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Random walks on carbon nanotubes and quasicrystals

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Abstract. An analytic formula for the total number of k-step walks between given sites on a carbon nanotube is obtained by using a new mathematical model based on a three-axes description of the honeycomb lattice. The new model represents an alternate mathematical description which may be useful in certain applications. It is similar to the four-axes description existing in the case of hexagonal crystals. The use of one or more additional axes is a fundamental method in quasicrystal physics. We show that the mathematical model we use for the honeycomb lattice can be defined in terms of a strip projection method, and present a method to associate some finite graphs to a quasicrystal. The random walks on these graphs are connected with random walks on a quasicrystal.

1. Introduction

The movement of an excitation (or a vacancy) on a carbon nanotube or a quasicrystal can be regarded as a sequence of jumps between neighbouring sites and described by a walk. Generally, the study of walks on the honeycomb lattice (usually regarded as a sublattice of the square lattice [14, p 48]) and on quasicrystals is done by generating all walks up to a certain length [1, 8] or by Monte Carlo simulations [16]. We restrict ourselves to the problem of enumerating all walks of a given number of steps between given sites (many other problem related to walks can be reduced to this important problem [14]), and our approach is different.

We use a three-axes description in the case of the honeycomb lattice and some finite graphs in the case of quasicrystals. This allows us to obtain some exact mathematical formulae. The use of an additional axis in the case of the honeycomb lattice is an old method [2, 20].

Starting from our description of the honeycomb lattice we obtain a new mathematical model for the single-wall carbon nanotubes, and an analytic formula for the total number of k-step walks between given sites. In order to illustrate other facilities offered by this new description we re-obtain in an elegant way some known results [5, 9, 12, 13, 21].

The use of one or more additional axes is a fundamental method in quasicrystal physics, but in the case of a 'rational cut' the model defined by the strip projection method [7, 15, 18] is periodic. The model we use for the honeycomb lattice can be defined in a natural way in terms of this method.

Some finite graphs can be associated with a quasicrystal by using a finite partition of the window of selection. The existence of certain connections between the random walks on the quasicrystal and the random walks on these graphs shows that they may be useful in the study of random walks on quasicrystals.

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2. A mathematical model

In this section we present an abstract model for the honeycomb lattice. Let $\mathbb{Z}$ be the set of all integers, and let

$$\mathcal{M} = \left\{ n = (n_0, n_1, n_2) \in \mathbb{Z}^3 \middle| \, n_0 + n_1 + n_2 \in \{0, 1\} \right\} = \mathcal{T} \cup (\mathcal{T} + \tau) \tag{1}$$

where $\tau = (1, 0, 0)$ and $\mathcal{T} = \left\{ n = (n_0, n_1, n_2) \in \mathbb{Z}^3 \middle| \, n_0 + n_1 + n_2 = 0 \right\}$. The mapping

$$\delta : \mathcal{M} \times \mathcal{M} \longrightarrow \mathbb{N} \qquad \delta(n, m) = |n_0 - m_0| + |n_1 - m_1| + |n_2 - m_2| \tag{2}$$

is a distance on $\mathcal{M}$. Each point $n \in \mathcal{M}$ has three *nearest neighbours*, namely,

$$n^0 = (n_0 + \nu(n), n_1, n_2) \qquad n^1 = (n_0, n_1 + \nu(n), n_2) \qquad n^2 = (n_0, n_1, n_2 + \nu(n))$$

where $\nu(n) = (-1)^{n_0+n_1+n_2}$. The six points $n^{ij} = (n^i)^j$ corresponding to $i \neq j$ are the *second neighbours* of n, and one can remark that $n^{ii} = n$, $n^{ijk} = n^{kji}$, for any $i, j, k \in \{0, 1, 2\}$. An *isometry* of the metric space $(\mathcal{M}, \delta)$ is a bijection $g : \mathcal{M} \longrightarrow \mathcal{M} : n \mapsto gn$ such that $\delta(gn, gm) = \delta(n, m)$, for all $n, m \in \mathcal{M}$.

Theorem 1. *The group G of all the isometries of the metric space $(\mathcal{M}, \delta)$ is isomorphic to the symmetry group of the honeycomb lattice [17, 22], the diperiodic group $Dg80 = p(6/m)(2/m)(2/m)$.*

Proof. Let $I, i : \mathbb{Z}^3 \longrightarrow \mathbb{Z}^3$, $In = n$, $in = -n$, and let S_3 be the group of all the permutations $\sigma : \{0, 1, 2\} \longrightarrow \{0, 1, 2\}$. The transformations

$$\begin{aligned} &g_\sigma : \mathcal{M} \longrightarrow \mathcal{M} : (n_0, n_1, n_2) \mapsto (n_{\sigma(0)}, n_{\sigma(1)}, n_{\sigma(2)}) \\ &t : \mathcal{M} \longrightarrow \mathcal{M} : (n_0, n_1, n_2) \mapsto (n_0 + t_0, n_1 + t_1, n_2 + t_2) \\ &\{i|\tau\} : \mathcal{M} \longrightarrow \mathcal{M} : (n_0, n_1, n_2) \mapsto (-n_0 + 1, -n_1, -n_2) \end{aligned} \tag{3}$$

are isometries of $(\mathcal{M}, \delta)$ for any $\sigma \in S_3$, and any $t = (t_0, t_1, t_2) \in \mathcal{T}$. The point $(0, 0, 0)$ can be transformed into an arbitrary point of $\mathcal{M}$ by composing these transformations. More than that, one can see that

$$G = \bigcup_{\sigma \in S_3} \mathcal{T} \circ g_\sigma \cup \bigcup_{\sigma \in S_3} \mathcal{T} \circ \{i \circ g_\sigma | \tau\} \tag{4}$$

where $\{i \circ g_\sigma|\tau\}n = -g_\sigma n + \tau$. If $\sigma \in S_3$ is the permutation $\sigma(0) = 2, \sigma(1) = 0, \sigma(2) = 1$ we have $(i \circ g_\sigma)^6 = I$ and $(i \circ g_\sigma)^j \neq I$ for $j < 6$. □

The unoriented graph $(\mathcal{M}, L)$ having

$$L = \{\{n, m\} | \delta(n, m) = 1\} = \{\{n, n^i\} | n \in \mathcal{M}, i \in \{0, 1, 2\}\} \tag{5}$$

as the set of all lines can be associated in a natural way with the metric space $(\mathcal{M}, \delta)$. Two points $n, m \in \mathcal{M}$ are *adjacent* if $\delta(n, m) = 1$. The group G is simultaneously the group of all the automorphisms of the graph $(\mathcal{M}, L)$. One can prove that the number $\delta(n, m)$ represents the minimal length of a walk from n to m.

3. The honeycomb lattice

Let us consider in the two-dimensional Euclidean space $\mathbb{E}_2$, the vectors $\boldsymbol{e}_0 = (1, 0)$, $\boldsymbol{e}_1 = \left(-\frac{1}{2}, \frac{1}{2}\sqrt{3}\right)$, $\boldsymbol{e}_2 = \left(-\frac{1}{2}, -\frac{1}{2}\sqrt{3}\right)$, $\boldsymbol{a}_1 = \boldsymbol{e}_0 - \boldsymbol{e}_1$ and $\boldsymbol{a}_2 = \boldsymbol{e}_0 - \boldsymbol{e}_2$, with respect to an orthonormal basis. The endpoints of $\boldsymbol{e}_0$, $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ are the vertices of an equilateral triangle, and $\boldsymbol{e}_0 = (\boldsymbol{a}_1 + \boldsymbol{a}_2)/3$. The periodic set (figure 1)

$$\mathcal{L} = \{\alpha_1\boldsymbol{a}_1 + \alpha_2\boldsymbol{a}_2 | (\alpha_1, \alpha_2) \in \mathbb{L}\} \tag{6}$$

where $\mathbb{L} = \mathbb{Z}^2 \cup (\mathbb{Z}^2 + (\frac{1}{3}, \frac{1}{3}))$, is called a *honeycomb lattice*. It is described [5, 12, 13, 21] with respect to the basis $\{\boldsymbol{a}_1, \boldsymbol{a}_2\}$ by the set $\mathbb{L}$, and its symmetry group is $Dg80 = D_{6h}T$, where T is the translational group $T = \{\alpha_1\boldsymbol{a}_1 + \alpha_2\boldsymbol{a}_2 | (\alpha_1, \alpha_2) \in \mathbb{Z}^2\}$.

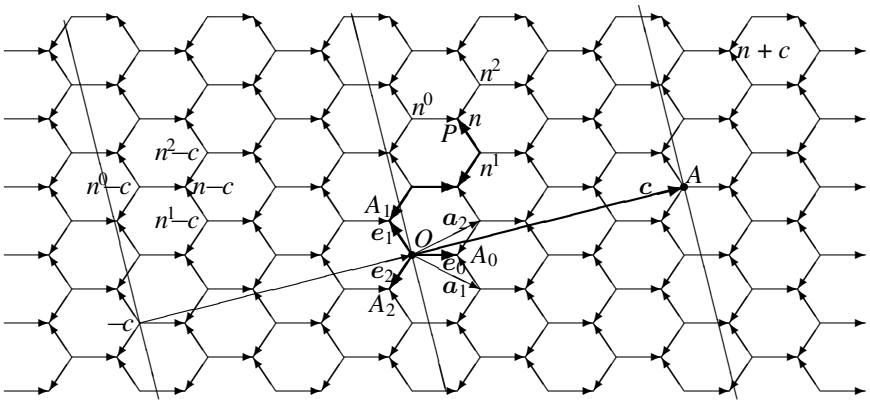

Figure 1. The *honeycomb lattice* $\mathcal{L}$ can be generated by constructing alternately representatives of $\boldsymbol{e}_0, \boldsymbol{e}_1, \boldsymbol{e}_2$ and of $\overline{\boldsymbol{e}}_0, \overline{\boldsymbol{e}}_1, \overline{\boldsymbol{e}}_2$ in the last obtained points. The point P can be described by the sequence $\boldsymbol{e}_1\overline{\boldsymbol{e}}_2\boldsymbol{e}_0\overline{\boldsymbol{e}}_2\boldsymbol{e}_1$. The vector $\boldsymbol{c}$ (in this case, $\boldsymbol{c} = \boldsymbol{a}_1 + 3\boldsymbol{a}_2 = 4\boldsymbol{e}_0 - \boldsymbol{e}_1 - 3\boldsymbol{e}_2$) defines an equivalence relation on $\mathcal{L}$.

Instead of the basis $\{\boldsymbol{a}_1, \boldsymbol{a}_2\}$ we have the possibility to use the vectors $\boldsymbol{e}_0, \boldsymbol{e}_1, \boldsymbol{e}_2$. This leads to a description which is useful in the study of random walks, and will be presented in detail.

Theorem 2. *We have* $\mathcal{L} = \{n_0\boldsymbol{e}_0 + n_1\boldsymbol{e}_1 + n_2\boldsymbol{e}_2 | (n_0, n_1, n_2) \in \mathcal{M}\}$.

Proof. Let $\overline{\boldsymbol{e}}_0 = -\boldsymbol{e}_0, \overline{\boldsymbol{e}}_1 = -\boldsymbol{e}_1, \overline{\boldsymbol{e}}_2 = -\boldsymbol{e}_2$. The honeycomb lattice $\mathcal{L}$ can be generated as follows (figure 1). The origin O of the plane belongs to $\mathcal{L}$. By starting from O we construct the oriented segments $\overrightarrow{OA}_0$, $\overrightarrow{OA}_1$, $\overrightarrow{OA}_2$ corresponding to the vectors $\boldsymbol{e}_0, \boldsymbol{e}_1, \boldsymbol{e}_2$. The points A_0, A_1, A_2 belong to $\mathcal{L}$. In each of the points A_0, A_1, A_2 considered as a starting point we construct representatives of the vectors $\overline{\boldsymbol{e}}_0, \overline{\boldsymbol{e}}_1, \overline{\boldsymbol{e}}_2$. The endpoints of these oriented segments belong to $\mathcal{L}$. By taking each of the last obtained points as starting point we construct representatives of the vectors $\boldsymbol{e}_0, \boldsymbol{e}_1, \boldsymbol{e}_2$. The endpoints of these oriented segments belong to $\mathcal{L}$. We continue by constructing alternatively representatives of $\boldsymbol{e}_0, \boldsymbol{e}_1, \boldsymbol{e}_2$ and $\overline{\boldsymbol{e}}_0, \overline{\boldsymbol{e}}_1, \overline{\boldsymbol{e}}_2$ in the extremities of the last obtained segments. The extremities of all the segments obtained in this way form the honeycomb lattice $\mathcal{L}$.

Each point $P \in \mathcal{L}$ can be described by using a formal sequence

$$\gamma = \boldsymbol{e}_{i_1}\overline{\boldsymbol{e}}_{i_2}\boldsymbol{e}_{i_3}\overline{\boldsymbol{e}}_{i_4} \ldots \boldsymbol{e}'_{i_k} \tag{7}$$

where $e'_{i_k} = e_{i_k}$ if k is odd, $e'_{i_k} = \overline{e}_{i_k}$ if k is even, and

$$\overrightarrow{OP} = e_{i_1} - e_{i_2} + e_{i_3} - e_{i_4} + \cdots + (-1)^{k-1} e_{i_k}.$$

Two sequences γ and γ' describe the same point if and only if one of them can be obtained from the other one by using the following operations:

$$\ldots e_i \overline{e}_j e_k \ldots \longrightarrow \ldots e_k \overline{e}_j e_i \ldots$$

(permutation of two neighbouring non-barred components),

$$\ldots \overline{e}_i e_j \overline{e}_k \ldots \longrightarrow \ldots \overline{e}_k e_j \overline{e}_i \ldots$$

(permutation of two neighbouring barred components),

$$\ldots e_i \overline{e}_j e_j \overline{e}_k \ldots \longrightarrow \ldots e_i \overline{e}_k \ldots \qquad \text{or} \qquad \ldots \overline{e}_i e_j \overline{e}_j e_k \ldots \longrightarrow \ldots \overline{e}_i e_k \ldots$$

(elimination of a sequence of the form $\overline{e}_j e_j$ or $e_j \overline{e}_j$),

$$\ldots e_i \overline{e}_k \ldots \longrightarrow \ldots e_i \overline{e}_j e_j \overline{e}_k \ldots \qquad \text{or} \qquad \ldots \overline{e}_i e_k \ldots \longrightarrow \ldots \overline{e}_i e_j \overline{e}_j e_k \ldots$$

(insertion of a sequence of the form $\overline{e}_j e_j$ or $e_j \overline{e}_j$). In this case we write $\gamma \sim \gamma'$. The relation '$\sim$' is an equivalence relation on the space

$$\mathcal{F} = \{\gamma = e_{i_1} \overline{e}_{i_2} e_{i_3} \overline{e}_{i_4} \ldots e'_{i_k} | k \in \mathbb{N}, i_1, i_2, \ldots, i_k \in \{0, 1, 2\}\}$$

of all the sequences (7), and we can identify $\mathcal{L}$ with the corresponding factor set, that is, $\mathcal{L} = \mathcal{F}/\sim$. If we associate to each sequence $\gamma = e_{i_1} \overline{e}_{i_2} e_{i_3} \overline{e}_{i_4} \ldots e'_{i_k}$ the element $(n_0, n_1, n_2) \in \mathbb{Z}^3$, where n_j is the difference between the number of appearances of e_j and the number of appearances of $\overline{e}_j$ in γ, then γ corresponds to the point $n_0 e_0 + n_1 e_1 + n_2 e_2$, and the mapping $\mathcal{L} \longrightarrow \mathcal{M} : \gamma \mapsto (n_0, n_1, n_2)$ is a bijection. □

Since $e_0 = (a_1 + a_2)/3$, $e_1 = (-2a_1 + a_2)/3$, $e_2 = (a_1 - 2a_2)/3$ we obtain

$$n_0 e_0 + n_1 e_1 + n_2 e_2 = \tfrac{1}{3}(n_0 - 2n_1 + n_2) a_1 + \tfrac{1}{3}(n_0 + n_1 - 2n_2) a_2. \tag{8}$$

The correspondence between the two descriptions of $\mathcal{L}$ is given by the bijection

$$\mathcal{M} \longrightarrow \mathbb{L} : (n_0, n_1, n_2) \mapsto \left(\tfrac{1}{3}(n_0 - 2n_1 + n_2), \tfrac{1}{3}(n_0 + n_1 - 2n_2)\right) \tag{9}$$

the inverse of which is

$$\mathbb{L} \longrightarrow \mathcal{M} : (\alpha_1, \alpha_2) \mapsto \begin{cases} (\alpha_1 + \alpha_2, -\alpha_1, -\alpha_2) & \text{if} \quad (\alpha_1, \alpha_2) \in \mathbb{Z}^2 \\ \left(\alpha_1 + \alpha_2 + \frac{1}{3}, -\alpha_1 + \frac{1}{3}, -\alpha_2 + \frac{1}{3}\right) & \text{if} \quad (\alpha_1, \alpha_2) \in \mathbb{Z}^2 + \left(\frac{1}{3}, \frac{1}{3}\right). \end{cases}$$

If at least one of n and m belongs to $\mathcal{T}$ then

$$\sum_{i=0}^{2} n_i m_i + \sum_{i \neq j} n_i m_j = (n_0 + n_1 + n_2)(m_0 + m_1 + m_2) = 0$$

whence

$$\langle n_0 e_0 + n_1 e_1 + n_2 e_2, m_0 e_0 + m_1 e_1 + m_2 e_2 \rangle = \tfrac{3}{2}(n_0 m_0 + n_1 m_1 + n_2 m_2). \tag{10}$$

The honeycomb lattice can be defined in terms of the strip projection method [7, 15, 18] in a natural way. The vector subspaces

$$\begin{aligned} \mathbb{E}_3^{\parallel} &= \{(x_0, x_1, x_2) \in \mathbb{E}_3 | x_0 + x_1 + x_2 = 0\} \\ \mathbb{E}_3^{\perp} &= \{(x_0, x_1, x_2) \in \mathbb{E}_3 | x_0 = x_1 = x_2\} \end{aligned} \tag{11}$$

of the Euclidean space $\mathbb{E}_3$ are orthogonal, and $\mathbb{E}_3 = \mathbb{E}_3^{\parallel} \oplus \mathbb{E}_3^{\perp}$. For each $x \in \mathbb{E}_3$ there exist $x^{\parallel} \in \mathbb{E}_3^{\parallel}$ and $x^{\perp} \in \mathbb{E}_3^{\perp}$ uniquely determined such that $x = x^{\parallel} + x^{\perp}$. Denoting

$$\begin{aligned} \boldsymbol{e}_0' &= (1,0,0)^{\parallel} = (\tfrac{2}{3}, -\tfrac{1}{3}, -\tfrac{1}{3}) \\ \boldsymbol{e}_1' &= (0,1,0)^{\parallel} = (-\tfrac{1}{3}, \tfrac{2}{3}, -\tfrac{1}{3}) \\ \boldsymbol{e}_2' &= (0,0,1)^{\parallel} = (-\tfrac{1}{3}, -\tfrac{1}{3}, \tfrac{2}{3}) \end{aligned} \tag{12}$$

we find $(x_0, x_1, x_2)^{\parallel} = x_0\boldsymbol{e}_0' + x_1\boldsymbol{e}_1' + x_2\boldsymbol{e}_2'$.

Let $S = \{x \in \mathbb{E}_3 | x^{\perp} \in W\}$ be the strip corresponding to the window $W = \{(\alpha, \alpha, \alpha) | \alpha \in [0, \frac{1}{3}]\}$. One can remark that $\mathcal{M} = S \cap \mathbb{Z}^3$. Since the endpoints of the vectors $\boldsymbol{e}_0', \boldsymbol{e}_1', \boldsymbol{e}_2'$ belonging to the plane $\mathbb{E}_3^{\parallel}$ are the vertices of an equilateral triangle, the set

$$\{x^{\parallel} | x \in \mathbb{Z}^3, x^{\perp} \in W\} = \{x_0\boldsymbol{e}_0' + x_1\boldsymbol{e}_1' + x_2\boldsymbol{e}_2' | x \in \mathcal{M}\} \tag{13}$$

represents a honeycomb lattice.

The bijection $\mathcal{L} \longrightarrow \mathcal{M}$ obtained in the proof of the theorem allows us to identify the honeycomb lattice with its abstract model, that is, to consider directly $\mathcal{L} = \{n = (n_0, n_1, n_2) \in \mathbb{Z}^3 | n_0 + n_1 + n_2 \in \{0; 1\}\}$. The nearest neighbours of the point described by $n \in \mathcal{M}$ are exactly the points corresponding to n^0, n^1, n^2. Each sequence γ corresponding to n represents a random walk on $\mathcal{L}$ from $o = (0, 0, 0)$ to n.

4. Random walks on the honeycomb lattice

The number $\mathcal{N}_k$ of all the k-step walks connecting the points $(0, 0)$ and (n_1, n_2) on the Cartesian lattice graph $\mathbb{Z}^2$ coincides with the coefficient of $x_1^{n_1}x_2^{n_2}$ in the expression $(x_1 + x_1^{-1} + x_2 + x_2^{-1})^k$. Since

$$\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}k\varphi}\,\mathrm{d}\varphi = \begin{cases} 0 & \text{for} \quad k \neq 0 \\ 2\pi & \text{for} \quad k = 0 \end{cases} \tag{14}$$

the number $\mathcal{N}_k$ is given by the formula [14, pp 60–1]

$$\mathcal{N}_k = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \left(\mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{-\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2} + \mathrm{e}^{-\mathrm{i}\varphi_2}\right)^k \mathrm{e}^{-\mathrm{i}(n_1\varphi_1 + n_2\varphi_2)}\,\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2. \tag{15}$$

The description of the honeycomb lattice presented in the previous section allows us to express the number $\mathcal{N}_k(m, n)$ of all the k-step walks from $m \in \mathcal{L}$ to $n \in \mathcal{L}$ in a similar way.

Theorem 3. *We have*

$$\mathcal{N}_k(o, n) = \begin{cases} \left\langle \left|\mathrm{e}^{\mathrm{i}\varphi_0} + \mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2}\right|^k \mathrm{e}^{-\mathrm{i}n\varphi} \right\rangle & \text{if } k \text{ is even} \\ \left\langle \left|\mathrm{e}^{\mathrm{i}\varphi_0} + \mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2}\right|^{k-1} \left(\mathrm{e}^{\mathrm{i}\varphi_0} + \mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2}\right) \mathrm{e}^{-\mathrm{i}n\varphi} \right\rangle & \text{if } k \text{ is odd} \end{cases} \tag{16}$$

where $o = (0, 0, 0)$, $n\varphi = n_0\varphi_0 + n_1\varphi_1 + n_2\varphi_2$, *and*

$$\langle f(\varphi) \rangle = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} f(\varphi)\,\mathrm{d}\varphi_0\,\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2. \tag{17}$$

Proof. There is a bijective correspondence between the k-step walks from o to $n = (n_0, n_1, n_2)$ and the sequences $\boldsymbol{e}_{i_1}\overline{\boldsymbol{e}}_{i_2}\boldsymbol{e}_{i_3}\overline{\boldsymbol{e}}_{i_4}\ldots\boldsymbol{e}_{i_k}'$ satisfying the relation

$$\boldsymbol{e}_{i_1} - \boldsymbol{e}_{i_2} + \boldsymbol{e}_{i_3} - \boldsymbol{e}_{i_4} + \cdots + (-1)^{k+1}\boldsymbol{e}_{i_k} = n_0\boldsymbol{e}_0 + n_1\boldsymbol{e}_1 + n_2\boldsymbol{e}_2.$$

If k is even, $k = 2j$, then $\mathcal{N}_k(o, n)$ is the coefficient of $x_0^{n_0}x_1^{n_1}x_2^{n_2}$ in

$$((x_0 + x_1 + x_2)(x_0^{-1} + x_1^{-1} + x_2^{-1}))^j$$

and if k is odd, $k = 2j + 1$, then $\mathcal{N}_k(o, n)$ is the coefficient of $x_0^{n_0}x_1^{n_1}x_2^{n_2}$ in

$$((x_0 + x_1 + x_2)(x_0^{-1} + x_1^{-1} + x_2^{-1}))^j(x_0 + x_1 + x_2). \qquad \square$$

Let $\mathcal{W}_k(m, n)$ be the set of all the k-step walks from m to n. For any $m \in \mathcal{L}$, the transformation

$$g : \mathcal{L} \longrightarrow \mathcal{L} \qquad g(n_0, n_1, n_2) = \begin{cases} (n_0 - m_0, n_1 - m_1, n_2 - m_2) & \text{if} \quad \nu(m) = 1 \\ (m_0 - n_0, m_1 - n_1, m_2 - n_2) & \text{if} \quad \nu(m) = -1 \end{cases} \tag{18}$$

belongs to G, and $gm = o$. It transforms each k-step walk from m to n into a k-step walk from $gm = o$ to gn. Since this transformation from $\mathcal{W}_k(m, n)$ to $\mathcal{W}_k(o, gn)$ is bijective, we have $\mathcal{N}_k(m, n) = \mathcal{N}_k(o, gn)$.

In a very similar way one can obtain a mathematical model for diamond-type crystals and a formula for the number of k-step walks between given sites by using the metric space $(\mathcal{D}, \delta)$, where

$$\begin{aligned} &\mathcal{D} = \{n = (n_0, n_1, n_2, n_3) \in \mathbb{Z}^4 | n_0 + n_1 + n_2 + n_3 \in \{0, 1\}\} \\ &\delta : \mathcal{D} \times \mathcal{D} \longrightarrow \mathbb{N} \qquad \delta(n, m) = |n_0 - m_0| + |n_1 - m_1| + |n_2 - m_2| + |n_3 - m_3| \end{aligned} \tag{19}$$

as an abstract mathematical model [3, 4]. The group of all the isometries of this metric space is isomorphic to the space group $O_h^7 = Fd\bar{3}m$.

5. Single-wall carbon nanotubes

The carbon nanotubes, discovered by Iijima [10] in 1991, form an important class of materials with many potential applications. Extensive experimental and theoretical investigations have been carried out on the mechanical and electronic properties of these novel fibres [5, 6, 9, 12, 13, 21]. They exhibit variations in electronic transport from metallic to semiconducting with narrow and moderate band gaps depending on the diameter of the tubule and the arrangement of the carbon hexagons. Their structure observed by high-resolution transmission electron microscopy can be visualized as the structure obtained by rolling a graphene sheet (that is, a sheet containing a honeycomb lattice) such that the origin O and a lattice point A are folded one onto the other (figure 1). Such a tubule is determined by the corresponding vector $\vec{OA} = \alpha_1\boldsymbol{a}_1 + \alpha_2\boldsymbol{a}_2 \in T$, called the *chiral vector.* Without loss of generality, we can consider only the cases where $\alpha_1 \geqslant \alpha_2 \geqslant 0$. A tubule with $\alpha_1 = \alpha_2$ is called an *armchair tubule*, and a tubule with $\alpha_2 = 0$ is called a *zig-zag tubule.*

In our three-axes description, a carbon nanotube is described by the element $c = (c_0, c_1, c_2) \in \mathcal{T}$ satisfying the relation $\vec{OA} = c_0\boldsymbol{e}_0 + c_1\boldsymbol{e}_1 + c_2\boldsymbol{e}_2$, called the *chirality* of the tubule. As in the case of the usual description, we can restrict ourselves to $0 \leqslant c_1 \leqslant c_2$. An armchair tubule corresponds to $c_1 = c_2$, and a zig-zag tubule to $c_1 = 0$.

After the graphene sheet rolling, the points $\ldots, n - 2c, n - c, n, n + c, n + 2c, \ldots$ are folded onto one another, for any $n = (n_0, n_1, n_2) \in \mathcal{L}$. Thus, each point of the set

$$[n_0, n_1, n_2] = n + \mathbb{Z}c = \{(n_0 + jc_0, n_1 + jc_1, n_2 + jc_2) | j \in \mathbb{Z}\} \tag{20}$$

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.

From a mathematical point of view, our model is a subset of the factor space $\mathbb{Z}^3/(\mathbb{Z}c) = \{(n_0, n_1, n_2) + \mathbb{Z}c | n_0, n_1, n_2 \in \mathbb{Z}\}$, namely,

$$\tilde{\mathcal{L}}_c = \left\{[n_0, n_1, n_2] \in \mathbb{Z}^3/(\mathbb{Z}c) | n_0 + n_1 + n_2 \in \{0; 1\}\right\}. \tag{21}$$

We remark that this set is well defined since the condition $n_0 + n_1 + n_2 \in \{0; 1\}$ we impose to $[n_0, n_1, n_2]$ does not depend on the representative we choose. Indeed,

$$(n_0 + jc_0) + (n_1 + jc_1) + (n_2 + jc_2) = n_0 + n_1 + n_2$$

for all $j \in \mathbb{Z}$. Each point $[n] \in \tilde{\mathcal{L}}_c$ has three *first neighbours*, namely, $[n^0]$, $[n^1]$, $[n^2]$, and six *second neighbours*, namely, $[n^{01}]$, $[n^{10}]$, $[n^{02}]$, $[n^{20}]$, $[n^{12}]$, $[n^{21}]$.

In order to illustrate the formalism of our mathematical model we present (in a rather formal way) some known results concerning the symmetry group [5, 12, 13, 21] and the band structure [9, 21] of carbon nanotubes. A symmetry transformation of the honeycomb lattice $\mathcal{L} \longrightarrow \mathcal{L} : n \mapsto gn$ defines the *symmetry transformation* $\tilde{\mathcal{L}}_c \longrightarrow \tilde{\mathcal{L}}_c : [n] \mapsto [gn]$ of the carbon nanotube $\tilde{\mathcal{L}}_c$ if $[n] = [m] \Longrightarrow [gn] = [gm]$, that is, if $n - m \in \mathbb{Z}c \Longrightarrow gn - gm \in \mathbb{Z}c$.

Theorem 4. *The mappings*

$$\begin{aligned} &t : \tilde{\mathcal{L}}_c \longrightarrow \tilde{\mathcal{L}}_c : [n_0, n_1, n_2] \mapsto [n_0 + t_0, n_1 + t_1, n_2 + t_2] \\ &\{i|\tau\} : \tilde{\mathcal{L}}_c \longrightarrow \tilde{\mathcal{L}}_c : [n_0, n_1, n_2] \mapsto [-n_0 + 1, -n_1, -n_2] \end{aligned} \tag{22}$$

are symmetry transformations of $\tilde{\mathcal{L}}_c$ for all $t \in \mathcal{T}$.

Proof. We have $(n + t) - (m + t) = n - m$ and $\{i|\tau\}n - \{i|\tau\}m = m - n$. □

Additional symmetries may appear for the zig-zag and armchair tubules. Since $(c_1 - c_2)c_0 + (c_2 - c_0)c_1 + (c_0 - c_1)c_2 = 0$, in view of the relation (10) the vector corresponding to $b = (c_1 - c_2, c_2 - c_0, c_0 - c_1)$ is orthogonal to the vector corresponding to c. It defines a translation in the direction of the axis of the tubule, called *a pure translation.* Let d be the greatest common divisor of c_0, c_1, c_2, and let $c_0 = dc_0'$, $c_1 = dc_1'$, $c_2 = dc_2'$. Generally, $b' = (c_1' - c_2', c_2' - c_0', c_0' - c_1')$ is not the shortest pure translation since in the case where $c_1' - c_2'$ is a multiple of 3, the numbers

$$c_2' - c_0' = (c_1' - c_2') + 3c_2' \qquad c_0' - c_1' = (c_1' - c_2') - 3c_1'$$

are also multiples of 3. The length of b' can be computed by using (10).

Let $\alpha, \beta_0, \beta_1, \beta_2$ be four real numbers. The relation

$$(H\psi)[n] = \alpha\psi[n] + \sum_{j=0}^{2} \beta_j \psi[n^j] \tag{23}$$

defines a linear operator on the space of all complex functions $\psi : \tilde{\mathcal{L}}_c \longrightarrow \mathbb{C}$. A number E belongs to the *spectrum* of H if there is a bounded non-trivial function $\psi : \tilde{\mathcal{L}}_c \longrightarrow \mathbb{C}$ such that $H\psi = E\psi$.

Theorem 5. *For any* $k = (k_0, k_1, k_2) \in \mathbb{R}^3$ *satisfying the conditions*

$$k_0 + k_1 + k_2 = 0 \qquad k_0c_0 + k_1c_1 + k_2c_2 \in 2\pi\mathbb{Z} \tag{24}$$

the numbers

$$E_{1,2}(k) = \alpha \pm [\beta_0^2 + \beta_1^2 + \beta_2^2 + 2\beta_0\beta_1\cos(k_0 - k_1) + 2\beta_1\beta_2\cos(k_1 - k_2) + 2\beta_2\beta_0\cos(k_2 - k_0)]^{1/2} \tag{25}$$

belong to the spectrum of H.

Proof. If k satisfies the conditions (24) then the function $\psi_k : \tilde{\mathcal{L}}_c \longrightarrow \mathbb{C}$

$$\psi_k[n] = \begin{cases} a\mathrm{e}^{\mathrm{i}(k_0n_0+k_1n_1+k_2n_2)} & \text{if} \quad \nu(n) = 1 \\ b\mathrm{e}^{\mathrm{i}(k_0n_0+k_1n_1+k_2n_2)} & \text{if} \quad \nu(n) = -1 \end{cases} \tag{26}$$

where a and b are two real constants, is well defined and the relation $H\psi_k = E\psi_k$ is verified if and only if (a, b) is a solution of the system of equations

$$\alpha a + (\beta_0\mathrm{e}^{\mathrm{i}k_0} + \beta_1\mathrm{e}^{\mathrm{i}k_1} + \beta_2\mathrm{e}^{\mathrm{i}k_2})b = Ea$$
$$\alpha b + (\beta_0\mathrm{e}^{-\mathrm{i}k_0} + \beta_1\mathrm{e}^{-\mathrm{i}k_1} + \beta_2\mathrm{e}^{-\mathrm{i}k_2})a = Eb.$$

This system has non-trivial solutions if and only if

$$\begin{vmatrix} \alpha - E & \beta_0\mathrm{e}^{\mathrm{i}k_0} + \beta_1\mathrm{e}^{\mathrm{i}k_1} + \beta_2\mathrm{e}^{\mathrm{i}k_2} \\ \beta_0\mathrm{e}^{-\mathrm{i}k_0} + \beta_1\mathrm{e}^{-\mathrm{i}k_1} + \beta_2\mathrm{e}^{-\mathrm{i}k_2} & \alpha - E \end{vmatrix} = 0$$

that is, if and only if E is one of the numbers

$$E_{1,2}(k) = \alpha \pm |\beta_0\mathrm{e}^{\mathrm{i}k_0} + \beta_1\mathrm{e}^{\mathrm{i}k_1} + \beta_2\mathrm{e}^{\mathrm{i}k_2}|.$$

This relation is equivalent to (25). □

If we neglect the differences that arise because of different C–C bonding directions on the tubule surface, that is, if we consider $\beta_0 = \beta_1 = \beta_2 = \beta$ then we find

$$E_{1,2}(k) = \alpha \pm \beta[3 + 2\cos(k_0 - k_1) + 2\cos(k_1 - k_2) + 2\cos(k_2 - k_0)]^{1/2}. \tag{27}$$

The relations (24) defines a countable family of straight lines orthogonal to the vector corresponding to c. Evidently, we can restrict ourselves to the vectors k belonging to the first Brillouin zone.

6. Random walks on carbon nanotubes

The number $\tilde{\mathcal{N}}_k([m], [n])$ of all the k-step walks from $[m]$ to $[n]$ on a carbon nanotube can be expressed in a simple way by using the model presented in the previous section.

Theorem 6. *We have*

$$\tilde{\mathcal{N}}_k([o], [n]) = \sum_{j\in\mathbb{Z}} \mathcal{N}_k(o, n + jc) \tag{28}$$

with $\mathcal{N}_k(o, n + jc)$ *given by theorem 3.*

Proof. Each k-step walk from o to $n + jc$ on the graphene sheet corresponds after rolling it to a k-step walk from $[o]$ to $[n]$ on the carbon nanotube $\tilde{\mathcal{L}}_c$. There is a one-to-one correspondence between the set of all k-step walks from $[o]$ to $[n]$ on the carbon nanotube and the union $\cup_{j\in\mathbb{Z}}\mathcal{W}_k(o, n + jc)$. Evidently, the number of non-empty sets $\mathcal{W}_k(o, n + jc)$ is finite. □

For any $m \in \mathcal{L}$, using the transformation (18) we can consider the symmetry transformation $\tilde{\mathcal{L}}_c \longrightarrow \tilde{\mathcal{L}}_c : [n] \mapsto [gn]$ of $\tilde{\mathcal{L}}_c$, and hence $\tilde{\mathcal{N}}_k([m], [n]) = \tilde{\mathcal{N}}_k([o], [gn])$.

7. Finite graphs associated with a quasicrystal

Some finite graphs can be associated in a natural way with a quasicrystal defined in terms of the strip projection method. In order to simplify the notation we shall consider the case of a one-dimensional quasicrystal, but extensions to other quasicrystals can be immediately obtained. Let $\mathbb{E}_2 = \mathbb{E}_2^{\parallel} \oplus \mathbb{E}_2^{\perp}$ be a decomposition of $\mathbb{E}_2$ into a sum of two orthogonal one-dimensional subspaces (figure 2). For each $\boldsymbol{x} \in \mathbb{E}_2$ there are the elements $\boldsymbol{x}^{\parallel} \in \mathbb{E}_2^{\parallel}$ and $\boldsymbol{x}^{\perp} \in \mathbb{E}_2^{\perp}$ uniquely determined such that $\boldsymbol{x} = \boldsymbol{x}^{\parallel} + \boldsymbol{x}^{\perp}$. Consider a segment $W \subset \mathbb{E}_2^{\perp}$ of finite length (the window) and the corresponding quasicrystal

$$\mathcal{Q} = \left\{ \boldsymbol{x}^{\parallel} \,\middle|\, \boldsymbol{x} \in \mathbb{Z}^2, \boldsymbol{x}^{\perp} \in W \right\}.$$

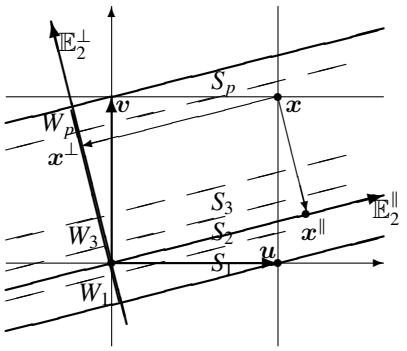

Figure 2. The partition $S = S_1 \cup S_2 \cup \ldots \cup S_p$ of the strip $S = \{\boldsymbol{x} \in \mathbb{R}^2 | \boldsymbol{x}^{\perp} \in W\}$ corresponding to a partition $W = W_1 \cup W_2 \cup \ldots \cup W_p$ of the window W determines a partition $\mathcal{Q} = \mathcal{Q}_1 \cup \mathcal{Q}_2 \cup \ldots \cup \mathcal{Q}_p$ of the *quasicrystal* $\mathcal{Q} = \{\boldsymbol{x}^{\parallel} | \boldsymbol{x} \in \mathbb{Z}^2, \boldsymbol{x}^{\perp} \in W\}$.

Each equidistant partition $W = W_1 \cup W_2 \cup W_3 \cup \ldots \cup W_p$ of the segment W determines a partition of the corresponding strip $S = S_1 \cup S_2 \cup \ldots \cup S_p$, where $S_j = \{\boldsymbol{x} \in \mathbb{R}^2 | \boldsymbol{x}^{\perp} \in W_j\}$, and indirectly a partition of the set $\mathcal{Q}$

$$\mathcal{Q} = \mathcal{Q}_1 \cup \mathcal{Q}_2 \cup \mathcal{Q}_3 \cup \ldots \cup \mathcal{Q}_p \tag{29}$$

where $\mathcal{Q}_j = \left\{ \boldsymbol{x}^{\parallel} \,\middle|\, \boldsymbol{x} \in \mathbb{Z}^2, \boldsymbol{x}^{\perp} \in W_j \right\}$.

It is known [15] that the occurrence frequency of the points of $\mathcal{Q}_j$ in $\mathcal{Q}$ is $|W_j|/|W|$, where $|W_j|$ is the length of W_j and $|W|$ is the length of W.

Let $\boldsymbol{u} = (1, 0)$ and $\boldsymbol{v} = (0, 1)$. The nearest arithmetical neighbours of a point $\boldsymbol{x} = (x_1, x_2) \in \mathbb{Z}^2$ are $\boldsymbol{x} + \boldsymbol{u}, \boldsymbol{x} - \boldsymbol{u}, \boldsymbol{x} + \boldsymbol{v}, \boldsymbol{x} - \boldsymbol{v}$. If $\boldsymbol{x} \in \mathbb{Z}^2 \cap S_j$ then

$$\begin{aligned} \boldsymbol{x} \pm \boldsymbol{u} \in S_j \pm \boldsymbol{u} &= \left\{ \boldsymbol{y} \in \mathbb{R}^2 \,\middle|\, \boldsymbol{y}^{\perp} \in W_j \pm \boldsymbol{u}^{\perp} \right\} \\ \boldsymbol{x} \pm \boldsymbol{v} \in S_j \pm \boldsymbol{v} &= \left\{ \boldsymbol{y} \in \mathbb{R}^2 \,\middle|\, \boldsymbol{y}^{\perp} \in W_j \pm \boldsymbol{v}^{\perp} \right\}. \end{aligned} \tag{30}$$

If p is large enough, then the sets $W_j + \boldsymbol{u}^{\perp}$, $W_j - \boldsymbol{u}^{\perp}$, $W_j + \boldsymbol{v}^{\perp}$, $W_j - \boldsymbol{v}^{\perp}$ are disjoint, and each set W_i can intersect at most one of the sets $W_j + \boldsymbol{u}^{\perp}$, $W_j - \boldsymbol{u}^{\perp}$, $W_j + \boldsymbol{v}^{\perp}$, $W_j - \boldsymbol{v}^{\perp}$.

Let $W_j' = (W_j + \boldsymbol{u}^{\perp}) \cup (W_j - \boldsymbol{u}^{\perp}) \cup (W_j + \boldsymbol{v}^{\perp}) \cup (W_j - \boldsymbol{v}^{\perp})$, for all $j \in \{1, 2, \ldots, p\}$. The set $\mathcal{Q}_i$ can contain a nearest arithmetical neighbour of a point $\boldsymbol{x}^{\parallel} \in \mathcal{Q}_j$ only if $W_i \cap W_j' \neq \emptyset$. In addition, we can consider that $\alpha_{ij} = |W_i \cap W_j'|/|W \cap W_j'|$ is the probability for a point belonging to $\mathcal{Q}_j$ to have a nearest neighbour belonging to $\mathcal{Q}_i$. The points of $\mathcal{Q}$ are the vertices of a tiling of the real axis with two tiles. If the distance between $\boldsymbol{x}^{\perp}$ and $\boldsymbol{y}^{\perp}$ is small then,

generally, the local configurations of the neighbours of $\boldsymbol{x}^{\parallel}$ and $\boldsymbol{y}^{\parallel}$ are similar. For p large enough, the local configurations of the points belonging to the same set $\mathcal{Q}_j$ are similar, for almost all $\mathcal{Q}_j$.

The numbers α_{ij} allow us to define the finite graph

$$\mathcal{G} = (\{\mathcal{Q}_1, \mathcal{Q}_2, \ldots, \mathcal{Q}_p\}, \{\{\mathcal{Q}_i, \mathcal{Q}_j\} | \alpha_{ij} \neq 0\}) \tag{31}$$

with the vertices $\mathcal{Q}_1, \mathcal{Q}_2, \ldots, \mathcal{Q}_p$, and to consider the projector $\pi : \mathcal{Q} \longrightarrow \{\mathcal{Q}_1, \mathcal{Q}_2, \ldots, \mathcal{Q}_p\}$, $\pi(x) = \mathcal{Q}_j$ for $x \in \mathcal{Q}_j$. The projection of a random walk on $\mathcal{Q}$ is a random walk on $\mathcal{G}$. In order to pass from $\mathcal{Q}$ to $\mathcal{G}$ it is sufficient not to distinguish the points of $\mathcal{Q}$ belonging to the same subset $\mathcal{Q}_j$.

The adjacency matrix of $\mathcal{G}$ is $\mathcal{A} = (a_{ij})_{1 \leqslant i,j \leqslant p}$, where $a_{ij} = 1$ if $\alpha_{ij} \neq 0$, and $a_{ij} = 0$ if $\alpha_{ij} = 0$. The number $w_n(\mathcal{Q}_i \to \mathcal{Q}_j)$ of n-step walks on $\mathcal{G}$ from $\mathcal{Q}_i$ to $\mathcal{Q}_j$ is [14]

$$w_n(\mathcal{Q}_i \to \mathcal{Q}_j) = (\mathcal{A}^n)_{ij}. \tag{32}$$

The number α_{ij} can be regarded as the probability for a generic point of $\mathcal{Q}_i$ to have a first neighbour belonging to $\mathcal{Q}_j$. This suggests that we should associate with each line $\{\mathcal{Q}_i, \mathcal{Q}_j\}$ the weight α_{ij}, and to define the weight of a walk on $\mathcal{G}$ as the product of the weights of the corresponding steps. The sum $\tilde{w}_n(\mathcal{Q}_i \to \mathcal{Q}_j)$ of the weights of all the n-step walks from $\mathcal{Q}_i$ to $\mathcal{Q}_j$ is

$$\tilde{w}_n(\mathcal{Q}_i \to \mathcal{Q}_j) = (\mathcal{B}^n)_{ij} \tag{33}$$

where $\mathcal{B} = (\alpha_{ij})_{1 \leqslant i,j \leqslant p}$ is the corresponding adjacency weight matrix. We think that the numbers $\tilde{w}_n(\mathcal{Q}_i \to \mathcal{Q}_j)$ might contain some statistical information concerning the random walks on the quasicrystal $\mathcal{Q}$.

8. Conclusions

In the case of certain problems concerning the hexagonal crystals it is convenient to use an additional axis [2, 20]. In this paper we try to prove that a similar situation occurs in the case of carbon nanotubes. The proposed alternate description seems to be more advantageous than the usual one in the case of certain problems and less advantageous in other cases. The choice of an adequate description may simplify the solution of a problem, and hence, the existence of two or more descriptions may offer some facilities.

The absence of periodicity in the case of quasicrystals leads to important difficulties in the mathematical modelling of these materials. Generally, the quasicrystal is replaced either by a periodic approximant or by a finite fragment generated by using a computer [11, 19]. In the last section we present a different approach which may be useful in problems concerning random walks on quasicrystals.

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