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Journal of Geometry and Physics 55 (2005) 123–134
JOURNAL OF GEOMETRY AND PHYSICS
www.elsevier.com/locate/jgp

An alternate mathematical model for single-wall carbon nanotubes

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Received 6 March 2004; accepted 13 December 2004
Available online 11 January 2005

Abstract

The positions of atoms forming a carbon nanotube are usually described by using a system of generators of the symmetry group. Each atomic position corresponds to an element of the set $\mathbb{Z} \times \{0, 1, \ldots, n\} \times \{0, 1\}$, where n is a natural number depending on the considered nanotube. We obtain an alternate rather different description by starting from a description of the honeycomb lattice in terms of Miller indices. In our mathematical model which is a factor space defined by an equivalence relation in the set $\{(v_0, v_1, v_2) \in \mathbb{Z}^3 | v_0 + v_1 + v_2 \in \{0, 1\}\}$ the neighbours of an atomic position can be described in a simpler way, and the mathematical objects with geometric or physical significance have a simpler and more symmetric form.

PACS: 61.46.+w; 73.63.Fg

MSC: 81V55

JGP SC: Quantum mechanics

Keywords: Single-wall carbon nanotube; Honeycomb lattice; Energy levels

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doi:10.1016/j.geomphys.2004.12.007

1. Introduction

The carbon nanotubes, discovered by Iijima in 1991, have several remarkable physical properties (geometry-dependent electronic transport from metallic to semiconducting with narrow and moderate band gaps, record-high elastic modulus, light weight) and many potential applications (molecular electronic devices, fiber reinforcement technologies, flat displays, carbon-based nanotips). Extensive experimental and theoretical investigations have been carried out on the mechanical and electronic properties of these novel fibers.

The structure of a single-wall carbon nanotube observed by scanning tunneling microscopy [14] can be visualized as the structure obtained by rolling a graphene sheet such that the endpoints of a translation vector are folded one onto the other. The geometric and physical properties of the obtained carbon nanotube depend on this vector, called the *chirality* of the tubule. The position of the atoms forming a carbon nanotube are usually described by using a system of generators of the corresponding symmetry group. Our purpose is to present an alternate mathematical model obtained by starting from a three-axes description (that is, a description in terms of Miller indices [13]) of the honeycomb lattice.

2. Honeycomb lattice in a three-axes description

The vectors $e_0 = (2/\sqrt{6}, 0)$, $e_1 = (-1/\sqrt{6}, 1/\sqrt{2})$, $e_2 = (-1/\sqrt{6}, -1/\sqrt{2})$ corresponding to the vertices of an equilateral triangle form a system of coherent vectors [2], that is, for any $v = (v_x, v_y)$, $u = (u_x, u_y) \in \mathbb{R}^2$ we have

$$v = \sum_{i=0}^{2} \langle v, e_i\rangle e_i, \qquad \langle v, u\rangle = \sum_{i=0}^{2} \langle v, e_i\rangle\langle u, e_i\rangle, \qquad \|v\|^2 = \sum_{i=0}^{2} \langle v, e_i\rangle^2, \tag{1}$$

where $\langle\cdot,\cdot\rangle$ is the usual scalar product. The numbers $\tilde{v}_0 = \langle v, e_0\rangle$, $\tilde{v}_1 = \langle v, e_1\rangle$, $\tilde{v}_2 = \langle v, e_2\rangle$ satisfy the relation $\tilde{v}_0 + \tilde{v}_1 + \tilde{v}_2 = 0$ and can be regarded as the *canonical coordinates* of v with respect to the system of vectors $\{e_0, e_1, e_2\}$. The space

$$\mathcal{E} = \{(u_0, u_1, u_2) \in \mathbb{R}^3 | u_0 + u_1 + u_2 = 0\} \tag{2}$$

becomes in this way a mathematical model for the geometric plane. The correspondence between this description and the usual one is given by the isometry

$$\mathcal{I} : \mathbb{R}^2 \longrightarrow \mathcal{E}, \qquad \mathcal{I}v = (\tilde{v}_0, \tilde{v}_1, \tilde{v}_2), \qquad \mathcal{I}^{-1}(u_0, u_1, u_2) = \sum_{i=0}^{2} u_i e_i. \tag{3}$$

The representation of a vector $v \in \mathbb{R}^2$ as a linear combination of e_0, e_1, e_2 is not unique. More exactly, we have

$$v = \sum_{i=0}^{2} v_i e_i \Longleftrightarrow (v_0, v_1, v_2) \in \{(\tilde{v}_0 + \alpha, \tilde{v}_1 + \alpha, \tilde{v}_2 + \alpha) | \alpha \in \mathbb{R}\}.$$

For each $v \in \mathbb{R}^2$ we denote by (v_0, v_1, v_2) (or simply by v) an element of $\mathbb{R}^3$ such that $v = v_0 e_0 + v_1 e_1 + v_2 e_2$. One can verify by direct computation that

$$\langle u, v\rangle = \sum_{i=0}^{2} \tilde{u}_i \tilde{v}_i = \sum_{i=0}^{2} \tilde{u}_i v_i = \sum_{i=0}^{2} u_i \tilde{v}_i \tag{4}$$

for any $u, v \in \mathbb{R}^2$.

The points of the plane $\mathbb{R}^2$ corresponding to the elements of the set

$$\mathcal{L} = \{v = (v_0, v_1, v_2) \in \mathbb{Z}^3 | v_0 + v_1 + v_2 \in \{0, 1\}\} \tag{5}$$

are distinct and form [3] the *honeycomb lattice*

$$\Lambda = \left\{ \sum_{i=0}^{2} v_i e_i \middle| v = (v_0, v_1, v_2) \in \mathcal{L} \right\}. \tag{6}$$

The bijection $\mathcal{L} \longrightarrow \Lambda : v \mapsto \sum_{i=0}^{2} v_i e_i$ allows us to describe Λ by using $\mathcal{L}$.

The *nearest neighbours* of v are

$$v^0 = (v_0 + \nu(v), v_1, v_2), \qquad v^1 = (v_0, v_1 + \nu(v), v_2), \qquad v^2 = (v_0, v_1, v_2 + \nu(v)),$$

where $\nu(v) = (-1)^{v_0+v_1+v_2}$. The six points $v^{ij} = (v^i)^j$ corresponding to $i \neq j$ are the *next-to-nearest neighbours* of v, and one can remark that $v^{ii} = v$, $v^{ijl} = v^{lji}$, for any $i, j, l \in \{0, 1, 2\}$. The mapping [4]

$$d : \mathcal{L} \times \mathcal{L} \longrightarrow \mathbb{N}, \quad d(v, u) = |v_0 - u_0| + |v_1 - u_1| + |v_2 - u_2| \tag{7}$$

is a distance on $\mathcal{L}$, and a point u is a *neighbour of order* l of v if $d(v, u) = l$.

We have $\mathcal{L} = \mathcal{T} \cup (\mathcal{T} + \vartheta)$, where $\vartheta = (1, 0, 0)$ and

$$\mathcal{T} = \{v = (v_0, v_1, v_2) \in \mathbb{Z}^3 | v_0 + v_1 + v_2 = 0\} = \mathcal{E} \cap \mathbb{Z}^3. \tag{8}$$

The symmetry group G of the honeycomb lattice coincides with the group of all the isometries of the metric space $(\mathcal{L}, d)$, and is generated by the transformations [4]

$$\begin{aligned}
&\sigma : \mathcal{L} \longrightarrow \mathcal{L}, \quad \sigma(v_0, v_1, v_2) = (v_1, v_2, v_0),\\
&\varrho : \mathcal{L} \longrightarrow \mathcal{L}, \quad \varrho(v_0, v_1, v_2) = (v_0, v_2, v_1),\\
&\tau : \mathcal{L} \longrightarrow \mathcal{L}, \quad \tau(v_0, v_1, v_2) = -(v_0, v_1, v_2) + \vartheta.
\end{aligned} \tag{9}$$

The group G contains the subgroup of translations (also denoted by $\mathcal{T}$)

$$\{\mathcal{L} \longrightarrow \mathcal{L} : v \mapsto v + u | u \in \mathcal{T}\}$$

generated by $\sigma^2\tau\sigma\tau$ and $\sigma\tau\sigma^2\tau$

$$\begin{aligned}
&\sigma^2\tau\sigma\tau(v_0, v_1, v_2) = (v_0, v_1, v_2) + (-1, 1, 0),\\
&\sigma\tau\sigma^2\tau(v_0, v_1, v_2) = (v_0, v_1, v_2) + (-1, 0, 1).
\end{aligned} \tag{10}$$

It is known [12] that the C–C bond length in the case of a graphene sheet is 1.44 Å. If we use the honeycomb lattice $\mathcal{L}$ as a mathematical model for a graphene sheet then we have to multiply the position vectors of the points of the lattice by the constant $a = 1.44\sqrt{6}/2$ in order to get their lengths in Å.

Consider the Hilbert space $(l^2(\mathcal{L}), \langle\cdot,\cdot\rangle)$, where

$$l^2(\mathcal{L}) = \left\{ \psi : \mathcal{L} \longrightarrow \mathbb{C} \left| \sum_{v\in\mathcal{L}} |\psi(v)|^2 < \infty \right. \right\},$$

$$\langle \psi_1, \psi_2 \rangle = \sum_{v\in\mathcal{L}} \bar{\psi}_1(v)\psi_2(v) \tag{11}$$

and the unitary representation of G in $l^2(\mathcal{L})$ defined by

$$g : l^2(\mathcal{L}) \longrightarrow l^2(\mathcal{L}), \qquad (g\psi)(v) = \psi(g^{-1}v). \tag{12}$$

Let ε be a real number, and $\gamma_0, \gamma_1, \gamma_2$ be three complex numbers. The linear operator

$$H : l^2(\mathcal{L}) \longrightarrow l^2(\mathcal{L}), \qquad (H\psi)(v) = \varepsilon\psi(v) + \sum_{j=0}^{2} \gamma(v, v^j)\psi(v^j), \tag{13}$$

where

$$\gamma(v, v^j) = \begin{cases} \gamma_j \text{ if } \nu(v) = 1, \\ \bar{\gamma}_j \text{ if } \nu(v) = -1 \end{cases} \tag{14}$$

is a self-adjoint operator

$$\begin{aligned} \langle H\psi_1, \psi_2 \rangle &= \varepsilon \sum_{v\in\mathcal{L}} \bar{\psi}_1(v)\psi_2(v) + \sum_{j=0}^{2} \sum_{v\in\mathcal{L}} \bar{\gamma}(v, v^j)\bar{\psi}_1(v^j)\psi_2(v) \\ &= \varepsilon \sum_{v\in\mathcal{L}} \bar{\psi}_1(v)\psi_2(v) + \sum_{j=0}^{2} \sum_{v\in\mathcal{L}} \gamma(v, v^j)\bar{\psi}_1(v)\psi_2(v^j) = \langle \psi_1, H\psi_2 \rangle. \end{aligned}$$

The Hamiltonian used in the tight-binding description of π bands in 2D graphite, with only first-neighbour C–C interaction, has the form (13).

Theorem 1. *For any $k = (k_0, k_1, k_2) \in \mathcal{E}$ the real numbers*

$$E_{\pm}(k) = \varepsilon \pm |\gamma_0 \, \mathrm{e}^{\mathrm{i}k_0 a} + \gamma_1 \, \mathrm{e}^{\mathrm{i}k_1 a} + \gamma_2 \, \mathrm{e}^{\mathrm{i}k_2 a}| \tag{15}$$

belong to the spectrum of H.

Proof. The function

$$\varphi : \mathcal{L} \longrightarrow \mathbb{C}, \qquad \varphi(v) = \begin{cases} \alpha \text{ for } v \in \mathcal{T}, \\ \beta \text{ for } v \in \mathcal{T} + \vartheta, \end{cases}$$

where α, β are two constants, is invariant under any translation $u \in \mathcal{T}$

$$\varphi(v+u) = \varphi(v) \quad \text{for all } v \in \mathcal{L}.$$

The Bloch type function

$$\psi_k : \mathcal{L} \longrightarrow \mathbb{C}, \qquad \psi_k(v) = \varphi(v)\, \mathrm{e}^{\mathrm{i}\langle k, v\rangle a} \tag{16}$$

belonging to an extension of the space $l^2(\mathcal{L})$ satisfies the relation $H\psi_k = E\psi_k$ if and only if (α, β) is a solution of the system of equations

$$\varepsilon\alpha + (\gamma_0\, \mathrm{e}^{\mathrm{i}k_0 a} + \gamma_1\, \mathrm{e}^{\mathrm{i}k_1 a} + \gamma_2\, \mathrm{e}^{\mathrm{i}k_2 a})\beta = E\alpha,$$
$$(\overline{\gamma}_0\, \mathrm{e}^{-\mathrm{i}k_0 a} + \overline{\gamma}_1\, \mathrm{e}^{-\mathrm{i}k_1 a} + \overline{\gamma}_2\, \mathrm{e}^{-\mathrm{i}k_2 a})\alpha + \varepsilon\beta = E\beta.$$

This system has non-trivial solutions if and only if

$$\begin{vmatrix} \varepsilon - E & \gamma_0\, \mathrm{e}^{\mathrm{i}k_0 a} + \gamma_1\, \mathrm{e}^{\mathrm{i}k_1 a} + \gamma_2\, \mathrm{e}^{\mathrm{i}k_2 a} \\ \overline{\gamma}_0\, \mathrm{e}^{-\mathrm{i}k_0 a} + \overline{\gamma}_1\, \mathrm{e}^{-\mathrm{i}k_1 a} + \overline{\gamma}_2\, \mathrm{e}^{-\mathrm{i}k_2 a} & \varepsilon - E \end{vmatrix} = 0,$$

that is, if and only if E is one of the numbers $E_{\pm}(k)$.

The origin on the energy axis is usually chosen such that $\varepsilon = 0$. If $\gamma_0 = \gamma_1 = \gamma_2 = \gamma$ is a real positive number then H is a G-invariant self-adjoint operator and its spectrum contains for each $k \in \mathcal{E}$ the numbers $\pm E(k)$, where

$$\begin{aligned} E(k) &= \gamma|\mathrm{e}^{\mathrm{i}k_0 a} + \mathrm{e}^{\mathrm{i}k_1 a} + \mathrm{e}^{\mathrm{i}k_2 a}| \\ &= \gamma\sqrt{3 + 2\cos(k_0 - k_1)a + 2\cos(k_1 - k_2)a + 2\cos(k_2 - k_0)a}. \end{aligned} \tag{17}$$

The relation (17) allows us to extend the function $E : \mathcal{E} \longrightarrow \mathbb{R}$ to a periodic function $E : \mathbb{R}^3 \longrightarrow \mathbb{R}$

$$\begin{aligned} E(k_0, k_1, k_2) &= E\left(k_0 + \frac{2\pi}{a}, k_1, k_2\right) = E\left(k_0, k_1 + \frac{2\pi}{a}, k_2\right) \\ &= E\left(k_0, k_1, k_2 + \frac{2\pi}{a}\right) \end{aligned} \tag{18}$$

with the property

$$E(k_0, k_1, k_2) = E(k_0 + \alpha, k_1 + \alpha, k_2 + \alpha) \quad \text{for all } \alpha \in \mathbb{R}.$$

The corresponding first Brillouin zone is the hexagonal set (Fig. 2)

$$\mathcal{B} = \left\{ (k_0, k_1, k_2) \in \mathcal{E} \,\middle|\, -\frac{2\pi}{3a} \le k_i \le \frac{2\pi}{3a} \right\} \tag{19}$$

(certain points lying on the frontier of $\mathcal{B}$ are equivalent).

The intervals $[-3\gamma, 0] = \{-E(k) | k \in \mathcal{B}\}$ and $[0, 3\gamma] = \{E(k) | k \in \mathcal{B}\}$ correspond to the valence π and the conduction π^* energy bands, respectively. The graphene sheet is a conductor since the gap between these bands is null.

Since $E(k)$ can be written as

$$E(k) = \gamma\sqrt{(\cos k_0 a + \cos k_1 a + \cos k_2 a)^2 + (\sin k_0 a + \sin k_1 a + \sin k_2 a)^2},$$

we have $E(k) \geq 0$, and the only points of $\mathcal{B}$ with $E(k) = 0$ are

$$\pm\left(\frac{2\pi}{3a}, -\frac{2\pi}{3a}, 0\right), \qquad \pm\left(\frac{2\pi}{3a}, 0, -\frac{2\pi}{3a}\right), \qquad \pm\left(0, \frac{2\pi}{3a}, -\frac{2\pi}{3a}\right), \tag{20}$$

that is, the vertices of the Brillouin zone (usually denoted by K) [10].

It is known that the Fermi level for a graphene sheet occurs at the K points. The function $E : \mathbb{R}^3 \longrightarrow \mathbb{R}$ is not differentiable at these points. We have, for example,

$$\lim_{k_0 \to 2\pi/3a} \frac{E(k_0, -2\pi/3a, 0) - 0}{k_0 - 2\pi/3a} = \gamma \qquad \lim_{k_0 \to 2\pi/3a} \frac{\sqrt{2 + 2\cos(k_0 a + \pi/3)}}{k_0 - 2\pi/3a} = 2\gamma$$
$$\lim_{k_0 \to 2\pi/3a} \frac{|\cos(k_0 a/2 + \pi/6)|}{k_0 - 2\pi/3a} \tag{21}$$

whence

$$\lim_{\substack{k_0 \to 2\pi/3a \\ k_0 > 2\pi/3a}} \frac{E(k_0, -2\pi/3a, 0) - 0}{k_0 - 2\pi/3a} = \gamma a, \qquad \lim_{\substack{k_0 \to 2\pi/3a \\ k_0 < 2\pi/3a}} \frac{E(k_0, -2\pi/3a, 0) - 0}{k_0 - 2\pi/3a} = -\gamma a.$$

The function $E : \mathbb{R}^3 \longrightarrow \mathbb{R}$ is differentiable at any point k with $E(k) \neq 0$, and

$$\frac{\partial E}{\partial k_0}(k) = \gamma \frac{-a\sin(k_0 - k_1)a + a\sin(k_2 - k_0)a}{\sqrt{3 + 2\cos(k_0 - k_1)a + 2\cos(k_1 - k_2)a + 2\cos(k_2 - k_0)a}}, \tag{22}$$

etc. The stationary points lying in the Brillouin zone $\mathcal{B}$ are

$$(0, 0, 0), \qquad \pm\left(\frac{2\pi}{3a}, -\frac{\pi}{3a}, -\frac{\pi}{3a}\right), \qquad \pm\left(-\frac{\pi}{3a}, \frac{2\pi}{3a}, -\frac{\pi}{3a}\right),$$
$$\pm\left(-\frac{\pi}{3a}, -\frac{\pi}{3a}, \frac{2\pi}{3a}\right),$$

that is, the center (a maximum point, denoted by Γ) and the middle of the edges of the Brillouin zone (saddle points, denoted by M).

3. Chiral single-wall carbon nanotubes

A single-wall carbon nanotube can be visualized as the structure obtained by rolling a graphene sheet such that the endpoints O and A of a translation vector $\vec{OA}$ are folded one onto the other (Fig. 1). The geometric and physical properties of the obtained nanotube depend on this vector, called the *chirality* of the tubule and represented in our approach by an element $c \in \mathcal{T}$. Without loss of generality, we can restrict us to the tubules with $c_0 > c_1 \geq c_2$. In the case $c_1 = c_2$ we have an *armchair* tubule, and in the case $c_1 = 0$ a

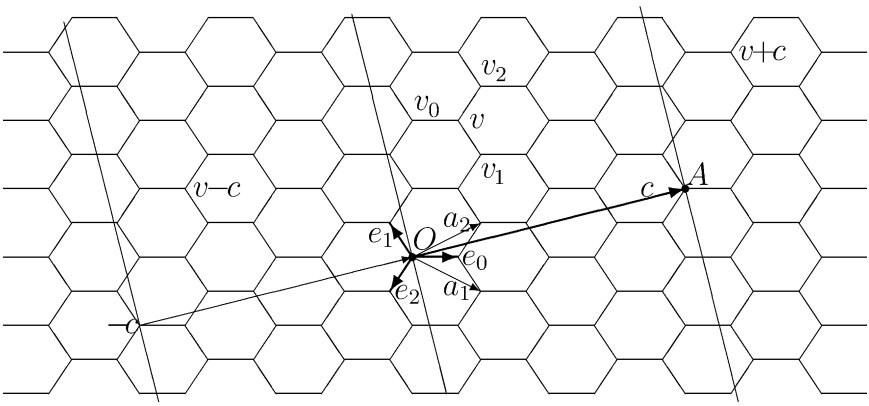

Fig. 1. The honeycomb lattice and the partition defined by a vector $c \in \mathcal{T}$.

zig-zag tubule. The nanotubes with $0 \neq c_1 \neq c_2$ are called *chiral nanotubes*. The diameter of the nanotube of chirality c is $\|c\|a/\pi$.

After the graphene sheet rolling, the points $\ldots, v-2c, v-c, v, v+c, v+2c, \ldots$ are folded one onto the other, for any $v = (v_0, v_1, v_2) \in \mathcal{L}$. Thus, each point of the set

$$[v_0, v_1, v_2] = v + \mathbb{Z}c = \{(v_0 + jc_0, v_1 + jc_1, v_2 + jc_2) | j \in \mathbb{Z}\} \tag{23}$$

describes the same point of the carbon nanotube of chirality c. Each rational number is a class of equivalent fractions, called its representatives. In a similar way, for each point of a carbon nanotube we have an infinite number of possibilities to describe it in our model. A mathematical expression containing the coordinates of a point is well defined only if it does not depend on the representative we choose. We describe the atomic positions on a carbon nanotube by using the subset

$$\mathcal{L}_c = \left\{ [v_0, v_1, v_2] \in \frac{\mathbb{Z}^3}{\mathbb{Z}c} \middle| \, v_0 + v_1 + v_2 \in \{0; 1\} \right\}. \tag{24}$$

of the factor space

$$\frac{\mathbb{Z}^3}{\mathbb{Z}c} = \{[v] = (v_0, v_1, v_2) + \mathbb{Z}c | v_0, v_1, v_2 \in \mathbb{Z}\} \tag{25}$$

as a mathematical model. One can remark that $\mathcal{L}_c$ is well defined since the condition $v_0 + v_1 + v_2 \in \{0; 1\}$ we impose to $[v_0, v_1, v_2]$ does not depend on the representative we choose. Indeed, $(v_0 + jc_0) + (v_1 + jc_1) + (v_2 + jc_2) = v_0 + v_1 + v_2$ for all $j \in \mathbb{Z}$.

Each point $[v] \in \mathcal{L}_c$ has three *nearest neighbours*, namely, $[v^0]$, $[v^1]$, $[v^2]$, and six *next-to-nearest neighbours*, namely, $[v^{01}]$, $[v^{10}]$, $[v^{12}]$, $[v^{21}]$, $[v^{20}]$, $[v^{02}]$.

A symmetry transformation of the honeycomb lattice $\mathcal{L} \longrightarrow \mathcal{L} : v \mapsto gv$ defines the *symmetry transformation* $\mathcal{L}_c \longrightarrow \mathcal{L}_c : [v] \mapsto [gv]$ of the carbon nanotube $\mathcal{L}_c$ if

$$[v] = [u] \Longrightarrow [gv] = [gu],$$

that is, if

$$v - u \in \mathbb{Z}c \Longrightarrow gv - gu \in \mathbb{Z}c.$$

Theorem 2. *The transformations*

$$g_w : \mathcal{L}_c \longrightarrow \mathcal{L}_c, \quad g_w[v] = [v + w], \qquad \tau : \mathcal{L}_c \longrightarrow \mathcal{L}_c, \quad \tau[v] = [-v + \vartheta] \quad (26)$$

are symmetry transformation of $\mathcal{L}_c$ for all $w \in \mathcal{T}$.

Proof. We have $v - u \in \mathbb{Z}c \Longrightarrow (v + w) - (u + w) = v - u \in \mathbb{Z}c$, and $v - u \in \mathbb{Z}c \Longrightarrow (-v + \vartheta) - (-u + \vartheta) = u - v \in \mathbb{Z}c$.

Let $n = \gcd\{c_0, c_1, c_2\}$ be the greatest common divisor of c_0, c_1, c_2, and let $c = nc'$, that is, $c'_0 = c_0/n$, $c'_1 = c_1/n$ and $c'_2 = c_2/n$. The transformation $g_{c'}$ represents a rotation of angle $2\pi/n$ of the nanotube with respect to its axis. Since $(c_1 - c_2)c_0 + (c_2 - c_0)c_1 + (c_0 - c_1)c_2 = 0$, the vector $w = (c_1 - c_2, c_2 - c_0, c_0 - c_1)$ is orthogonal to c, and the corresponding transformation g_w is a pure translation, that is, a translation in the direction of the nanotube symmetry axis. The vector $b = (1/\mathcal{R})(c_1 - c_2, c_2 - c_0, c_0 - c_1)$, where

$$\mathcal{R} = \gcd\{c_1 - c_2, c_2 - c_0, c_0 - c_1\} = \begin{cases} n & \text{if } c'_1 - c'_2 \notin 3\mathbb{Z}, \\ 3n & \text{if } c'_1 - c'_2 \in 3\mathbb{Z} \end{cases} \quad (27)$$

defines the shortest pure translation of $\mathcal{L}_c$.

From $c_0 + c_1 + c_2 = 0$, we get $(c_1 - c_2)^2 + (c_2 - c_0)^2 + (c_0 - c_1)^2 = 3(c_0^2 + c_1^2 + c_2^2)$, that is, $\mathcal{R}^2\|b\|^2 = 3\|c\|^2$, whence

$$q = \frac{1}{\mathcal{R}}(c_0^2 + c_1^2 + c_2^2) \in n\mathbb{Z}. \quad (28)$$

For any $w \in \mathcal{T}$ the projections of w on c and b can be written as

$$\frac{\langle w, c\rangle}{||c||^2}c = \left(w_1\frac{c_1 - c_0}{\mathcal{R}} + w_2\frac{c_2 - c_0}{\mathcal{R}}\right)\frac{c}{q}, \qquad \frac{\langle w, b\rangle}{||b||^2}b = \left(w_1\frac{c_2}{n} - w_2\frac{c_1}{n}\right)\frac{b}{q'},$$

where $q' = q/n$. It is well known that in the case of two integer numbers $\eta, \mu \in \mathbb{Z}$ with $\gcd\{\eta, \mu\} = 1$ there exist $\alpha, \beta \in \mathbb{Z}$ with $\alpha\eta + \beta\mu = 1$. Since $\gcd\{(c_1 - c_0)/\mathcal{R}, (c_2 - c_0)/\mathcal{R}\} = 1$ and $\gcd\{c_2/n, c_1/n\} = 1$ it follows that the projection of $\mathcal{T}$ on c is $\mathbb{Z}c/q$ and the projection of $\mathcal{T}$ on b is $\mathbb{Z}b/q'$. Let $\omega \in \mathcal{T}$ be the shortest vector with

$$\frac{\langle \omega, b\rangle}{\|b\|^2}b = \frac{b}{q'}. \quad (29)$$

If $\mathcal{L}_c$ is a chiral nanotube then its symmetry group G_c is generated by the transformations $g_{c'}$, g_ω and τ (additional symmetry operations, namely, mirror and glide planes occur only in the case of armchair and zig-zag nanotubes). More than that, for any $[v] \in \mathcal{L}_c$ there exist $s \in \mathbb{Z}$, $m \in \{0, 1, \ldots, n - 1\}$ and $p \in \{0, 1\}$ uniquely determined such that

$$[v] = \tau^p g_\omega^s g_{c'}^m [0, 0, 0]. \quad (30)$$

The usual description of the atomic positions of the atoms forming a carbon nanotube [15,16] is based on this remark, and the set

$$\{(s, m, p)|s \in \mathbb{Z}, m \in \{0, 1, \ldots, n-1\}, p \in \{0, 1\}\} \tag{31}$$

is used as a mathematical model.

The subgroup $\tilde{G}_c$ of G_c generated by $g_{c'}$ and g_ω is a commutative index-2 subgroup, and $g_{c'}^n = I$, $g_\omega^{q'} = g_b$, where I is the transformation $I[v] = [v]$ for all $[v] \in \mathcal{L}_c$. The irreducible representations of $\tilde{G}_c$ are one-dimensional and can be described in terms of generators as [5]

$$\begin{aligned} &T_{(\kappa,m)}(g_{c'}) = \mathrm{e}^{-\mathrm{i}2\pi m/n}, \quad \text{where } m \in \{0, 1, \ldots, n-1\}, \\ &T_{(\kappa,m)}(g_\omega) = \mathrm{e}^{-\mathrm{i}\kappa a/q'}, \quad \text{where } \kappa \in \left[0, \frac{2\pi q'}{a}\right). \end{aligned} \tag{32}$$

The irreducible representations of G_c can be obtained from the irreducible representations of $\tilde{G}_c$ by using the index-2 subgroup induction.

Consider the Hilbert space $(l^2(\mathcal{L}_c), \langle\cdot,\cdot\rangle)$, where

$$l^2(\mathcal{L}_c) = \left\{ \psi : \mathcal{L}_c \longrightarrow \mathbb{C} \,\middle|\, \sum_{v\in\mathcal{L}_c} |\psi(v)|^2 < \infty \right\}, \qquad \langle\psi_1, \psi_2\rangle = \sum_{v\in\mathcal{L}_c} \bar{\psi}_1(v)\psi_2(v) \tag{33}$$

and the unitary representation of G_c in $l^2(\mathcal{L}_c)$ defined by

$$g : l^2(\mathcal{L}_c) \longrightarrow l^2(\mathcal{L}_c), \qquad (g\psi)[v] = \psi(g^{-1}[v]). \tag{34}$$

If ε is a real number and $\gamma_0, \gamma_1, \gamma_2$ are three complex numbers, then the linear operator

$$H : l^2(\mathcal{L}_c) \longrightarrow l^2(\mathcal{L}_c), \qquad (H\psi)[v] = \varepsilon\psi[v] + \sum_{j=0}^{2} \gamma(v, v^j)\psi[v^j] \tag{35}$$

with $\gamma(v, v^j)$ defined by (14), is a self-adjoint operator.

Theorem 3. *For any $k = (k_0, k_1, k_2) \in \mathcal{E}$ satisfying the relation*

$$\langle k, c\rangle = k_0c_0 + k_1c_1 + k_2c_2 \in \left(\frac{2\pi}{a}\right)\mathbb{Z} \tag{36}$$

the real numbers

$$E_\pm(k) = \varepsilon \pm |\gamma_0\,\mathrm{e}^{\mathrm{i}k_0a} + \gamma_1\,\mathrm{e}^{\mathrm{i}k_1a} + \gamma_2\,\mathrm{e}^{\mathrm{i}k_2a}| \tag{37}$$

belong to the spectrum of H.

Proof. For $k \in \mathcal{E}$ satisfying (36) we have

$$v - u \in \mathbb{Z}c \Longrightarrow \varphi(v)\,\mathrm{e}^{\mathrm{i}\langle k,v\rangle a} = \varphi(u)\,\mathrm{e}^{\mathrm{i}\langle k,u\rangle a}$$

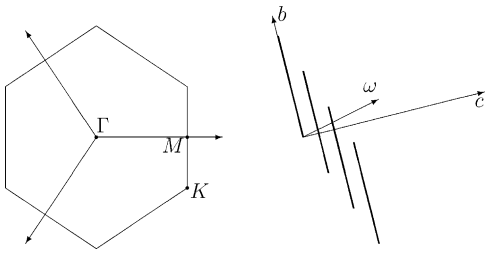

Fig. 2. The first Brillouin zone $\mathcal{B}$ (left) and the set $\mathcal{B}_c$ in case $n = 4$ (right).

and hence the Bloch type function

$$\psi_k : \mathcal{L}_c \longrightarrow \mathbb{C}, \qquad \psi_k[v] = \varphi(v)\, \mathrm{e}^{\mathrm{i}\langle k, v\rangle a} \tag{38}$$

is well defined. If $E \in \{E_+(k), E_-(k)\}$ then there exists a non-null function of this form satisfying the relation $H\psi_k = E\psi_k$.

If $\gamma_0, \gamma_1, \gamma_2$ are real then H is G_c-invariant. Indeed, since $g_{c'} v^j = (g_{c'} v)^j$, $g_\omega v^j = (g_\omega v)^j$ and $\tau v^j = (\tau v)^j$ we have $gHg^{-1} = H$, for any $g \in G_c$. Denoting $\langle k, c\rangle = 2m\pi/a$ and $\langle k, \omega\rangle = \kappa/q'$ we get

$$\begin{aligned}
(g_{c'}\psi_k)[v] &= \varphi(v)\, \mathrm{e}^{\mathrm{i}\langle k, v-c'\rangle a} = \mathrm{e}^{-\mathrm{i}\langle k, c'\rangle a}\psi_k[v] = \mathrm{e}^{-\mathrm{i}2m\pi/n}\psi_k[v],\\
(g_\omega\psi_k)[v] &= \varphi(v)\, \mathrm{e}^{\mathrm{i}\langle k, v-\omega\rangle a} = \mathrm{e}^{-\mathrm{i}\langle k, \omega\rangle a}\psi_k[v] = \mathrm{e}^{-\mathrm{i}\kappa a/q'}\psi_k[v],\\
(\tau\psi_k)[v] &= \varphi(\tau v)\, \mathrm{e}^{\mathrm{i}\langle k, -v+\vartheta\rangle a} = \left(\frac{\varphi(\tau v)}{\varphi(v)}\right) \mathrm{e}^{\mathrm{i}k_0 a}\psi_{-k}[v]
\end{aligned} \tag{39}$$

that is, the subspace generated by ψ_k and ψ_{-k} is G_c-invariant. More than that, these relations allow us [5] to classify the eigenstates ψ_k by using the quantum numbers m and κ. The set (Fig. 2)

$$\mathcal{B}_c = \left\{ k \in \mathcal{E} \;\middle|\; \begin{array}{l} \langle k, c\rangle = \dfrac{2m\pi}{a} \text{ with } m \in \{0, 1, \ldots, n-1\} \\ \langle k, \omega\rangle = \dfrac{\kappa}{q'} \text{ with } \kappa \in \left[0, \dfrac{2q'\pi}{a}\right) \end{array} \right\}. \tag{40}$$

contains a k corresponding to each class. The conduction m-band

$$\left\{ E_+(k) | \langle k, c\rangle = \frac{2m\pi}{a}, \langle k, \omega\rangle \in \left[0, \frac{2\pi q'}{a}\right) \right\} \tag{41}$$

and the valence m-band

$$\left\{ E_-(k) | \langle k, c\rangle = \frac{2m\pi}{a}, \langle k, \omega\rangle \in \left[0, \frac{2\pi q'}{a}\right) \right\} \tag{42}$$

can easily be determined by using (37). A graphic representation of these conduction bands can be found in [5].

The relation (36) defines a family of equidistant straight lines orthogonal to c with the distance between neighbouring lines equal to $\delta = 2\pi/a\|c\|$. Since the length of the

projection of the vector $(2\pi/3a, -2\pi/3a, 0)$ on c is $2\pi(c_0 - c_1)/3a\|c\| = (c_0 - c_1)\delta/3$, the K points belong to the straight lines (36) if and only if $c_0 - c_1 \in 3\mathbb{Z}$.

The Hamiltonian used in the tight-binding description of π bands in $\mathcal{L}_c$, with only first-neighbour C–C interaction, has the form (35). Except for very small diameter nanotubes, the constants γ_0, γ_1, γ_2 keep almost the same values as in the case of a graphene sheet [1,16]. Neglecting the effects of the curvature of the graphite sheet, we can assume $\varepsilon = 0$, $\gamma_0 = \gamma_1 = \gamma_2 = \gamma \in (0, \infty)$, and we get the energy levels

$$E_{\pm}(k) = \pm\gamma\sqrt{3 + 2\cos(k_0 - k_1)a + 2\cos(k_1 - k_2)a + 2\cos(k_2 - k_0)a}. \tag{43}$$

From the form of the surface $E(k)$ [12], it follows that the gap between the valence and conduction bands is given by:

$$\Delta E_c = \min_{k\in\mathcal{B}_c} E_+(k) - \max_{k\in\mathcal{B}_c} E_-(k) = 2\min_{k\in\mathcal{B}_c} E(k) \tag{44}$$

and we have $\Delta E_c = 0$ if and only if $c_0 - c_1 \in 3\mathbb{Z}$. Therefore [7,16], the nanotube $\mathcal{L}_c$ is a conductor if $c_0 - c_1 \in 3\mathbb{Z}$, and a semiconductor if $c_0 - c_1 \notin 3\mathbb{Z}$. The minimum $\min_{k\in\mathcal{B}_c} E(k)$ is achieved [12] at a point lying on a straight line (36) in the vicinity of a point K.

In the case of a magnetic field parallel to the nanotube axis the Hamiltonian also has the form (35), but $\gamma_0 = \gamma\,\mathrm{e}^{\mathrm{i}\beta c_0 a}$, $\gamma_1 = \gamma\,\mathrm{e}^{\mathrm{i}\beta c_1 a}$, $\gamma_2 = \gamma\,\mathrm{e}^{\mathrm{i}\beta c_2 a}$, where β is a real constant describing the magnetic field strength threading the nanotube [9]. Choosing $\varepsilon = 0$, $\gamma \in (0, \infty)$, we get the energy levels

$$E_{\pm}^{\mathrm{mag}}(k) = \pm\gamma|\mathrm{e}^{\mathrm{i}(k_0+\beta c_0)a} + \mathrm{e}^{\mathrm{i}(k_1+\beta c_1)a} + \mathrm{e}^{\mathrm{i}(k_2+\beta c_2)a}| = E_{\pm}(k + \beta c) \tag{45}$$

for any k satisfying (36). From this relation it follows that the presence of a magnetic field parallel to the nanotube axis can modify drastically the electronic properties of the nanotube, and this modification depends essentially on the nanotube chirality [9].

4. Concluding remarks

The alternate description presented in this paper offers certain formal advantages and is significantly different from the usual one. We think that it can be used as a complementary description, and may stimulate the interest of mathematicians in the fascinating geometry of carbon nanotubes. We have re-obtained some known results [5,6,8,9,11,12,16] concerning the chiral carbon nanotubes in order to illustrate the proposed approach.

Since our model is a factor space, we have to verify the independence of the representative (v_0, v_1, v_2) we choose for $[v_0, v_1, v_2]$ in the case of any mathematical object we consider on $\mathcal{L}_c$. This is not an inconvenience for our approach but a useful criterion when we look for mathematical objects with possible geometric or physical significance.

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