$$\Phi_{3,k}(\boldsymbol{v}) = 0 \quad \forall \boldsymbol{v} \in L_0 \backslash \{\boldsymbol{v}_{2k+1}^{-k}\}, \quad \Phi_{3,k}(\boldsymbol{v}_{2k+1}^{-k}) = 1, \tag{36}$$

$$\Phi_{4,k}(\boldsymbol{v}) = 0 \quad \forall \boldsymbol{v} \in L_0 \backslash \{\hat{\boldsymbol{v}}_{2k+1}^{-k}\}, \quad \Phi_{4,k}(\hat{\boldsymbol{v}}_{2k+1}^{-k}) = 1. \tag{37}$$

If we have defined this functions in the profile L_0, we can extend it to G thanks to Proposition 1, and thus we obtain a canonical basis for the complete graphene G (Fig. 5).

In (34)–(37), we introduced the functions $\Phi_{1,k}$, $\Phi_{2,k}$, $\Phi_{3,k}$, $\Phi_{4,k}$, $k \in \mathbb{Z}$, that form the canonical base of the graphene. Also, by definition, we know the value of these functions in the vertices of the profile L_0. In this section, we are interested in calculating the values of these functions in the others profiles L_q, for $q \in \mathbb{Z}\backslash\{0\}$.

The support is bounded in the profile L_0. One of the questions that we want to address is whether the support is still bounded in the rest of the profiles and in the complete graphene. Using the periodicity of the L_0, all the analyses in this section can be concentrated in the study of the functions $\Phi_{1,0}$,$\Phi_{2,0}$, $\Phi_{3,0}$ y $\Phi_{4,0}$. Once we know completely these functions, the other ones are horizontal translations (respect to the vector $2\boldsymbol{e}_1 - \boldsymbol{e}_2$) (Fig. 6).

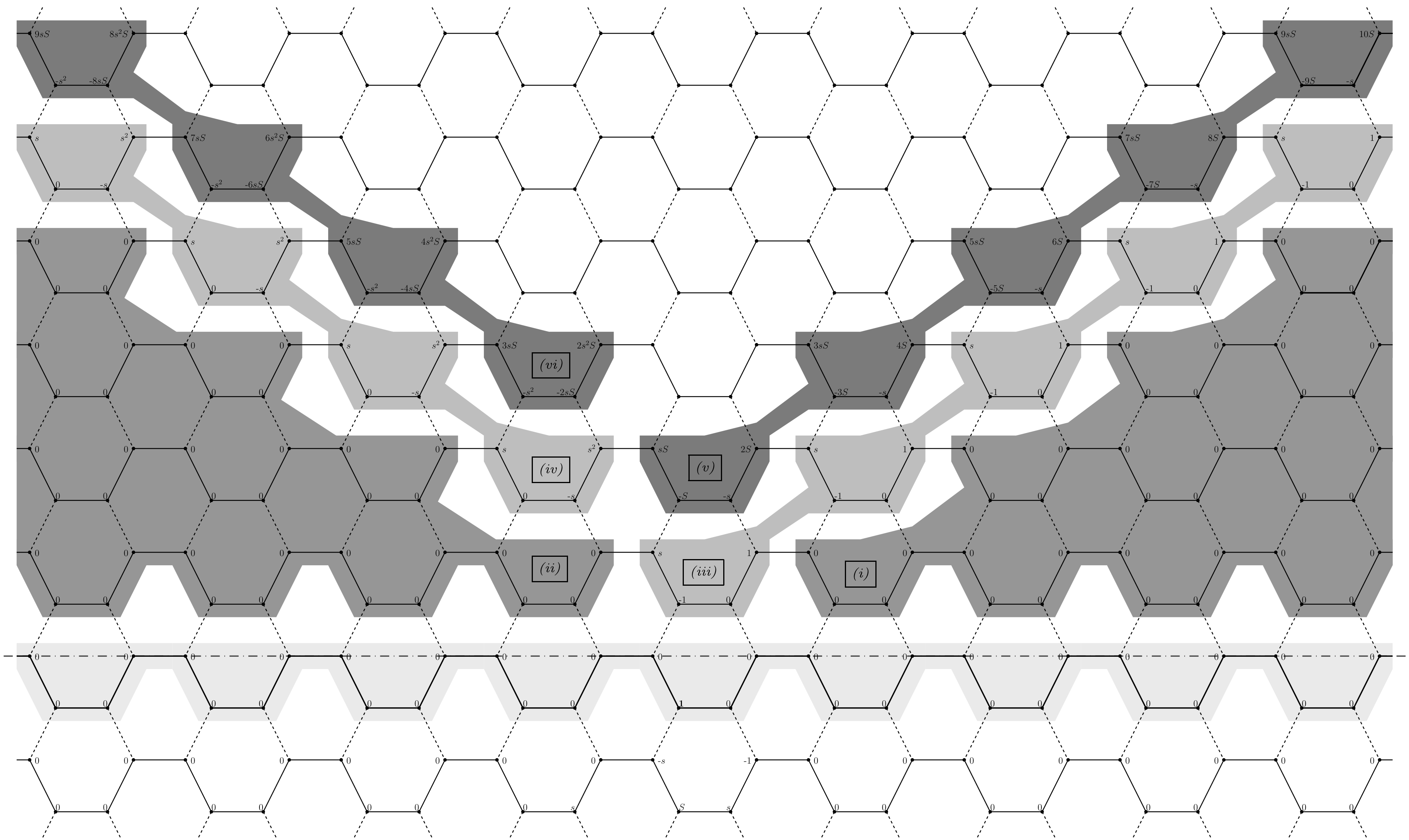

Fig. 6 Function $\Phi_{1,0}$ evaluated at each vertex of G. The different colors illustrate the respective parts (i)–(vi) of Theorem 3. Here, $S = s^2 - 1$

Theorem 3 *Let us consider the function $\Phi_{1,0}$ defined in* (34) *and the vector* $\boldsymbol{X} = 2\boldsymbol{e}_1 - \boldsymbol{e}_2 = (3, 0)$.

(i) *In all the profiles L_q, with $q \geq 1$, we have that for all $j \geq q$*

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_1^q + (j-1)\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_0^q + j\boldsymbol{X}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_0^q + j\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_1^q + j\boldsymbol{X}) = 0. \tag{38}$$

(ii) *In all the profiles L_q, with $q \geq 1$, we have that for all $j \geq -q$*

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_1^q + (j-1)\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_0^q + j\boldsymbol{X}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_0^q + j\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_1^q + j\boldsymbol{X}) = 0. \tag{39}$$

(iii) *In all the profiles L_q, with $q \geq 1$, we have that for $j = q - 1$*

$$\begin{array}{ll} \Phi_{1,0}(\hat{\boldsymbol{v}}_1^q + (j-1)\boldsymbol{X}) = s, & \Phi_{1,0}(\boldsymbol{v}_0^q + j\boldsymbol{X}) = -1, \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^q + j\boldsymbol{X}) = 0, & \Phi_{1,0}(\boldsymbol{v}_1^q + j\boldsymbol{X}) = 1. \end{array} \tag{40}$$

(iv) *In all the profiles L_q, with $q \geq 2$, we have that for $j = -q + 1$*

$$\begin{array}{ll} \Phi_{1,0}(\hat{\boldsymbol{v}}_1^q + (j-1)\boldsymbol{X}) = s, & \Phi_{1,0}(\boldsymbol{v}_0^q + j\boldsymbol{X}) = 0, \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^q + j\boldsymbol{X}) = -s, & \Phi_{1,0}(\boldsymbol{v}_1^q + j\boldsymbol{X}) = s^2. \end{array} \tag{41}$$

(v) *In all the profiles L_q, with $q \geq 2$, we have that for $j = q - 2$*

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}_1^q + (j-1)\boldsymbol{X}) &= (2q-3)s(s^2-1), \\ \Phi_{1,0}(\boldsymbol{v}_0^q + j\boldsymbol{X}) &= -(2q-3)(s^2-1), \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^q + j\boldsymbol{X}) &= -s, \\ \Phi_{1,0}(\boldsymbol{v}_1^q + j\boldsymbol{X}) &= (2q-2)(s^2-1). \end{aligned} \tag{42}$$

(vi) *In all the profiles L_q, with $q \geq 3$, we have that for $j = -q + 2$*

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}_1^q + (j-1)\boldsymbol{X}) &= (2q-3)s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}_0^q + j\boldsymbol{X}) &= -s^2, \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^q + j\boldsymbol{X}) &= -(2q-4)s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}_1^q + j\boldsymbol{X}) &= (2q-4)s^2(s^2+1). \end{aligned} \tag{43}$$

(vii) *The values of $\Phi_{1,0}$ in the profiles L_q with $q < 0$ can be obtained from the previous items considering the antisymmetry as follows:*

$$\frac{y_1 + y_2}{2} = \frac{\sqrt{3}}{2} \Rightarrow \Phi_{1,0}(x, y_1) + \Phi_{1,0}(x, y_2) = 0. \tag{44}$$

Moreover, we can characterize the functions $\Phi_{2,0}$, $\Phi_{3,0}$ y $\Phi_{4,0}$. Considering the respective symmetries, we can write

$$\begin{aligned} \Phi_2(x, y) &= \Phi_1\left(1 - x, y\right) \\ \Phi_3(x, y) &= \Phi_1\left(x - \frac{3}{2}, \frac{\sqrt{3}}{2} - y\right) \\ \Phi_4(x, y) &= \Phi_1\left(\frac{5}{2} - x, \frac{\sqrt{3}}{2} - y\right) \end{aligned}$$

Therefore, from here, we have that

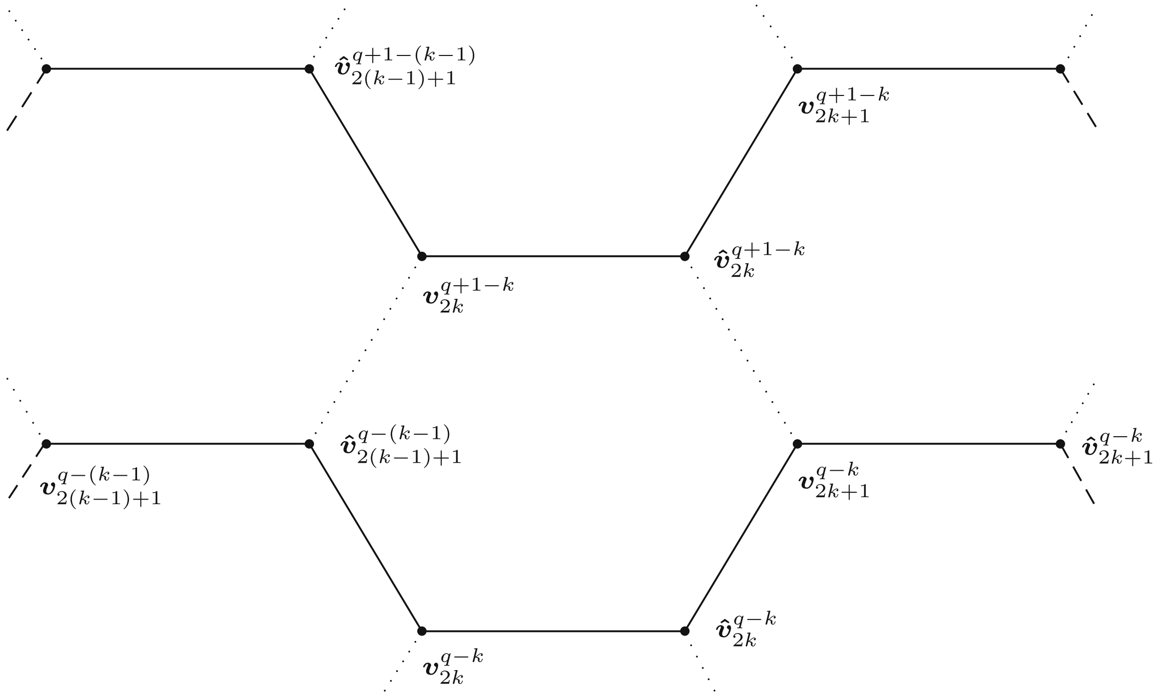

Fig. 7 Vertices of L_q and L_{q+1}, $k \in \mathbb{Z}$

- From (iii) of Theorem 3, we can conclude that $\Phi_{1,0}$, $\Phi_{2,0}$, $\Phi_{3,0}$ and $\Phi_{4,0}$ are not bounded.
- From (v) of Theorem 3, we can conclude that $\Phi_{1,0}$, $\Phi_{2,0}$, $\Phi_{3,0}$ and $\Phi_{4,0}$ do not have compact support.
- It is possible to prove that the finite linear combinations of $\Phi_{1,0}$, $\Phi_{2,0}$, $\Phi_{3,0}$ and $\Phi_{4,0}$ are not bounded and do not have compact support.

2 Proof of the main results

Now, we will prove the main results stated in Sect. 1.2.

2.1 A canonical basis for the graphene

This subsection is devoted to the proof of Proposition 1, and its respective corollary.

For $q, k \in \mathbb{Z}$, we consider the vertices in the sets L_q and L_{q+1}, as Fig. 7 shows. We recall that L_q is 4-periodic, for all $q \in \mathbb{Z}$.

To make notation simpler, we write Ψ_i^j instead of $\Psi(\boldsymbol{v}_i^j)$ and $\hat{\Psi}_i^j$ instead of $\Psi(\hat{\boldsymbol{v}}_i^j)$.

Using (21), with $i = 2(k-1)+1$ y $j = q-k$, and (20), with $i = 2k+1$ y $j = k-q$, we get the following equations (see Fig. 7):

$$\Psi_{2k}^{(q+1)-k} = -\left(\Psi_{2(k-1)+1}^{q-(k-1)} + s\hat{\Psi}_{2(k-1)+1}^{q-(k-1)} + \Psi_{2k}^{q-k}\right) \tag{45}$$

$$\hat{\Psi}_{2k}^{(q+1)-k} = -\left(\hat{\Psi}_{2k}^{q-k} + s\Psi_{2k+1}^{q-k} + \hat{\Psi}_{2k+1}^{q-k}\right). \tag{46}$$

Similarly, from (20) and (21), both with $i = 2k$ y $j = (q+1)-k$, we obtain the system

$$\hat{\Psi}_{2(k-1)+1}^{(q+1)-(k-1)} = -\left(\hat{\Psi}_{2(k-1)+1}^{q-(k-1)} + s\Psi_{2k}^{(q+1)-k} + \hat{\Psi}_{2k}^{(q+1)-k}\right) \tag{47}$$

$$\Psi_{2k+1}^{(q+1)-k} = -\left(\Psi_{2k}^{(q+1)-k} + s\hat{\Psi}_{2k}^{(q+1)-k} + \Psi_{2k+1}^{q-k}\right). \tag{48}$$

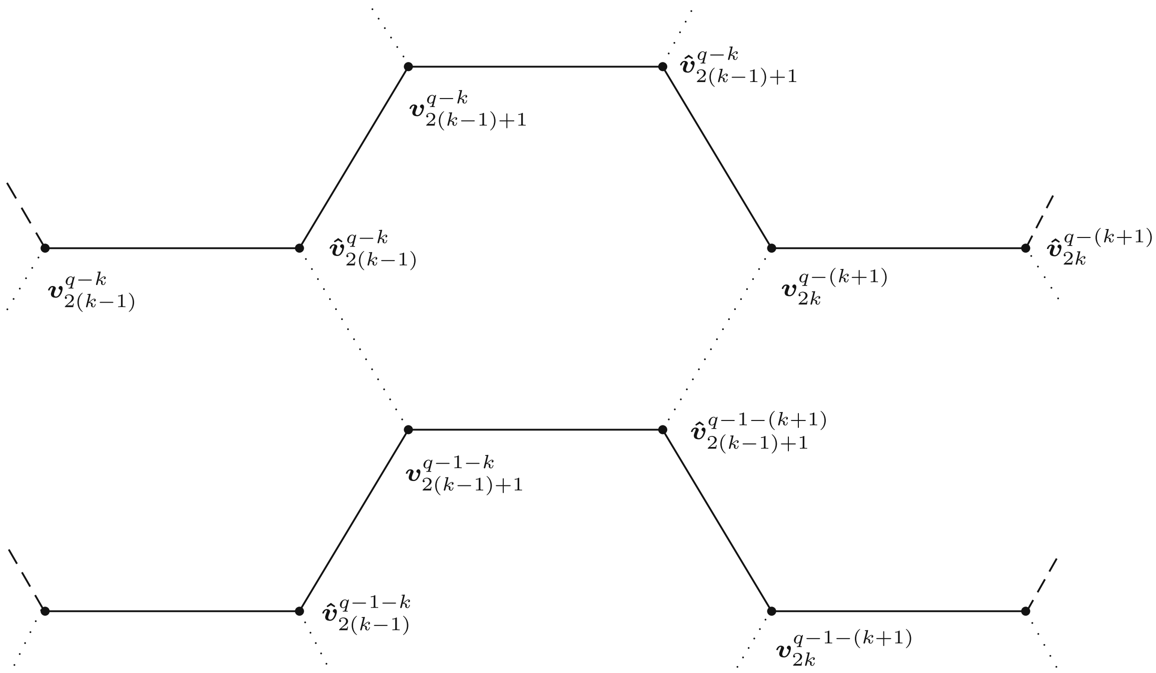

Fig. 8 Vertices of L_q and L_{q-1}, $k \in \mathbb{Z}$

Replacing (45) and (46) in (47) and (48), and factorizing we obtain (31).

We analyze now the vertices in L_{q-1} (see Fig. 8). Following the same procedure as before, from (20), with $i = 2(k-1)+1$ y $j = (q-1)-k$, and (21), with $i = 2(k-1)$ y $j = q-k$, we get

$$\begin{aligned} \hat{\Psi}^{(q-1)-k}_{2(k-1)} &= -\left(\hat{\Psi}^{q-k}_{2(k-1)} + s\Psi^{(q-1)-k}_{2(k-1)+1} + \hat{\Psi}^{(q-1)-k}_{2(k-1)+1}\right), \\ \Psi^{(q-1)-k}_{2(k-1)+1} &= -\left(\Psi^{q-k}_{2(k-1)} + s\hat{\Psi}^{q-k}_{2(k-1)} + \Psi^{q-k}_{2(k-1)+1}\right). \end{aligned}$$

Using (20), with $i = 2k$ y $j = q-k$, and (21), with $i = 2(k-1)+1$ y $j = (q-1)-k$, we also obtain

$$\begin{aligned} \hat{\Psi}^{(q-1)-k}_{2(k-1)+1} &= -\left(\hat{\Psi}^{q-k}_{2(k-1)+1} + s\Psi^{q-k}_{2k} + \hat{\Psi}^{q-k}_{2k}\right) \\ \Psi^{(q-1)-k}_{2k} &= -\left(\Psi^{(q-1)-k}_{2(k-1)+1} + s\hat{\Psi}^{(q-1)-k}_{2(k-1)+1} + \Psi^{q-k}_{2k}\right). \end{aligned}$$

This completes the proof of Proposition 1.

If $\Psi \equiv 0$ at each vertex of L_q, then, from (20) and (21), we can conclude that $\Psi(\mathbf{x})$ at each vertex of L_{q+k}, for all $k \in \mathbb{Z}$. Thus, Ψ is zero on each edge of G, hence it is zero in all G.

2.2 Properties of the canonical basis

In this subsection, we will prove parts (i)–(vii) of Theorem 3, one by one.

(i) We will prove that (38) is true for all $q \geq 1$ by induction over q.

For $q = 1$, we have to show that

$$\Phi_{1,0}(\hat{\boldsymbol{v}}^1_1 + (j-1)\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}^1_0 + j\boldsymbol{X}) = \Phi_{1,0}(\hat{\boldsymbol{v}}^1_0 + j\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}^1_1 + j\boldsymbol{X}) = 0, \forall j \geq 1,$$

i.e.,

$$\Phi_{1,0}(\hat{\boldsymbol{v}}^{1-(j-1)}_{2(j-1)+1}) = \Phi_{1,0}(\boldsymbol{v}^{1-j}_{2j}) = \Phi_{1,0}(\hat{\boldsymbol{v}}^{1-j}_{2j}) = \Phi_{1,0}(\boldsymbol{v}^{1-j}_{2j+1}) = 0, \quad \forall j \geq 1. \tag{49}$$

Using (31) with $q = 0$ and $k = j$, we have that

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{1-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{1-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{1-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{1-j}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}_{2(j-1)+1}^{-(j-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j+1}^{-j}) \end{pmatrix}.$$

In the right-hand side, we have the values of $\Phi_{1,0}$ in L_0, that are given by (34), and we can see that they are all zero when $j > 0$. Thus, (49) is true.

Suppose now that (38) is true for q. Let us see that it is also true for $q + 1$, i.e., we will show it for all $j \geq q + 1$

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_1^{q+1} + (j-1)\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_0^{q+1} + j\boldsymbol{X}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_0^{q+1} + j\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_1^{q+1} + j\boldsymbol{X}) = 0,$$

i.e.,

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{(q+1)-(j-1)}) = \Phi_{1,0}(\boldsymbol{v}_{2j}^{(q+1)-j}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{(q+1)-j}) = \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{(q+1)-j}) = 0, \quad \forall j \geq q+1.$$

Using (31) with $k = j$,

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{(q+1)-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{(q+1)-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{(q+1)-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{(q+1)-j}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}_{2(j-1)+1}^{q-(j-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{q-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{q-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{q-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{q-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j+1}^{q-j}) \end{pmatrix}.$$

Here, again the right-hand side is the null vector. Indeed, from the induction hypothesis, the four central terms are zero, because $j \geq q$. The lower term is zero using the induction hypothesis for $j + 1 \geq q$. Finally, the first term is null using the induction hypothesis for $j - 1 \geq q$.

In this way, (38) is true for all $q \geq 1$.

(ii) We will prove that (39) is true for all $q \geq 1$ by induction over q.

For $q = 1$, we have to show that

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_1^1 + (j-1)\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_0^1 + j\boldsymbol{X}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_0^1 + j\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_1^1 + j\boldsymbol{X}) = 0,$$

i.e.,

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{1-(j-1)}) = \Phi_{1,0}(\boldsymbol{v}_{2j}^{1-j}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{1-j}) = \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{1-j}) = 0, \quad \forall j \leq -1. \quad (50)$$

Using (31) with $q = 0$ and $k = j$, we have that

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{1-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{1-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{1-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{1-j}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}_{2(j-1)+1}^{-(j-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j+1}^{-j}) \end{pmatrix}.$$

In the right-hand side, we have the values of $\Phi_{1,0}$ in the profile L_0, that are given by (34), and we can see that they are all zero when $j \leq -1$. Thus, (50) is true.

Suppose now that (50) is true for q. Let us see that it is also true for $q + 1$, i.e., we will show it for all $j \leq -q - 1$

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_1^{q+1} + (j-1)\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_0^{q+1} + j\boldsymbol{X}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_0^{q+1} + j\boldsymbol{X}) = \Phi_{1,0}(\boldsymbol{v}_1^{q+1} + j\boldsymbol{X}) = 0,$$

i.e.,

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{(q+1)-(j-1)}) = \Phi_{1,0}(\boldsymbol{v}_{2j}^{(q+1)-j}) = \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{(q+1)-j}) = \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{(q+1)-j}) = 0, \quad \forall j \leq -q-1.$$

Using (31) with $k = j$.

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{(q+1)-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{(q+1)-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{(q+1)-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{(q+1)-j}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}_{2(j-1)+1}^{q-(j-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(j-1)+1}^{q-(j-1)}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j}^{q-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j}^{q-j}) \\ \Phi_{1,0}(\boldsymbol{v}_{2j+1}^{i-j}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2j+1}^{q-j}) \end{pmatrix}.$$

Here, again the right-hand side is the null vector. Indeed, from the induction hypothesis, the four central terms are zero, because $j \leq -q - 1 \leq -q$. The lower term is zero using the induction hypothesis for $j + 1 \leq -q$. Finally, the first term is null using the induction hypothesis for $j - 1 \leq -q$.

In this way, (39) is true for all $q \geq 1$ by induction over q.

(iii) We will show that (40) is true for all $q \geq 1$ by induction over q.

For $q = 1$, we have to show that

$$\begin{aligned} &\Phi_{1,0}(\hat{\boldsymbol{v}}_1^1 + (j-1)\boldsymbol{X}) = s, && \Phi_{1,0}(\boldsymbol{v}_0^1 + j\boldsymbol{X}) = -1, \\ &\Phi_{1,0}(\hat{\boldsymbol{v}}_0^1 + j\boldsymbol{X}) = 0, && \Phi_{1,0}(\boldsymbol{v}_1^1 + j\boldsymbol{X}) = 1, \end{aligned}$$

for $j = q - 1 = 0$, i.e.,

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_{-1}^2) = s, \quad \Phi_{1,0}(\boldsymbol{v}_0^1) = -1, \quad \Phi_{1,0}(\hat{\boldsymbol{v}}_0^1) = 0, \quad \Phi_{1,0}(\boldsymbol{v}_1^1) = 1. \tag{51}$$

Using (31) with $q = 0$ and $k = 0$, (51) comes from the following calculation

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{-1}^2) \\ \Phi_{1,0}(\boldsymbol{v}_0^1) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^1) \\ \Phi_{1,0}(\boldsymbol{v}_1^1) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}_{-1}^1) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{-1}^1) \\ \Phi_{1,0}(\boldsymbol{v}_0^0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^0) \\ \Phi_{1,0}(\boldsymbol{v}_1^0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_1^0) \end{pmatrix} = \mathcal{M} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \mathcal{M}_{\bullet,3}.$$

Suppose now that (40) is true for q. We will see that it is also true for $q+1$, i.e., we will show that

$$\begin{aligned} &\Phi_{1,0}(\hat{\boldsymbol{v}}_1^{q+1} + (j-1)\boldsymbol{X}) = s, \ \Phi_{1,0}(\boldsymbol{v}_0^{q+1} + j\boldsymbol{X}) = -1, \\ &\Phi_{1,0}(\hat{\boldsymbol{v}}_0^{q+1} + j\boldsymbol{X}) = 0, \qquad\quad \Phi_{1,0}(\boldsymbol{v}_1^{q+1} + j\boldsymbol{X}) = 1, \end{aligned}$$

for $j = (q+1) - 1 = q$, i.e.,

$$\Phi_{1,0}(\hat{\boldsymbol{v}}_{2(q-1)+1}^2) = s, \quad \Phi_{1,0}(\boldsymbol{v}_{2q}^1) = -1, \quad \Phi_{1,0}(\hat{\boldsymbol{v}}_{2q}^1) = 0, \quad \Phi_{1,0}(\boldsymbol{v}_{2q+1}^1) = 1. \tag{52}$$

Using (31) with $k = q$,

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(q-1)+1}^2) \\ \Phi_{1,0}(\boldsymbol{v}_{2q}^1) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2q}^1) \\ \Phi_{1,0}(\boldsymbol{v}_{2q+1}^1) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}_{2(q-1)+1}^1) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(q-1)+1}^1) \\ \Phi_{1,0}(\boldsymbol{v}_{2q}^0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2q}^0) \\ \Phi_{1,0}(\boldsymbol{v}_{2q+1}^0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2q+1}^0) \end{pmatrix}. \tag{53}$$

From (38) with $j = q$ we have $\Phi_{1,0}(\hat{\boldsymbol{v}}_{2(q-1)+1}^1) = \Phi_{1,0}(\boldsymbol{v}_{2q}^0) = \Phi_{1,0}(\hat{\boldsymbol{v}}_{2q}^0) = \Phi_{1,0}(\boldsymbol{v}_{2q+1}^0) = 0$. Also, from (38) with $j = q+1$ we have $\Phi_{1,0}(\hat{\boldsymbol{v}}_{2q+1}^0) = 0$. Finally, using the induction hypothesis (40) we have $\Phi_{1,0}(\boldsymbol{v}_{2(q-1)+1}^1) = 1$. Thus, (53) is reduced to

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}_{2(q-1)+1}^2) \\ \Phi_{1,0}(\boldsymbol{v}_{2q}^1) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}_{2q}^1) \\ \Phi_{1,0}(\boldsymbol{v}_{2q+1}^1) \end{pmatrix} = \mathcal{M} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \mathcal{M}_{\bullet,1}.$$

Therefore, (52) is true thanks to (33).

Thus, we proved (40) for all $q \geq 1$.

(iv) We will prove that (41) is true for all $q \geq 2$ by induction over q.

For $q=2$, we have to show that

$$\begin{aligned}\Phi_{1,0}(\hat{\boldsymbol{v}}_1^2+(j-1)\boldsymbol{X})&=s,\ \Phi_{1,0}(\boldsymbol{v}_0^2+j\boldsymbol{X})=0,\\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^2+j\boldsymbol{X})&=-s,\qquad \Phi_{1,0}(\boldsymbol{v}_1^2+j\boldsymbol{X})=s^2,\end{aligned}$$

for $j=-q+1=-1$, i.e.,

$$\begin{aligned}\Phi_{1,0}(\hat{\boldsymbol{v}}^4_{-3})&=s,\quad \Phi_{1,0}(\boldsymbol{v}^3_{-2})=0,\\ \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-2})&=-s,\ \Phi_{1,0}(\boldsymbol{v}^3_{-1})=s^2.\end{aligned}\tag{54}$$

Using (31) with $q=1$ and $k=-1$, (54) comes from the following calculation

$$\begin{pmatrix}\Phi_{1,0}(\hat{\boldsymbol{v}}^4_{-3})\\ \Phi_{1,0}(\boldsymbol{v}^3_{-2})\\ \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-2})\\ \Phi_{1,0}(\boldsymbol{v}^3_{-1})\end{pmatrix}=\mathcal{M}\begin{pmatrix}\Phi_{1,0}(\boldsymbol{v}^3_{-3})\\ \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-3})\\ \Phi_{1,0}(\boldsymbol{v}^2_{-2})\\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_{-2})\\ \Phi_{1,0}(\boldsymbol{v}^2_{-1})\\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_{-1})\end{pmatrix},\tag{55}$$

From (50) with $j=-1$, $\Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-3})=\Phi_{1,0}(\boldsymbol{v}^2_{-2})=\Phi_{1,0}(\hat{\boldsymbol{v}}^2_{-2})=\Phi_{1,0}(\boldsymbol{v}^2_{-1})=0$, from (50) with $j=-2$, $\Phi_{1,0}(\boldsymbol{v}^3_{-3})=0$ and from (40) with $q=1$, $\Phi_{1,0}(\hat{\boldsymbol{v}}^2_{-1})=s$. Thus, the right-hand side of (55) is equal to

$$\mathcal{M}\begin{pmatrix}0\\0\\0\\0\\0\\s\end{pmatrix}=\begin{pmatrix}s\\0\\-s\\s^2\end{pmatrix}.$$

Suppose now that (41) is true for q. Let us see that it is also true for $q+1$, i.e., we will show that

$$\begin{aligned}\Phi_{1,0}(\hat{\boldsymbol{v}}_1^{q+1}+(j-1)\boldsymbol{X})&=s,\ \Phi_{1,0}(\boldsymbol{v}_0^{q+1}+j\boldsymbol{X})=0,\\ \Phi_{1,0}(\hat{\boldsymbol{v}}_0^{q+1}+j\boldsymbol{X})&=-s,\qquad \Phi_{1,0}(\boldsymbol{v}_1^{q+1}+j\boldsymbol{X})=s^2,\end{aligned}$$

with $j=-(q+1)+1=-q$, i.e.,

$$\begin{aligned}\Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+2}_{-2(q+1)+1})&=s,\ \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2q})=0,\\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2q})&=-s,\qquad \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2q+1})=s^2.\end{aligned}\tag{56}$$

Using (31) with $k = -q$,

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+2}_{-2(q+1)+1}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2q}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2q}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2q+1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2(q+1)+1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2(q+1)+1}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2q}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2q}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2q+1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2q+1}) \end{pmatrix}. \tag{57}$$

From (39) with $j = -q$, $\Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2(q+1)+1}) = \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2q}) = \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2q}) = \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2q+1}) = 0$, from (39) with $j = -q-1$, $\Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2(q+1)+1}) = 0$ and from the induction hypothesis (41), $\Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2q+1}) = s$. Thus, (57) is reduced to

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+2}_{-2(q+1)+1}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2q}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2q}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q+1}_{-2q+1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ s \end{pmatrix} = \begin{pmatrix} s \\ 0 \\ -s \\ s^2 \end{pmatrix}.$$

Therefore, (56) is true thanks to(33).

Thus, we proved (41) for all $q \geq 1$.

(v) We will prove that (42) is true for all $q \geq 2$ by induction over q.

For $q = 2$, we will show that

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}^2_1 + (j-1)\boldsymbol{X}) &= s(s^2-1), \\ \Phi_{1,0}(\boldsymbol{v}^2_0 + j\boldsymbol{X}) &= -(s^2-1), \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_0 + j\boldsymbol{X}) &= -s, \\ \Phi_{1,0}(\boldsymbol{v}^2_1 + j\boldsymbol{X}) &= 2(s^2-1), \end{aligned}$$

for $j = q - 2 = 0$, i.e.,

$$\begin{array}{ll} \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-1}) = s(s^2-1), & \Phi_{1,0}(\boldsymbol{v}^2_0) = -(s^2-1), \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_0) = -s, & \Phi_{1,0}(\boldsymbol{v}^2_1) = 2(s^2-1). \end{array} \tag{58}$$

Using (31) with $q = 1$ and $k = 0$, we have

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-1}) \\ \Phi_{1,0}(\boldsymbol{v}^2_0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_0) \\ \Phi_{1,0}(\boldsymbol{v}^2_1) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}^2_{-1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_{-1}) \\ \Phi_{1,0}(\boldsymbol{v}^1_0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^1_0) \\ \Phi_{1,0}(\boldsymbol{v}^1_1) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^1_1) \end{pmatrix}.$$

From (50) with $j = -1$ we have $\Phi_{1,0}(\boldsymbol{v}^2_{-1}) = 0$, from (49) with $j = 1$ we have $\Phi_{1,0}(\hat{\boldsymbol{v}}^1_1) = 0$, and using (51), we obtain

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-1}) \\ \Phi_{1,0}(\boldsymbol{v}^2_0) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_0) \\ \Phi_{1,0}(\boldsymbol{v}^2_1) \end{pmatrix} = \mathcal{M} \begin{pmatrix} 0 \\ s \\ -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

Therefore, (58) comes from the product between a matrix and a vector, considering the definition of $\mathcal{M}$ given in (33).

Suppose now that (42) is true for q. Let us see that it is also true for $q + 1$, i.e., we will show that

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}^{q+1}_1 + (j-1)\boldsymbol{X}) &= (2q-1)s(s^2-1), \\ \Phi_{1,0}(\boldsymbol{v}^{q+1}_0 + j\boldsymbol{X}) &= -(2q-1)(s^2-1), \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{q+1}_0 + j\boldsymbol{X}) &= -s, \\ \Phi_{1,0}(\boldsymbol{v}^{q+1}_1 + j\boldsymbol{X}) &= 2q(s^2-1), \end{aligned}$$

for $j = (q+1) - 2 = q - 1$, i.e.,

$$\begin{aligned} &\Phi_{1,0}(\hat{\boldsymbol{v}}^3_{2(q-2)+1}) = (2q-1)s(s^2-1), && \Phi_{1,0}(\boldsymbol{v}^2_{2(q-1)}) = -(2q-1)(s^2-1), \\ &\Phi_{1,0}(\hat{\boldsymbol{v}}^2_{2(q-1)}) = -s, && \Phi_{1,0}(\boldsymbol{v}^2_{2(q-1)+1}) = 2q(s^2-1). \end{aligned} \tag{59}$$

Using (31) with $k = q - 1$,

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{2(q-2)+1}) \\ \Phi_{1,0}(\boldsymbol{v}^2_{2(q-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_{2(q-1)}) \\ \Phi_{1,0}(\boldsymbol{v}^2_{2(q-1)+1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}^2_{2(q-2)+1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_{2(q-2)+1}) \\ \Phi_{1,0}(\boldsymbol{v}^1_{2(q-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^1_{2(q-1)}) \\ \Phi_{1,0}(\boldsymbol{v}^1_{2(q-1)+1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^1_{2(q-1)+1}) \end{pmatrix} \tag{60}$$

From the induction hypothesis (42), we have $\Phi_{1,0}(\boldsymbol{v}^2_{2(q-2)+1}) = (2q-2)(s^2-1)$. Also, using (38) with $j = q$ we have $\Phi_{1,0}(\hat{\boldsymbol{v}}^1_{2(q-1)+1}) = 0$. Finally, thanks to (40), (60) can be written as

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{2(q-2)+1}) \\ \Phi_{1,0}(\boldsymbol{v}^2_{2(q-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^2_{2(q-1)}) \\ \Phi_{1,0}(\boldsymbol{v}^2_{2(q-1)+1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} (2q-2)(s^2-1) \\ s \\ -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

Multiplying by the matrix defined in (33), we have that (59) is true.

With this, (42) is true for all $q \geq 2$.

(vi) We will prove that (43) is true for all $q \geq 3$ by induction over q.

For $q = 3$, we have to show that

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}^3_1 + (j-1)\boldsymbol{X}) &= 3s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}^3_0 + j\boldsymbol{X}) &= -s^2, \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^3_0 + j\boldsymbol{X}) &= -2s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}^3_1 + j\boldsymbol{X}) &= 2s^2(s^2+1), \end{aligned}$$

for $j = -q + 2 = -1$, i.e.,

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}^5_{-3}) &= 3s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}^4_{-2}) &= -s^2, \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^4_{-2}) &= -2s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}^4_{-1}) &= 2s^2(s^2+1). \end{aligned} \tag{61}$$

Using (31) with $q = 2$ and $k = -1$, we obtain

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^5_{-3}) \\ \Phi_{1,0}(\boldsymbol{v}^4_{-2}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^4_{-2}) \\ \Phi_{1,0}(\boldsymbol{v}^4_{-1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}^4_{-3}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^4_{-3}) \\ \Phi_{1,0}(\boldsymbol{v}^3_{-2}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-2}) \\ \Phi_{1,0}(\boldsymbol{v}^3_{-1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-1}) \end{pmatrix}.$$

Using (39) with $q = 2$ and $j = -2$ to obtain $\Phi_{1,0}(\boldsymbol{v}^4_{-3}) = 0$, the equality(54) and (58) to obtain $\Phi_{1,0}(\hat{\boldsymbol{v}}^3_{-1}) = s(s^2-1)$, the expression above is equivalent to

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^5_{-3}) \\ \Phi_{1,0}(\boldsymbol{v}^4_{-2}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^4_{-2}) \\ \Phi_{1,0}(\boldsymbol{v}^4_{-1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} 0 \\ s \\ 0 \\ -s \\ s^2 \\ s(s^2-1) \end{pmatrix}.$$

Therefore, (61) comes from the product between a matrix and a vector, considering the definition of $\mathcal{M}$ given in (33).

Suppose now that (43) is true for q. Let us see that it is also true for $q+1$, i.e., we will show that

$$\begin{aligned} \Phi_{1,0}(\hat{\boldsymbol{v}}^{q+1}_1 + (j-1)\boldsymbol{X}) &= (2q-1)s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}^{q+1}_0 + j\boldsymbol{X}) &= -s^2, \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{q+1}_0 + j\boldsymbol{X}) &= -(2q-2)s(s^2+1), \\ \Phi_{1,0}(\boldsymbol{v}^{q+1}_1 + j\boldsymbol{X}) &= (2q-2)s^2(s^2+1), \end{aligned}$$

for $j = -(q+1)+2 = -(q-1)$, i.e.,

$$\begin{aligned} &\Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2q+1}) = (2q-1)s(s^2-1), \qquad \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2(q-1)}) = -s^2, \\ &\Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2(q-1)}) = -(2q-2)s(s^2-1),\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2(q-1)+1}) = (2q-2)s^2(s^2-1). \end{aligned} \tag{62}$$

Using (31) with $k = -(q-1)$,

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2q+1}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2(q-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2(q-1)}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2(q-1)+1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2q+1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2q+1}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q-1}_{-2(q-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q-1}_{-2(q-1)}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q-1}_{-2(q-1)+1}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q-1}_{-2(q-1)+1}) \end{pmatrix} \tag{63}$$

From (38) with $j = -q$, $\Phi_{1,0}(\boldsymbol{v}^{2q}_{-2q+1}) = 0$. From the induction hypothesis (43), we have $\Phi_{1,0}(\hat{\boldsymbol{v}}^{2q-1}_{-2(q-1)+1}) = (2q-3)s(s^2-1)$. Finally, thanks to (41), (60) can be written as

$$\begin{pmatrix} \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q+1}_{-2q+1}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2(q-1)}) \\ \Phi_{1,0}(\hat{\boldsymbol{v}}^{2q}_{-2(q-1)}) \\ \Phi_{1,0}(\boldsymbol{v}^{2q}_{-2(q-1)+1}) \end{pmatrix} = \mathcal{M} \begin{pmatrix} 0 \\ s \\ 0 \\ -s \\ s^2 \\ (2q-3)s(s^2-1) \end{pmatrix},$$

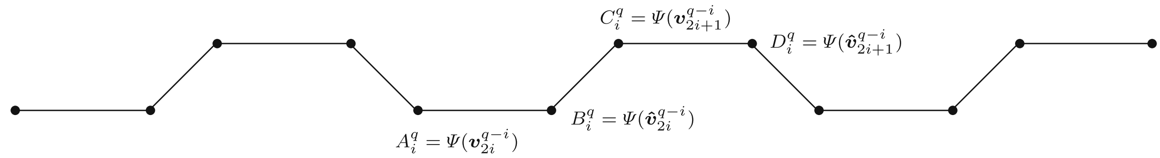

Fig. 9 Definition of the constants A_i^q, B_i^q, C_i^q y D_i^q

Multiplying by the matrix defined in (33), we have that (62) is true.

With this, (43) is true for all $q \geq 2$.

(vii) Using (38), (39) and (40), we have that the property is true for all the vertices of the graphene with y-coordinate $y = \sqrt{3}$.

The total symmetry is obtained considering that the line composed by all the vertices of y-coordinate $y = \sqrt{3}/2$ and $y = \sqrt{3}$ is a basis of graphene, symmetric to L_0, but with component $\Phi_{1,0}(0, \sqrt{3}) = -1$. This new basis generates the same solutions found in (38)–(43), but with opposite signs. Thus, we obtain the desired symmetry.

3 Basis with support in the semi-plane

We seek for solutions $\Psi \in L^2(G)$ such that $\mathcal{H}\Psi \equiv \lambda\Psi$ with compact support. In this section we use A_i^q, B_i^q, C_i^q and D_i^q, $i \in \mathbb{Z}$ to denote the value of $\Psi \in L^2(G)$ such that $\mathcal{H}\Psi \equiv \lambda\Psi$, at the four vertices which generate the profile L_q, i.e.,

$$A_i^q = \Psi(\boldsymbol{v}_{2i}^{q-i}), \quad B_i^q = \Psi(\hat{\boldsymbol{v}}_{2i}^{q-i}), \quad C_i^q = \Psi(\boldsymbol{v}_{2i+1}^{q-i}), \quad D_i^q = \Psi(\hat{\boldsymbol{v}}_{2i+1}^{q-i}). \tag{64}$$

See definition of the profile L_q in (26) and Fig. 9 for more details.

From (31) and (32), we can write all the values of Ψ at the vertices of L_{q+1} and L_{q-1} in terms of its values at the vertices of L_q as follows. For all $i \in \mathbb{Z}$,

$$A_i^{q+1} = -C_{i-1}^q - sD_{i-1}^q - A_i^q \tag{65}$$
$$B_i^{q+1} = -B_i^q - sC_i^q - D_i^q \tag{66}$$
$$C_i^{q+1} = C_{i-1}^q + sD_{i-1}^q + A_i^q + sB_i^q + (s^2-1)C_i^q + sD_i^q \tag{67}$$
$$D_i^{q+1} = sC_i^q + (s^2-1)D_i^q + sA_{i+1}^q + B_{i+1}^q + sC_{i+1}^q + D_{i+1}^q \tag{68}$$
$$A_i^{q-1} = A_{i-1}^q + sB_{i-1}^q + C_{i-1}^q + sD_{i-1}^q + (s^2-1)A_i^q + sB_i^q \tag{69}$$
$$B_i^{q-1} = sA_i^q + (s^2-1)B_i^q + sC_i^q + D_i^q + sA_{i+1}^q + B_{i+1}^q \tag{70}$$
$$C_i^{q-1} = -A_i^q - sB_i^q - C_i^q \tag{71}$$
$$D_i^{q-1} = -D_i^q - sA_{i+1}^q - B_{i+1}^q \tag{72}$$

If solutions $\Psi \in L^2(G)$ such that $\mathcal{H}\Psi \equiv \lambda\Psi$ with compact support exist, then there is an $i_0 \in \mathbb{Z}$ such that

$$A_i^q = B_i^q = C_i^q = D_i^q = 0, \ \forall i < i_0, \forall q \in \mathbb{Z}. \tag{73}$$

Without loss of generality, we can assume $i_0 = 0$. In other words, we study the case in which the function Ψ is zero in all the gray region of Fig. 10. In addition, we write "$-n$, with $n \in \mathbb{N}$" instead of "$i < 0$, with $i \in \mathbb{Z}$".

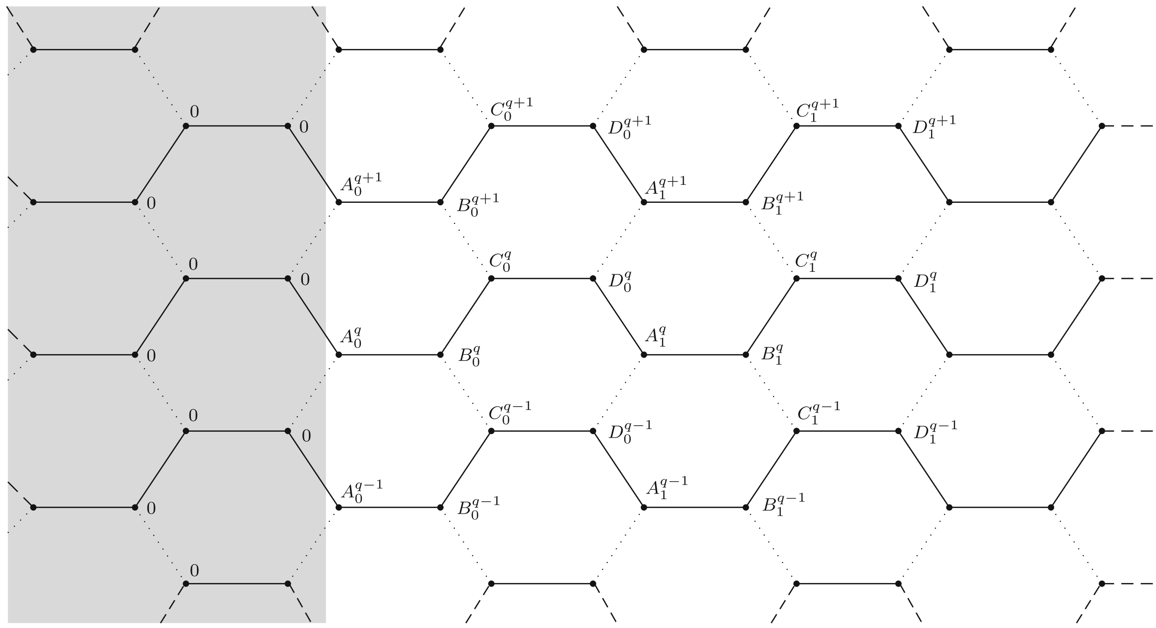

Fig. 10 Values non-zero of A_i^j, B_i^j, C_i^j y D_i^j, $i, j \in \mathbb{Z}, i \geq 0$

To prove the results in this section and determine the structure of all functions Ψ satisfying (73) (with $i_0 = 0$), the polynomials P_n, recursively defined as follows, play a crucial role.

The family of polynomials $(P_n)_{n\in\mathbb{N}}$ is defined by the recursive relation:

$$P_0(s) = -s \tag{74}$$

$$P_n(s) = P_{n-1}(s) + s \sum_{k=0}^{n-1} P_k(s) P_{n-1-k}(s) \quad \text{for } n \geq 1. \tag{75}$$

For $n = 1$, we notice that

$$P_1(s) = P_0 + s P_0^2 = -s + s^3 = s(s^2 - 1) = (s^2 - 1)s. \tag{76}$$

The degree of each polynomial P_n, $n \in \mathbb{N}$, is $2n + 1$.

Using these polynomials, we now present the main result of this section.

Theorem 4 *For $\Psi \in L^2(G)$ such that $\mathcal{H}\Psi \equiv \lambda\Psi$, let A_i^q, B_i^q, C_i^q, D_i^q be the values of Ψ at the vertices that generate L_q defined in* (64)*. The following propositions are equivalent:*

(a) *For each $q \in \mathbb{Z}$ it holds that*

$$A_{-n}^q = B_{-n}^q = C_{-n}^q = D_{-n}^q = 0 \qquad \forall n \in \mathbb{N}. \tag{77}$$

(b) *There exists $q_0 \in \mathbb{Z}$ such that $A_{-n}^{q_0} = B_{-n}^{q_0} = C_{-n}^{q_0} = D_{-n}^{q_0} = 0$ for all $n \in \mathbb{N}$. Moreover,*

$$B_n^q = \sum_{k=0}^{n} A_{n-k}^q P_k(s) \quad \forall n \in \mathbb{N}, \forall q \in \mathbb{Z} \tag{78}$$

and

$$D_n^q = \sum_{k=0}^{n} C_{n-k}^q P_k(s) \quad \forall n \in \mathbb{N}, \forall q \in \mathbb{Z}. \tag{79}$$

(c) *There exists* $q_0 \in \mathbb{Z}$ *such that* $A^{q_0}_{-n} = B^{q_0}_{-n} = C^{q_0}_{-n} = D^{q_0}_{-n} = 0$ *for all* $n \in \mathbb{N}$. *Moreover,*

$$B^{q_0}_n = \sum_{k=0}^{n} A^{q_0}_{n-k} P_k(s) \quad \forall n \in \mathbb{N} \tag{80}$$

and

$$D^{q_0}_n = \sum_{k=0}^{n} C^{q_0}_{n-k} P_k(s) \quad \forall n \in \mathbb{N}. \tag{81}$$

(d) *For each* $q \in \mathbb{Z}$ *it holds*

$$A^q_{-n} = B^q_{-n} = C^q_{-n} = D^q_{-n} = 0 \qquad \forall n \in \mathbb{N}, i < 0, \tag{82}$$

$$B^q_n = \sum_{k=0}^{n} A^q_{n-k} P_k(s) \quad \forall n \in \mathbb{N} \tag{83}$$

and

$$D^q_n = \sum_{k=0}^{n} C^q_{n-k} P_k(s) \quad \forall n \in \mathbb{N}. \tag{84}$$

To prove this result, we will show first several previous results which combine the definition of the polynomials P_n with the conditions (20) and (21). Let us begin with an algebraic lemma.

Lemma 1 *If there exists* $n_0 \in \mathbb{N}$ *such that*

$$B^q_n = \sum_{k=0}^{n} A^q_{n-k} P_k(s) \qquad \forall n \in \{0, \dots, n_0\} \tag{85}$$

and

$$D^q_n = \sum_{k=0}^{n} C^q_{n-k} P_k(s) \qquad \forall n \in \{0, \dots, n_0\}, \tag{86}$$

where P_n *are the polynomials given in* (74)*, then*

$$\sum_{k=0}^{n} \left(A^q_{n-k} + sB^q_{n-k}\right) P_k(s) = sA^q_{n+1} + B^q_{n+1} \quad \forall n \in \{0, \dots, n_0 - 1\}, \tag{87}$$

$$\sum_{k=0}^{n} (C^q_{n-k} + sD^q_{n-k}) P_k(s) = sC^q_{n+1} + D^q_{n+1} \quad \forall n \in \{0, \dots, n_0 - 1\} \tag{88}$$

and

$$s\sum_{k=0}^{n_0} B^q_{n_0-k} P_k(s) = \sum_{k=1}^{n_0+1} A^q_{n_0+1-k} P_k(s) - B^q_{n_0}, \tag{89}$$

$$s\sum_{k=0}^{n_0} D^q_{n_0-k} P_k(s) = \sum_{k=1}^{n_0+1} C^q_{n_0+1-k} P_k(s) - D^q_{n_0}. \tag{90}$$

Proof To show (87) we use the hypothesis (85) to deduce that, for each $n \in \{0, \dots, n_0\}$, we have

$$
\begin{aligned}
\sum_{k=0}^{n}(A^q_{n-k} + sB^q_{n-k})P_k &= \sum_{k=0}^{n} A^q_{n-k}P_k + s\sum_{k=0}^{n}\sum_{r=0}^{n-k} A^q_{n-(k+r)}P_rP_k \\
&= \sum_{k=0}^{n} A^q_{n-k}P_k + s\sum_{t=0}^{n}\sum_{j=0}^{t} A^q_{n-t}P_jP_{t-j} \\
&= \sum_{k=0}^{n} A^q_{n-k}\left(P_k + s\sum_{j=0}^{k} P_jP_{k-j}\right).
\end{aligned}
$$

Now, using the recursive relation (75), we obtain

$$
\begin{aligned}
\sum_{k=0}^{n}(A^q_{n-k} + sB^q_{n-k})P_k &= \sum_{k=0}^{n} A^q_{n-k}P_{k+1} \\
&= \sum_{k=1}^{n+1} A^q_{n+1-k}P_k. \qquad (91)
\end{aligned}
$$

This directly implies (90), using the hypothesis (85) on the sum of left-hand side.

To obtain (87), we restrict the range of the variable n to the set $\{0, \dots, n_0 - 1\}$, and thus we can use the hypothesis (85) in the sum of the right-hand side in (91), hence

$$
\sum_{k=0}^{n}(A^q_{n-k} + sB^q_{n-k})P_k = -A^q_{n+1}P_0 + B^q_{n+1}.
$$

The equality (87) is consequence of the last expression and the definition (74).

Finally, interchanging the name of the variables, the equalities (88) and (90) are the same as the ones that we have just shown. □

Lemma 2 *If*

$$
A^q_{-n} = B^q_{-n} = C^q_{-n} = D^q_{-n} = 0, \qquad \forall n \in \mathbb{N},\ \forall q \in \mathbb{Z}, \qquad (92)
$$

then

$$
\begin{aligned}
B^q_0 &= A^q_0 P_0, \quad \forall q \in \mathbb{Z}, && (93) \\
D^q_0 &= C^q_0 P_0, \quad \forall q \in \mathbb{Z}, && (94) \\
B^q_1 &= A^q_1 P_0 + A^q_0 P_1, \quad \forall q \in \mathbb{Z}, && (95) \\
D^q_1 &= C^q_1 P_0 + C^q_0 P_1, \quad \forall q \in \mathbb{Z}. && (96)
\end{aligned}
$$

Proof Using the identity (72) for $i = -1$, and the hypothesis (92), we obtain

$$
0 = 0 - sA^q_0 - B^q_0,
$$

which implies (93), since $P_0 = -s$.

To show (94), we begin by considering the identity (68) with $i = -1$, and obtain

$$
0 = 0 + 0 + sA^q_0 + B^q_0 + sC^q_0 + D^q_0.
$$

Thus, the property (94) follows from (93) and the fact that $P_0 = -s$.

Since equality (93) holds for all $q \in \mathbb{Z}$, we can write

$$B_0^{q-1} = A_0^{q-1} P_0. \tag{97}$$

Hence, using the identities (70) and (69), for $i = 0$, in (97), we obtain that

$$sA_0^q + (s^2 - 1)B_0^q + 0 + sA_1^q + B_1^q = -s(0 + 0 + 0 + 0 + (s^2 - 1)A_0^q + sB_0^q), \tag{98}$$

which implies that

$$sA_1^q + B_1^q = -s(A_0^q + sB_0^q) - (s^2 - 1) \cdot 0. \tag{99}$$

Thus (95), considering that $P_1(s) = (s^2 - 1)s$ (see (76)).

Finally, to obtain (96), we use (94) for $q + 1$, i.e.,

$$D_0^{q+1} = C_0^{q+1} P_0. \tag{100}$$

Hence, using the identities (68) and (67), for $i = 0$, in (100), we get

$$\begin{aligned} &sC_0^q + (s^2 - 1)D_0^q + sA_1^q + B_1^q + sC_1^q + D_1^q \\ &\quad = -s(0 + 0 + A_0^q + sB_0^q + (s^2 - 1)C_0^q + sD_0^q). \end{aligned}$$

Using (99), previous equality becomes

$$sC_0^q + (s^2 - 1)D_0^q + sC_1^q + D_1^q = -s((s^2 - 1)C_0^q + sD_0^q).$$

Since this equation is analog to the identity (98), the proofs follows similarly to the proof of the previous case. □

We will now see how these results can be generalized. Let us show the following lemma.

Lemma 3 *Let us assume that*

$$A_{-n}^q = B_{-n}^q = C_{-n}^q = D_{-n}^q = 0, \qquad \forall n \in \mathbb{N},\ \forall q \in \mathbb{Z}. \tag{101}$$

If there exists $n_0 \in \mathbb{N}$ *such that*

$$B_n^q = \sum_{k=0}^{n} A_{n-k}^q P_k(s) \quad \forall q \in \mathbb{Z}, \forall n \in \{0, \ldots, n_0\} \tag{102}$$

and

$$D_n^q = \sum_{k=0}^{n} C_{n-k}^q P_k(s) \quad \forall q \in \mathbb{Z}, \forall n \in \{0, \ldots, n_0\}, \tag{103}$$

then

$$B_{n_0+1}^q = \sum_{k=0}^{n_0+1} A_{n_0+1-k}^q P_k(s) \tag{104}$$

and

$$D_{n_0+1}^q = \sum_{k=0}^{n_0+1} C_{n_0+1-k}^q P_k(s). \tag{105}$$

Proof To show (104) we first write the hypothesis (102) for $q-1$ y n_0, i.e.,

$$B_{n_0}^{q-1} = \sum_{k=0}^{n_0} A_{n_0-k}^{q-1} P_k(s).$$

Using the identities (70) with $i = n_0$ and (69) with $i = n_0 - k$, we get

$$\begin{aligned} &sA_{n_0}^q + (s^2-1)B_{n_0}^q + sC_{n_0}^q + D_{n_0}^q + sA_{n_0+1}^q + B_{n_0+1}^q \\ &\quad = \sum_{k=0}^{n_0} (A_{n_0-k-1}^q + sB_{n_0-k-1}^q + C_{n_0-k-1}^q + sD_{n_0-k-1}^q + (s^2-1)A_{n_0-k}^q + sB_{n_0-k}^q) P_k. \end{aligned} \tag{106}$$

Considering the hypothesis (101), these sums can be rewritten as:

$$\begin{aligned} &sA_{n_0}^q + (s^2-1)B_{n_0}^q + sC_{n_0}^q + D_{n_0}^q + sA_{n_0+1}^q + B_{n_0+1}^q \\ &\quad = \sum_{k=0}^{n_0-1} (A_{n_0-k-1}^q + sB_{n_0-k-1}^q + C_{n_0-k-1}^q + sD_{n_0-k-1}^q) P_k \\ &\qquad + (s^2-1) \sum_{k=0}^{n_0} A_{n_0-k}^q P_k + s \sum_{k=0}^{n_0} B_{n_0-k}^q P_k. \end{aligned} \tag{107}$$

Here, thanks to hypotheses (103)–(102), we can use Lemma 1, in the first and third sums of the right-hand side. The second sum can be obtained directly from hypothesis (102). Thus, we get

$$\begin{aligned} &sA_{n_0}^q + (s^2-1)B_{n_0}^q + sC_{n_0}^q + D_{n_0}^q + sA_{n_0+1}^q + B_{n_0+1}^q \\ &\quad = B_{n_0}^q + sA_{n_0}^q + D_{n_0}^q + sC_{n_0}^q + (s^2-1)B_{n_0}^q + \sum_{k=1}^{n_0+1} A_{n_0+1-k}^q P_k(s) - B_{n_0}. \end{aligned} \tag{108}$$

Simplifying,

$$sA_{n_0+1}^q + B_{n_0+1}^q = \sum_{k=1}^{n_0+1} A_{n_0+1-k}^q P_k(s). \tag{109}$$

This, together with definition (74), implies.

To show (105), we write the hypothesis (103) for $q+1$ in the case $n = n_0$, i.e.,

$$D_{n_0}^{q+1} = \sum_{k=0}^{n_0} C_{n_0-k}^{q+1} P_k(s).$$

Replacing the identities (68), with $i = n_0$, and (67) with $i = n_0 - k$, the above expression becomes

$$\begin{aligned} &sC_{n_0}^q + (s^2-1)D_{n_0}^q + sA_{n_0+1}^q + B_{n_0+1}^q + sC_{n_0+1}^q + D_{n_0+1}^q \\ &\quad = \sum_{k=0}^{n_0} \left(C_{n_0-k-1}^q + sD_{n_0-k-1}^q + A_{n_0-k}^q + sB_{n_0-k}^q + (s^2-1)C_{n_0-k}^q + sD_{n_0-k}^q \right) P_k. \end{aligned} \tag{110}$$

Considering the hypothesis (101), these sums can be rewritten as follows:

$$\begin{aligned}&sC^q_{n_0} + (s^2-1)D^q_{n_0} + sA^q_{n_0+1} + B^q_{n_0+1} + sC^q_{n_0+1} + D^q_{n_0+1}\\&\quad = \sum_{k=0}^{n_0-1}(C^q_{n_0-k-1} + sD^q_{n_0-k-1})P_k + \sum_{k=0}^{n_0}(A^q_{n_0-k} + sB^q_{n_0-k})P_k + (s^2-1)\sum_{k=0}^{n_0} C^q_{n_0-k}P_k\\&\qquad + s\sum_{k=0}^{n_0} D^q_{n_0-k}P_k. \qquad (111)\end{aligned}$$

For the first and last sums on the right-hand side, we use(88) from Lemma 1, thanks to hypothesis (103). For the second sum, we also use the same lemma, since the identity (104) allows us to use the equality (87) up to $n = n_0$. Finally, the third sum can be obtained directly from hypothesis (103). Hence, we get

$$\begin{aligned}&sC^q_{n_0} + (s^2-1)D^q_{n_0} + sA^q_{n_0+1} + B^q_{n_0+1} + sC^q_{n_0+1} + D^q_{n_0+1}\\&\quad = sC^q_{n_0} + D^q_{n_0} + sA^q_{n_0+1} + B^q_{n_0+1} + (s^2-1)D^q_{n_0} + \sum_{k=1}^{n_0+1} C^q_{n_0+1-k}P_k - D^q_{n_0}. \qquad (112)\end{aligned}$$

Simplifying,

$$sC^q_{n_0+1} + D^q_{n_0+1} = \sum_{k=1}^{n_0+1} C^q_{n_0+1-k}P_k. \qquad (113)$$

Thus, (105) is consequence of definition (74). □

Lemma 4 *Suppose that there exists $q_0 \in \mathbb{Z}$ such that the following properties are satisfied in the profile L_{q_0}:*

$$A^{q_0}_i = B^{q_0}_i = C^{q_0}_i = D^{q_0}_i = 0 \quad \forall i \in \mathbb{Z}, i < 0, \qquad (114)$$

$$B^{q_0}_n = \sum_{k=0}^{n} A^{q_0}_{n-k}P_k(s) \quad \forall n \in \mathbb{N} \qquad (115)$$

and

$$D^{q_0}_n = \sum_{k=0}^{n} C^{q_0}_{n-k}P_k(s) \quad \forall n \in \mathbb{N}, \qquad (116)$$

where $P_k(s)$, $k \in \{0, \ldots, n\}$ are the polynomials defined in (74)–(75)*. Then, in the profiles L_{q_0+1} y L_{q_0-1} the following relations are satisfied*

$$A^{q_0+1}_i = B^{q_0+1}_i = C^{q_0+1}_i = D^{q_0+1}_i = 0 \quad \forall i \in \mathbb{Z}, i < 0, \qquad (117)$$

$$B^{q_0+1}_n = \sum_{k=0}^{n} A^{q_0+1}_{n-k}P_k(s) \quad \forall n \in \mathbb{N}, \qquad (118)$$

$$D^{q_0+1}_n = \sum_{k=0}^{n} C^{q_0+1}_{n-k}P_k(s) \quad \forall n \in \mathbb{N}, \qquad (119)$$

$$A^{q_0-1}_{-n} = B^{q_0-1}_{-n} = C^{q_0-1}_{-n} = D^{q_0-1}_{-n} = 0 \quad \forall n \in \mathbb{N}, \qquad (120)$$

$$B^{q_0-1}_n = \sum_{k=0}^{n} A^{q_0-1}_{n-k}P_k(s) \quad \forall n \in \mathbb{N}, \qquad (121)$$

$$D_n^{q_0-1} = \sum_{k=0}^{n} C_{n-k}^{q_0-1} P_k(s) \quad \forall n \in \mathbb{N}. \tag{122}$$

Proof We begin by showing the properties in the profile L_{q_0+1}.

To prove (117), we consider the identities (65)–(68) with $i < 0$ and $q = q_0$. Using the hypothesis (114), we obtain (117) for all i, except for the case

$$D_{-1}^{q_0+1} = sA_0^{q_0} + B_0^{q_0} + sC_0^{q_0} + D_0^{q_0},$$

which is also zero, thanks to the hypotheses (115)–(116) for $n = 0$ and the definition (74).

To show (118), we calculate the sum of the right-hand side. For each $k \in \{0, \ldots, n\}$, we consider the identity (65), with $i = n - k$ and $q = q_0$. Hence, we obtain that

$$\sum_{k=0}^{n} A_{n-k}^{q_0+1} P_k(s) = -\sum_{k=0}^{n} (C_{n-k-1}^{q_0} + sD_{n-k-1}^{q_0} + A_{n-k}^{q_0}) P_k(s).$$

Using hypothesis (114), we can write

$$\sum_{k=0}^{n} A_{n-k}^{q_0+1} P_k(s) = -\sum_{k=0}^{n-1} (C_{n-k-1}^{q_0} + sD_{n-k-1}^{q_0}) P_k(s) - \sum_{k=0}^{n} A_{n-k}^{q_0} P_k(s).$$

Since hypothesis (116) holds for all n, we can use the identity (88) from Lemma 1 in the first sum of the right-hand side. The second sum can be directly calculated using the hypothesis (115). Then,

$$\sum_{k=0}^{n} A_{n-k}^{q_0+1} P_k(s) = -(sC_n^{q_0} + D_n^{q_0} + B_n^{q_0}).$$

Thus, equality (118) is consequence of previous identity and equality (66) with the respective indices.

Similarly, to show (119), we first calculate the sum on the right-hand side. For each $k \in \{0, \ldots, n\}$, we use identity (67), with $i = n - k$ and $q = q_0$. Hence, we obtain

$$\sum_{k=0}^{n} C_{n-k}^{q_0+1} P_k = \sum_{k=0}^{n} \left(C_{n-k-1}^{q_0} + sD_{n-k-1}^{q_0} + A_{n-k}^{q_0} + sB_{n-k}^{q_0} + (s^2 - 1) C_{n-k}^{q_0} + sD_{n-k}^{q_0} \right) P_k,$$

which, thanks to hypothesis (114), can be rewritten as

$$\begin{aligned} \sum_{k=0}^{n} C_{n-k}^{q_0+1} P_k = & \sum_{k=0}^{n-1} (C_{n-k-1}^{q_0} + sD_{n-k-1}^{q_0}) P_k + \sum_{k=0}^{n} \left(A_{n-k}^{q_0} + sB_{n-k}^{q_0} \right) P_k \\ & + (s^2 - 1) \sum_{k=0}^{n} C_{n-k}^{q_0} P_k + s \sum_{k=0}^{n} D_{n-k}^{q_0} P_k. \end{aligned} \tag{123}$$

Since hypotheses (115)–(116) hold for all n, we can use the identities (87), (88) and (90) from Lemma 1 in order to calculate the first, second and fourth sums of the right-hand side. Thus, we get

$$\sum_{k=0}^{n} C_{n-k}^{q_0+1} P_k = sC_n^{q_0} + D_n^{q_0} + sA_{n+1}^{q_0} + B_{n+1}^{q_0} + (s^2-1)\sum_{k=0}^{n} C_{n-k}^{q_0} P_k + \sum_{k=1}^{n+1} C_{n+1-k}^{q_0} P_k - D_n^{q_0}.$$

Simplifying and using hypothesis (116), we calculate the two last sums of the right-hand side and obtain

$$\sum_{k=0}^{n} C_{n-k}^{q_0+1} P_k = sC_n^{q_0} + sA_{n+1}^{q_0} + B_{n+1}^{q_0} + (s^2-1)D_n^{q_0} + D_{n+1}^{q_0} - C_{n+1}^{q_0} P_0(s).$$

Since $P_0(s) = -s$, (see (74)), reordering terms we get

$$\sum_{k=0}^{n} C_{n-k}^{q_0+1} P_k = sC_n^{q_0} + (s^2-1)D_n^{q_0} + sA_{n+1}^{q_0} + B_{n+1}^{q_0} + sC_{n+1}^{q_0} + D_{n+1}^{q_0}.$$

Compering this identity with (68), with $i = n$ and $q = q_0$, we obtain equality (119).

Let us now prove the properties the profile L_{q_0-1}.

To show (120), we use the identities (69)–(72) with $i < 0$ and $q = q_0$. Using hypothesis (114), (120) is directly obtained for all i, except for the cases

$$B_{-1}^{q_0-1} = sA_0^{q_0} + B_0^{q_0}, \quad \text{y}$$
$$D_{-1}^{q_0-1} = -sA_0^{q_0} - B_0^{q_0}.$$

However, from (93), $sA_0^{q_0} + B_0^{q_0} = 0$ and thus we get $B_{-1}^{q_0-1} = D_{-1}^{q_0-1} = 0$.

To show (121), we begin by calculating the sum on the right-hand side. For each $k \in \{0, \ldots, n\}$, we use the identity (69), with $i = n - k$ and $q = q_0$. Hence, we obtain

$$\sum_{k=0}^{n} A_{n-k}^{q_0-1} P_k = \sum_{k=0}^{n} (A_{n-k-1}^{q_0} + sB_{n-k-1}^{q_0} + C_{n-k-1}^{q_0} + sD_{n-k-1}^{q_0} + (s^2-1)A_{n-k}^{q_0} + sB_{n-k}^{q_0}) P_k(s).$$

Using hypothesis (114), we can write

$$\sum_{k=0}^{n} A_{n-k}^{q_0-1} P_k = \sum_{k=0}^{n-1} (A_{n-k-1}^{q_0} + sB_{n-k-1}^{q_0}) P_k + \sum_{k=0}^{n-1} (C_{n-k-1}^{q_0} + sD_{n-k-1}^{q_0}) P_k + (s^2-1)\sum_{k=0}^{n} A_{n-k}^{q_0} P_k + s\sum_{k=0}^{n} B_{n-k}^{q_0} P_k(s). \tag{124}$$

Since hypotheses (115) and (116) hold for all n, we can use (87) in the first sum of the right-hand side, (88) in the second sum and (89) in the last sum. Hence,

$$\sum_{k=0}^{n} A_{n-k}^{q_0-1} P_k = sA_n^{q_0} + B_n^{q_0} + sC_n^{q_0} + D_n^{q_0} + (s^2-1)\sum_{k=0}^{n} A_{n-k}^{q_0} P_k + \sum_{k=1}^{n+1} A_{n+1-k}^{q_0} P_k - B_n^{q_0},$$

which, thanks to (115), is equivalent to

$$\sum_{k=0}^{n} A_{n-k}^{q_0-1} P_k = sA_n^{q_0} + B_n^{q_0} + sC_n^{q_0} + D_n^{q_0} + (s^2-1)B_n^{q_0} + B_{n+1}^{q_0} - A_{n+1}^{q_0} P_0 - B_n^{q_0}.$$

Since $P_0 = -s$, reordering terms we write

$$\sum_{k=0}^{n} A_{n-k}^{q_0-1} P_k = sA_n^{q_0} + (s^2-1)B_n^{q_0} + sC_n^{q_0} + D_n^{q_0} + sA_{n+1}^{q_0} + B_{n+1}^{q_0}.$$

This, equality (121) is a direct consequence from above identity and inequality (66) with the corresponding indices.

Similarly, to show (122), we begin by calculating the sum on the right-hand side. For each $k \in \{0, \ldots, n\}$, we use the identity (71), with $i = n - k$ and $q = q_0$. Hence, we obtain

$$\sum_{k=0}^{n} C_{n-k}^{q_0-1} P_k = -\sum_{k=0}^{n} (A_{n-k}^{q_0} + sB_{n-k}^{q_0} + C_{n-k}^{q_0}) P_k.$$

Thanks to (87), this can be rewritten as

$$\sum_{k=0}^{n} C_{n-k}^{q_0-1} P_k = -(sA_{n+1}^{q_0} + B_{n+1}^{q_0}) - \sum_{k=0}^{n} C_{n-k}^{q_0} P_k$$

and, from (116), we get

$$\sum_{k=0}^{n} C_{n-k}^{q_0-1} P_k(s) = -(sA_{n+1}^{q_0} + B_{n+1}^{q_0}) - D_n^{q_0}.$$

Thus, equality (122) is obtained directly from (72) with $i = n$ and $q = q_0$. □

Proof of Theorem 4 We begin by showing $(a) \Rightarrow (b)$. We will prove that the identities (78)–(79) hold for all $n \in \mathbb{N}$ using induction over n. The case $n = 0$ is consequence of identities (93)–(94) of Lemma 2. In fact, in this lemma, the case $n = 1$ has been explicitly studied. Now, let us suppose that the identities (78)–(79) hold up to $n \in \mathbb{N}$. Then, using Lemma 3 we can deduce that they are also true for $n + 1$. Thus, we have shown that $(a) \Rightarrow (b)$.

On the other hand, $(b) \Rightarrow (c)$ is true because the property (b) is more general than property (c).

We now show that $(c) \Rightarrow (d)$. To do that, we use double induction over $q \in \mathbb{Z}$. First of all, the hypothesis (c) is the case $q = q_0$ for which the equalities (82)–(84) are satisfied. Let us now assume that the identities (82)–(84) hold for $q \in \mathbb{Z}$. By using Lemma 4 we conclude that these equalities also hold for $q + 1$ and $q - 1$. Hence, property (d) is true for all $q \in \mathbb{Z}$.

Finally, $(d) \Rightarrow (a)$ is true since (d) is a more general property than (a). □

Theorem 5 *From the above result, the functions $\Psi \in L^2(G)$ such that $\mathcal{H}\Psi = \lambda\Psi$ are not bounded and do not have compact support.*

Using the properties in Theorem 4, we can deduce additional properties of the solutions of $\mathcal{H}\Psi \equiv \lambda\Psi$ that are zeros for all $i \in \mathbb{Z}, i < 0$. Recursively using identities (65)–(68), we obtain the following properties.

Theorem 6 *If A_i^q, B_i^q, C_i^q, D_i^q satisfy hypotheses* (77) *of Theorem* 4*, then*

$$A_0^{q+k} = (-1)^k A_0^q, \quad \forall q \in \mathbb{Z}, \forall k \in \mathbb{Z}, \tag{125}$$

$$C_0^{q+k} = (-1)^k (C_0^q + k(s^2-1)A_0^q), \quad \forall q \in \mathbb{Z}, \forall k \in \mathbb{Z}. \tag{126}$$

Proof Let $k \in \mathbb{N}$ and show (125) by induction on k. Clearly, the base case ($k = 0$) is true. We assume that (125) holds for $k \in \mathbb{N}$. In order to show that (125) is also true for $k + 1$, we consider the identity (65) with $i = 0$ and $q + k$ instead of q, i.e.,

$$A_0^{q+k+1} = -C_{-1}^{q+k} - sD_{-1}^{q+k} - A_0^{q+k}.$$

using hypothesis (77), we get

$$A_0^{q+k+1} = -A_0^{q+k}.$$

By induction hypothesis, the above equality becomes

$$A_0^{q+k+1} = -(-1)^k A_0^q,$$

i.e.,

$$A_0^{q+(k+1)} = (-1)^{k+1} A_0^q, \quad \forall q \in \mathbb{Z}.$$

Hence, for all $k \in \mathbb{N}$,

$$A_0^{q+k} = (-1)^k A_0^q. \tag{127}$$

To show that (127) is also true if $k < 0$, we take $r = q + k$ in (127) and obtain

$$A_0^r = (-1)^k A_0^{r-k},$$

which is the same as

$$A_0^{r-k} = (-1)^k A_0^r. \tag{128}$$

Thus, (125) holds.

We now prove (126) by induction on k. The base case is clearly true. Let us assume that (126) holds for $k \in \mathbb{N}$. We use the identity (67), with $i = 0$ and $q + k$ instead of q, i.e.,

$$C_0^{q+k+1} = C_{-1} + sD_{-1} + A_0^{q+k} + sB_0^{q+k} + (s^2 - 1)C_0^{q+k} + sD_0^{q+k}.$$

From hypothesis (77), we get that

$$C_0^{q+k+1} = A_0^{q+k} + sB_0^{q+k} + (s^2 - 1)C_0^{q+k} + sD_0^{q+k}$$

which is equivalent to

$$C_0^{q+k+1} = A_0^{q+k} - s^2 A_0^{q+k} + (s^2 - 1)C_0^{q+k} - s^2 C_0^{q+k},$$

thanks to (93) and (94) with $q + k$ instead of q. Thus,

$$C_0^{q+k+1} = -(s^2 - 1)A_0^{q+k} - C_0^{q+k}.$$

Using (125) and the induction hypothesis, we can write

$$C_0^{q+k+1} = -(s^2 - 1)(-1)^k A_0^q - (-1)^k (C_0^q + k(s^2 - 1)A_0^q),$$

i.e.,

$$C_0^{q+k+1} = (-1)^{k+1}(C_0^q + (k+1)(s^2 - 1)A_0^q), \quad \forall q \in \mathbb{Z}.$$

Then, for all $k \in \mathbb{N}$ we get

$$C_0^{q+k} = (-1)^k (C_0^q + k(s^2 - 1)A_0^q). \tag{129}$$

To show that (129) is also true for $k < 0$, we take $r = q + k$ in (129) and obtain

$$C_0^r = (-1)^k (C_0^{r-k} + k(s^2 - 1) A_0^{r-k}),$$

which is the same as

$$C_0^r = (-1)^k (C_0^{r-k} + (-1)^k k(s^2 - 1) A_0^r),$$

thanks to (128). From this expression, we get

$$C_0^{r-k} = (-1)^k (C_0^r - k(s^2 - 1) A_0^r),$$

which allows us to conclude (126). □

4 Conclusions

We found a recursive solution for the electron wave function in a graphene-like hexagonal lattice based on the physical conditions of wave continuity and flow incompressibility.

We defined the Hamiltonia $\mathcal{H}$ that describes graphene parameterizing the problem in three edges joined by the same vertex. The eigenfunctions of $\mathcal{H}$ together with the conditions of continuity and flow (15) and (16) led us to define a more convenient mathematical basis for the problem, namely the profiles L_q in (26). These profiles extend unidimensionally across the lattice, parallel to each other, and can describe any eigenfunction in the hexagonal network G. This means that if we know the value of the solution only in the vertices of the profile L_q, then it is possible to obtain the solution in each vertex in $\mathcal{V}$ and in each edge in $\mathcal{A}$ (see Remark 1).

This leads us to conclude that it is enough to analyze a one-dimensional problem in a "chain" of ordinary second-order differential equations (a L_q profile) to obtain the behavior of the solution in the whole graphene, which is two dimensional.

We defined four functions that form the canonical basis of G in the Remark 2 and deduced that these functions are unbounded and do not have compact support, as shown in Theorem 3. The same analysis is also valid for finite linear combinations of them.

We looked for eigenfunctions of $\mathcal{H}$ with compact support. Then we proved Theorem 4, which shows that the following statements are equivalent:

(i) The eigenfunctions are equal to zero in all vertices to the left of an arbitrary vertex i_0 for all the profiles L_q, where the vertices i_0 in different profiles are simply connected.
(ii) There exists a profile L_{q0} such that the eigenfunctions are equal to zero in all its vertices to the left i_0 and satisfies the recursive formulas given in (78)–(79). These formulas are valid for all profiles L_q.
(iii) There exists a profile L_{q0} such that the eigenfunctions are equal to zero in all its vertices to the left i_0 and satisfies the recursive formulas given in (78)–(79) that are unique for that profile.
(iv) The eigenfunctions are equal to zero in all vertex to the left of i_0 and in all profiles L_q, and satisfy the recursive formulas given in (78)–(79).

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