Quantum random walks on diamond-type crystals and carbon nanotubes

2001 J. Phys. A: Math. Gen. 34 5469

(http://iopscience.iop.org/0305-4470/34/27/301)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) 5469–5483 PII: S0305-4470(01)14216-2

Quantum random walks on diamond-type crystals and carbon nanotubes

Nicolae Cotfas

Faculty of Physics, University of Bucharest, PO Box 76-54, Postal Office 76, Bucharest, Romania

E-mail: ncotfas@yahoo.com

Received 25 May 2000, in final form 29 March 2001
Published 29 June 2001
Online at stacks.iop.org/JPhysA/34/5469

Abstract

A class of graphs including models for diamond-type crystals and carbon nanotubes is defined, and some results concerning random walks and symmetry transformations are presented. These graphs may be useful discrete approximants in a path integral approach to physical phenomena occurring in diamond-type crystals and carbon nanotubes. Some details concerning a possible application of Gudder's discrete quantum mechanics to these crystals are analysed.

PACS numbers: 0540F, 6146

1. Introduction

A crystal is a very complicated physical system. The study of the physical phenomena occurring in such a system cannot be done without assuming some rather drastic approximations. In many cases, it is useful [19] to approximate a crystal by a graph: the atoms are the vertices, and the chemical bonds are the edges of the graph. The first purpose of this paper is to present a class of graphs containing models for diamond-type crystals [1,10,24,30] and carbon nanotubes [6, 17, 18, 28, 32]. It is a more general and unitary view on some results published previously [2–4], which may facilitate a transfer of ideas and methods.

Since the movement of an electron (excitation, vacancy, etc) on a crystal can be regarded as a sequence of jumps between neighbouring sites, the random walks are expected to play an important role in the description of physical phenomena occurring in crystals. The second purpose of this paper is to present some mathematical results concerning random walks on our graphs, and to suggest some possible physical interpretations.

It is well known that the diffusion equation has an underlying microscopic model, namely Brownian motion, which can be approximated by random walks on a hypercubic lattice [27]. Consider a point particle which performs an erratic motion on a d-dimensional hypercubic lattice $(\mathbb{Z}h)^d$ with lattice constant h such that within a period of time of length τ, the particle

may proceed along any of the $2d$ directions of the lattice (steps of size h), the probability being $(2d)^{-1}$ in each direction. Denoting $e_1 = (1, 0, \ldots, 0)$, $e_2 = (0, 1, 0, \ldots, 0)$, $\ldots$, $e_d = (0, \ldots, 0, 1)$, and by $P(x, t; x', t')$ the probability that the particle arrives at site x' at time t' after having started from x at time t, we get the relation [27]

$$P(x_0, t_0; x, t+\tau) = \frac{1}{2d}\sum_{j=1}^{d}(P(x_0, t_0; x - he_j, t) + P(x_0, t_0; x + he_j, t)) \tag{1}$$

which can be written as

$$\frac{P(x_0, t_0; x, t+\tau) - P(x_0, t_0; x, t)}{\tau} = \frac{h^2}{2d\tau}\sum_{j=1}^{d}\frac{P(x_0, t_0; x - he_j, t) + P(x_0, t_0; x + he_j, t) - 2P(x_0, t_0; x, t)}{h^2}. \tag{2}$$

For an appropriate choice of the time unit, in the limit $h \to 0$, $\tau \to 0$, this finite difference equation corresponds to the d-dimensional diffusion equation $\frac{\partial}{\partial t}P = \frac{1}{2}\Delta P$, and the considered random walk describes what is called d-dimensional Brownian motion.

If the diffusion takes place inside a crystal, then there is a natural discrete approximant, namely the associated graph, which may be more adequate than the use of a hypercubic lattice. Thus, the study of random walks on the graph corresponding to a crystal may be useful in the description of the diffusion.

It is well known that

$$K(x, t) = (2\pi t)^{-d/2}\exp\left(-x^2/2t\right) \tag{3}$$

where $x^2 = \sum_{j=1}^{d} x_j^2$ is a solution of the diffusion equation, and $K(x, 0) = \lim_{t\to 0} K(x, t) = \delta(x)$. Hence, for a particle starting at the origin at time $t = 0$, the probability of finding it at some later time t within a region $A \subset \mathbb{R}^d$ is $\int_A \mathrm{d}x\, K(x, t)$.

A probabilistic model of Brownian motion is obtained [27] by using a probability space $(\Omega, \mathcal{F}, \boldsymbol{P})$, where the underlying space Ω is the space of all the sample paths $\omega : I \longrightarrow \mathbb{R}^d$ defined on an interval $I \subset \mathbb{R}$: for example $I = [0, \infty)$. The position of the particle at time $\mathrm{s} > 0$ is a random variable $X_\mathrm{s} : \Omega \longrightarrow \mathbb{R}^d$, $X_\mathrm{s}(\omega) = \omega(s)$. For any Borel set $A \subset \mathbb{R}^d$, the event $X_\mathrm{s} \in A$ means that the Brownian particle has passed the 'window' A at time s. The probability measure $A \mapsto \boldsymbol{P}(X_\mathrm{s} \in A) = \int_A \mathrm{d}x\, K(x, s)$, where $X_\mathrm{s} \in A$ stands for the set $\{\omega |\ X_\mathrm{s}(\omega) \in A\}$, is called the *distribution* of X_s.

A stochastic process is a map $s \mapsto X_\mathrm{s}$ defined over some interval, and in order to define such a process it is necessary to indicate how to compute the probabilities of general events, including a rule to determine the probabilities $\boldsymbol{P}(X_{\mathrm{s}_1} \in A_1, \ldots, X_{\mathrm{s}_n} \in A_n)$ of compound events [27]. In the case

$$\begin{aligned}\boldsymbol{P}(X_{s_1} \in A_1, \ldots, X_{s_n} \in A_n) &= \int_{A_n}\mathrm{d}x_n \ldots \int_{A_2}\mathrm{d}x_2\int_{A_1}\mathrm{d}x_1\, K(x_n - x_{n-1}, s_n - s_{n-1})\ldots \\ &\quad \times K(x_2 - x_1, s_2 - s_1)K(x_1, s_1)\end{aligned} \tag{4}$$

with K given by (3) and

$$\boldsymbol{P}(X_0 \in A_0) = \begin{cases} 1 & \text{if} \quad 0 \in A_0 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

the stochastic process X_s is the *Wiener process*.

If in the diffusion equation we replace the time variable t by an imaginary time variable $\mathrm{i}t$, then the obtained equation $\frac{\partial}{\partial(\mathrm{i}t)}P = \frac{1}{2}\Delta P$, coincides with the Schrödinger equation of a free

particle $\mathrm{i}\frac{\partial}{\partial t}\psi = -\frac{1}{2}\Delta\psi$, written in a suitable system of physical units. In addition, it follows that the wavefunction ψ satisfies the relation

$$\psi(x,t) = \int \mathrm{d}x'\, K(x-x', \mathrm{i}t)\psi(x',0). \tag{6}$$

The complex transition function

$$K(x,\mathrm{i}t) = \begin{cases} (2\pi \mathrm{i}t)^{-d/2}\exp(-x^2/2\mathrm{i}t) & \text{if} \quad t \neq 0 \\ \delta(x) & \text{if} \quad t = 0 \end{cases} \tag{7}$$

obtained from $K(x,t)$ by the analytic continuation $t \mapsto \mathrm{i}t$ is no longer positive but complex and of oscillatory character. The behaviour of the solutions of diffusion and Schrödinger equation is qualitatively very different [25–27]. The Wiener measure is transformed into a complex pseudo-measure.

The mathematical relation existing between the two equations is useful in calculations concerning the Schrödinger equation, but not very useful in the interpretation of the equation itself since the formal analytic continuation does not transfer the associated microscopic model. The random walks of Brownian particles have a correspondence in the Feynman paths [8,27], but the positive Boltzmann weights are replaced by complex numbers and an interpretation in terms of the classical probability is not possible.

There exist several attempts [12, 14, 15, 25, 26] to find an underlying stochastic model for the Schrödinger equation related to this equation as directly as the Brownian motion model is to the diffusion equation. We have seen that Brownian motion is a limit of random walks, and a random walk is associated with a discrete version of the diffusion equation. Gudder [12,14,15] has shown that an analogous situation occurs for the Schrödinger equation: there exists a quantum stochastic process whose associated evolution is given by the free Schrödinger equation.

An outcome of a quantum mechanical measurement is the result of various interfering alternatives each having an amplitude for occurring. The probability of this outcome is the absolute value squared of the sum of these amplitudes [7,8]. Using these two statements as a basic axiom, Gudder has formulated [12, 14, 16] a theory of quantum probability in terms of amplitude functions. Among the quantum stochastic processes defined within this framework there is the so-called *discrete quantum mechanics* [12,13,16].

The starting point of discrete quantum mechanics [16] is a non-empty discrete set S interpreted as a set of 'states' that a quantum particle can occupy. A function $K_1 : S\times S \longrightarrow \mathbb{C}$ is a *stochastic one-step transition amplitude* if for every $s_1, s_2 \in S$ we have

$$\begin{aligned} &\sum_s K_1(s_1,s) = 1 \\ &\sum_s K_1(s_1,s)\overline{K}_1(s_2,s) = \sum_s K_1(s,s_1)\overline{K}_1(s,s_2) = \delta_{s_1 s_2} \end{aligned} \tag{8}$$

where the summations converge absolutely. For $j \in \mathbb{N}$, a *j-path* is a $(j+1)$-tuple $\omega = (s_0, s_1, \ldots, s_j) \in S^{j+1}$. Let $\mathcal{P}_j(S)$ denote the set of j-paths in S and form the sample space $\Omega = \mathcal{P}_N(S)$. Starting from a unit vector $f_0 \in l^2(S)$ representing the initial distribution for a quantum particle we define the amplitude density [16]

$$\begin{aligned} &f : \Omega \longrightarrow \mathbb{C} \\ &f(s_0, s_1, \ldots, s_N) = f_0(s_0)\, K_1(s_0,s_1)\ldots K_1(s_{N-1}, s_N). \end{aligned} \tag{9}$$

For $j = 0, 1, \ldots, N$ define the map

$$X_j : \Omega \longrightarrow S \qquad X_j(s_0, s_1, \ldots, s_N) = s_j \tag{10}$$

which becomes a *measurement* if we consider on S and $X_j^{-1}(s)$ the counting measures [16]. For $j \in \mathbb{N}$ with $1 \leqslant j \leqslant N$, define $K_j : S \times S \longrightarrow \mathbb{C}$ by

$$K_j(s_0, s) = \Sigma\{K_1(s_0, s_1)K_1(s_1, s_2) \dots K_1(s_{j-1}, s) \mid (s_0, s_1, \dots, s_{j-1}, s) \in \mathcal{P}_j(S)\} \tag{11}$$

and define $K_0(s_0, s) = \delta_{s_0 s}$. The complex number $K_j(s_0, s)$ is interpreted as the conditional amplitude that a particle is at s at time j given that it was at s_0 at time 0, and it satisfies the Chapman–Kolmogorov equation [12, 13, 16]

$$K_j(s_0, s) = \sum_{s'} K_m(s_0, s')\, K_{j-m}(s', s) \tag{12}$$

for all $m \leqslant j$.

The wavefunction for X_j becomes [12, 13, 16]

$$f_j(s) = \Sigma\{f(\omega) \mid \omega \in \Omega,\ X_j(\omega) = s\} = \sum_{s_0} f_0(s_0)\, K_j(s_0, s). \tag{13}$$

Since the linear operator $U : l^2(S) \longrightarrow l^2(S)$, $(Ug)(s) = \sum_{s_0} K_1(s_0, s)\, g(s_0)$ is unitary and $f_j = U^j f_0$, from $||f_0|| = 1$ we get $||f_j|| = 1$, for all $j = 0, 1, \dots, N$. The main purpose of this paper is to present some mathematical results concerning random walks on diamond-type crystals and carbon nanotubes. As an illustration of the usefulness of these results we analyse some details concerning a possible application of the discrete quantum mechanics to crystal physics. The usual difficulties encountered in a path integral approach are avoided since we use finite spaces and counting measures.

2. Graphs defined by discrete metric spaces

Let $n \geqslant 2$ be a natural number and let

$$\mathcal{V}_n = \left\{ x = (x_1, x_2, \dots, x_n) \in \mathbb{Z}^n \;\middle|\; x_1 + x_2 + \dots + x_n \in \{0, 1\} \right\} = \mathcal{V}'_n \cup \mathcal{V}''_n \tag{14}$$

where $\mathcal{V}'_n = \{x \in \mathbb{Z}^n \mid x_1 + x_2 + \dots + x_n = 0\}$ and $\mathcal{V}''_n = (1, 0, \dots, 0) + \mathcal{V}'_n$. The mapping $d_n : \mathcal{V}_n \times \mathcal{V}_n \longrightarrow \mathbb{N}$

$$d_n(x, y) = |x_1 - y_1| + |x_2 - y_2| + \dots + |x_n - y_n| \tag{15}$$

is a distance on $\mathcal{V}_n$. Each point $x \in \mathcal{V}_n$ has n nearest neighbours, namely

$$x^i = x + \varepsilon(x) e_i \qquad i \in \mathcal{I}_n \tag{16}$$

where $e_1 = (1, 0, \dots, 0)$, $e_2 = (0, 1, 0, \dots, 0), \dots, e_n = (0, \dots, 0, 1)$, $\mathcal{I}_n = \{1, 2, \dots, n\}$ and

$$\varepsilon(x) = (-1)^{x_1 + x_2 + \dots + x_n} = \begin{cases} 1 & \text{if} \quad x_1 + x_2 + \dots + x_n = 0 \\ -1 & \text{if} \quad x_1 + x_2 + \dots + x_n = 1. \end{cases} \tag{17}$$

The $n(n-1)$ points $x^{ij} = (x^i)^j$ corresponding to $i \neq j$ are the next-nearest neighbours of x. One can remark that $x^{ii} = x$, and $x^{ijk} = x^{kji}$ for all $i, j, k \in \mathcal{I}_n$.

The graph $\mathcal{G}_n = (\mathcal{V}_n, \mathcal{E}_n)$, where

$$\mathcal{E}_n = \{\{x, y\} \mid x, y \in \mathcal{V}_n,\ d_n(x, y) = 1\} = \{\{x, x^i\} \mid x \in \mathcal{V}_n,\ i \in \mathcal{I}_n\}$$

can be associated to the metric space $\mathcal{M}_n = (\mathcal{V}_n, d_n)$ in a natural way. A k-step walk [19] on $\mathcal{G}_n$ with the starting point x has the form

$$\{x, x^{i_1}\}\{x^{i_1}, x^{i_1 i_2}\} \dots \{x^{i_1 i_2 \dots i_{k-1}}, x^{i_1 i_2 \dots i_{k-1} i_k}\} \tag{18}$$

and will be denoted by $(x, i_1 i_2 \dots i_k)$. The minimal length of a walk from x to y is $d_n(x, y)$. Since $x^{ijkijk} = x$, the walk $(x, ijkijk)$ is closed for any $i, j, k \in \mathcal{I}_n$. The walks $(x, ijkijk)$ with $i \neq j \neq k \neq i$ are called *hexagonal walks*.

An *isometry* of the metric space $\mathcal{M}_n$ is a bijection $g : \mathcal{V}_n \longrightarrow \mathcal{V}_n : x \mapsto gx$ such that $d_n(gx, gy) = d_n(x, y)$, for all $x, y \in \mathcal{V}_n$. Let $I, i : \mathbb{Z}^n \longrightarrow \mathbb{Z}^n$, $Ix = x$, $ix = -x$, and let S_n be the group of all the permutations $\sigma : \mathcal{I}_n \longrightarrow \mathcal{I}_n$. The transformations $g_\sigma,\ g_a : \mathcal{V}_n \longrightarrow \mathcal{V}_n$

$$g_\sigma(x_1, x_2, \ldots, x_n) = (x_{\sigma^{-1}(1)}, x_{\sigma^{-1}(2)}, \ldots, x_{\sigma^{-1}(n)})$$
$$g_a(x_1, x_2, \ldots, x_n) = \begin{cases} (x_1 + a_1, x_2 + a_2, \ldots, x_n + a_n) & \text{if} \quad a \in \mathcal{V}'_n \\ (-x_1 + a_1, -x_2 + a_2, \ldots, -x_n + a_n) & \text{if} \quad a \in \mathcal{V}''_n \end{cases} \tag{19}$$

are isometries of $\mathcal{M}_n$ for any $\sigma \in S_n$, $a \in \mathcal{V}_n$. One can remark that

$$g_\sigma(x^i) = (g_\sigma x)^{\sigma(i)} \qquad g_a(x^i) = (g_a x)^i \tag{20}$$

for all $\sigma \in S_n,\ a \in \mathcal{V}_n, i \in \mathcal{I}_n$.

A *graph-automorphism* of $\mathcal{G}_n$ is a bijection $g : \mathcal{V}_n \longrightarrow \mathcal{V}_n : x \mapsto gx$ such that $\{x, y\} \in \mathcal{E}_n \Longleftrightarrow \{gx, gy\} \in \mathcal{E}_n$. Any isometry of $\mathcal{M}_n$ is a graph-automorphism of $\mathcal{G}_n$.

Lemma 1. *Each graph-automorphism of $\mathcal{G}_n$ transforms a hexagonal walk into a hexagonal walk.*

Proof. If the graph-automorphism $g : \mathcal{V}_n \longrightarrow \mathcal{V}_n$ transforms the hexagonal walk $(x, ijkijk)$ into $(gx, i_1i_2i_3i_4i_5i_6)$ then we must have $i_1 \neq i_2 \neq i_3 \neq i_4 \neq i_5 \neq i_6$ and $e_{i_1} - e_{i_2} + e_{i_3} - e_{i_4} + e_{i_5} - e_{i_6} = (0, 0, \ldots, 0)$, whence $i_4 = i_1$, $i_5 = i_2$ and $i_6 = i_3$. □

Lemma 2. *(a) The point $o = (0, 0, \ldots, 0)$ is invariant under g_σ and*

$$g_\sigma(o^{i_1i_2\ldots i_k}) = o^{\sigma(i_1)\sigma(i_2)\ldots\sigma(i_k)} \tag{21}$$

for all $\sigma \in S_n$, $k \in \mathbb{N}$ and $i_1, i_2, \ldots, i_k \in \mathcal{I}_n$.
(b) If g is a graph-automorphism of $\mathcal{G}_n$ such that $go = o$ then $g \in \{g_\sigma \mid \sigma \in S_n\}$.

Proof. (a) The relation (21) is a consequence of the relations $g_\sigma o = o$ and $g_\sigma(x^i) = (g_\sigma x)^{\sigma(i)}$.
(b) If g is a graph-automorphism such that $go = o$ then $g\{o^1, o^2, \ldots, o^n\} = \{o^1, o^2, \ldots, o^n\}$, and hence there is $\sigma \in S_n$ such that $g(o^i) = o^{\sigma(i)}$, for all $i \in \mathcal{I}_n$. The transformation $h = g^{-1} \circ g_\sigma$ is a graph-automorphism of $\mathcal{G}_n$, $ho = o$, and $h(o^i) = o^i$ for all $i \in \mathcal{I}_n$. In order to prove that $h = I$ it is sufficient to prove the implication

$$\left.\begin{array}{l} hx = x \\ h(x^i) = x^i \qquad \text{for all} \quad i \in \mathcal{I}_n \end{array}\right\} \Longrightarrow h(x^{ij}) = x^{ij} \qquad \text{for all} \quad i, j \in \mathcal{I}_n \tag{22}$$

for any $x \in \mathcal{V}_n$. Let x be a fixed point of $\mathcal{V}_n$ such that $hx = x$, $h(x^i) = x^i$ for all $i \in \mathcal{I}_n$, and let $i, j \in \mathcal{I}_n$, $i \neq j$. If we assume that $h(x^{ij}) = x^{ik}$ with $k \neq j$ then h transforms the walk $(x^k, kij) = \{x^k, x\}\{x, x^i\}\{x^i, x^{ij}\}$ into the walk $\{x^k, x\}\{x, x^i\}\{x^i, x^{ik}\} = (x^k, kik)$, and hence h cannot transform the hexagonal walk $(x^k, kijkij)$ into a hexagonal walk. In view of lemma 1 we must have $h(x^{ij}) = x^{ij}$. □

Let us denote by $\mathcal{T}_n$ the group of all the 'translations' $\{\mathcal{V}_n \longrightarrow \mathcal{V}_n : x \mapsto x + a \mid a \in \mathcal{V}'_n\}$ and by $\{i|e_1\}$ the isometry $\mathcal{V}_n \longrightarrow \mathcal{V}_n : x \mapsto ix + e_1 = -x + e_1$. One can remark that $\{i|e_1\}\mathcal{V}'_n = \mathcal{V}''_n$, $\{i|e_1\}\mathcal{V}''_n = \mathcal{V}'_n$, and $\{i|e_1\} \circ \{i|e_1\} = I$.

Theorem 1. *The group G_n of all the graph-automorphisms of $\mathcal{G}_n$ coincides to the group of all the isometries of the metric space $\mathcal{M}_n$ and*

$$G_n = \bigcup_{\sigma \in S_n} \mathcal{T}_n \circ g_\sigma \ \cup \bigcup_{\sigma \in S_n} \mathcal{T}_n \circ \{i|e_1\} \circ g_\sigma . \tag{23}$$

Proof. Let g be a graph-automorphism of $\mathcal{G}_n$. If $a = go \in \mathcal{V}'_n$ then $h : \mathcal{V}_n \longrightarrow \mathcal{V}_n, hx = gx - a$ is a graph-automorphism and $ho = o$. In view of lemma 2 there is $\sigma \in S_n$ such that $h = g_\sigma$, and hence the transformation $gx = g_\sigma x + a$ belongs to $\mathcal{T}_n \circ g_\sigma$. If $go \in \mathcal{V}''_n$ then there is $a \in \mathcal{V}'_n$ such that $go = e_1 + a$, and $h : \mathcal{V}_n \longrightarrow \mathcal{V}_n$, $hx = e_1 + a - gx$ is a graph-automorphism with $ho = o$. In view of lemma 2 there is $\sigma \in S_n$ such that $h = g_\sigma$, whence $gx = -g_\sigma x + e_1 + a$, that is $g \in \mathcal{T}_n \circ \{i|e_1\} \circ g_\sigma$. Since $\mathcal{T}_n \subset G_n$, $\{g_\sigma \mid \sigma \in S_n\} \subset G_n$ and $\{i|e_1\} \in G_n$ the group of all the graph-automorphisms of $\mathcal{G}_n$ is given by (23). In addition, any graph-automorphism of $\mathcal{G}_n$ is an isometry of $\mathcal{M}_n$. □

The group-automorphisms G_4 is isomorphic [2] to the space group $O_h^7 = Fd\bar{3}m$, and the graph $\mathcal{G}_4$ can be used as a *mathematical model for a diamond-type crystal* [1, 10, 24, 30]. It corresponds to a four-axes description [2, 3] very similar to a well known description existing in the case of hexagonal crystals [29]. This description offers some facilities since the use of an additional axis leads to simpler expressions for the O_h^7-invariant mathematical objects, and allow us to index in a natural way the atoms of the crystal [2, 3].

The graph $\mathcal{G}_3$ can be used as a *mathematical model for the honeycomb lattice*, and as a starting point in the description of carbon nanotubes. We present the method which leads from $\mathcal{G}_3$ to a model for a nanotube [6, 18, 32], but in a more general version. Let $c = (c_1, c_2, \ldots, c_n)$ be a fixed element of $\mathcal{V}'_n$. The relation

$$x \sim y \Longleftrightarrow x - y \in \mathbb{Z}c \tag{24}$$

is an equivalence relation on $\mathcal{V}_n$. The equivalence class corresponding to $x \in \mathcal{V}_n$ is $[x] = x + \mathbb{Z}c$. Since $x \sim y \Longrightarrow x^i \sim y^i$, we can define $[x]^i = [x^i]$, and consider the graph $\mathcal{G}_{n,c} = (\mathcal{V}_{n,c}, \mathcal{E}_{n,c})$, where

$$\mathcal{V}_{n,c} = \{[x] \mid x \in \mathcal{V}_n\} \qquad \mathcal{E}_{n,c} = \{([x], [x]^i) \mid [x] \in \mathcal{V}_{n,c},\ i \in \mathcal{I}_n\}. \tag{25}$$

The set $\mathcal{V}_{n,c}$ can be regarded as a subset of the factor $\mathbb{Z}$-module $\mathbb{Z}^n/(\mathbb{Z}c)$, namely

$$\mathcal{V}_{n,c} = \{[x_1, x_2, \ldots, x_n] \in \mathbb{Z}^n/(\mathbb{Z}c) \mid x_1 + x_2 + \cdots + x_n \in \{0, 1\}\} \tag{26}$$

since $x_1 + x_2 + \cdots + x_n = (x_1 + kc_1) + (x_2 + kc_2) + \cdots + (x_n + kc_n)$, for any $k \in \mathbb{Z}$. The graph $\mathcal{G}_{3,c}$ can be used [4] as a *mathematical model for a carbon nanotube with chirality c*.

Theorem 2. *For each $a \in \mathcal{V}_n$, the transformation*

$$g_a : \mathcal{V}_{n,c} \longrightarrow \mathcal{V}_{n,c} \qquad g_a[x] = \begin{cases} [x + a] & \text{if} \quad a \in \mathcal{V}'_n \\ [-x + a] & \text{if} \quad a \in \mathcal{V}''_n \end{cases} \tag{27}$$

is a graph-automorphism of $\mathcal{G}_{n,c}$.

Proof. Since $x - y \in \mathbb{Z}c \Longleftrightarrow (\pm x + a) - (\pm y + a) \in \mathbb{Z}c$ the transformation g_a is well defined, and $g_a([x]^i) = (g_a[x])^i$. Indeed,

$$g_a[x^i] = \begin{cases} [x^i + a] = [(x + a)^i] = [x + a]^i & \text{if} \quad a \in \mathcal{V}'_n \\ [-x^i + a] = [(-x + a)^i] = [-x + a]^i & \text{if} \quad a \in \mathcal{V}''_n. \end{cases}$$

□

In order to simplify the mathematical computations, a crystal is usually finitized by using the Born–Karman periodic boundary conditions [1]. In the case of our models this reduction can be achieved by using a factor ring $\mathbb{Z}_m$ instead $\mathbb{Z}$ in the definition of $\mathcal{G}_n$. Let $m \neq 0$ be a fixed natural number, and let

$$\mathcal{V}_{n,m} = \{\hat{x} = (\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n) \in (\mathbb{Z}_m)^n \mid \hat{x}_1 + \hat{x}_2 + \cdots + \hat{x}_n \in \{\hat{0}, \hat{1}\}\} \tag{28}$$

where $\mathbb{Z}_m$ is the factor ring $\mathbb{Z}/(m\mathbb{Z})$ and $\hat{0} = m\mathbb{Z}$, $\hat{1} = 1 + m\mathbb{Z}$. The canonical projection $\mathbb{Z} \longrightarrow \mathbb{Z}_m : k \mapsto \hat{k} = k + m\mathbb{Z}$ allows us to consider the projector

$$\pi : \mathcal{V}_n \longrightarrow \mathcal{V}_{n,m} \qquad \pi(x_1, x_2, \ldots, x_n) = (\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n) \tag{29}$$

and to associate $\hat{x}^1 = \pi(x^1), \ldots, \hat{x}^n = \pi(x^n)$ to each $\hat{x} = \pi(x) \in \mathcal{V}_{n,m}$. The graph $\mathcal{G}_{n,m} = (\mathcal{V}_{n,m}, \mathcal{E}_{n,m})$, where $\mathcal{E}_{n,m} = \{\{\hat{x}, \hat{x}^i\} \mid \hat{x} \in \mathcal{V}_{n,m},\ i \in \mathcal{I}_n\}$ has $2m^{n-1}$ vertices, and each of them has n nearest neighbours. Particularly, the graphs $\mathcal{G}_{4,m}$ are useful in the description of diamond-type crystals [3].

Theorem 3. *The transformations* $g_\sigma,\ g_{\hat{a}} : \mathcal{V}_{n,m} \longrightarrow \mathcal{V}_{n,m}$

$$g_\sigma(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n) = (\hat{x}_{\sigma^{-1}(1)}, \hat{x}_{\sigma^{-1}(2)}, \ldots, \hat{x}_{\sigma^{-1}(n)}) \tag{30}$$

$$g_{\hat{a}}\hat{x} = \begin{cases} \hat{x} + \hat{a} & \text{if} \quad \hat{a}_1 + \hat{a}_2 + \cdots + \hat{a}_n = \hat{0} \\ -\hat{x} + \hat{a} & \text{if} \quad \hat{a}_1 + \hat{a}_2 + \cdots + \hat{a}_n = \hat{1} \end{cases} \tag{31}$$

are graph-automorphism of $\mathcal{G}_{n,m}$ *for any* $\sigma \in S_n$, $\hat{a} \in \mathcal{V}_{n,m}$.

Proof. We have $g_\sigma(\hat{x}^i) = (g_\sigma \hat{x})^{\sigma(i)}$ and $g_{\hat{a}}(\hat{x}^i) = (g_{\hat{a}}\hat{x})^i$, for all $i \in \mathcal{I}_n$ and $\hat{x} \in \mathcal{V}_{n,m}$. □

Let $\mathcal{F}(\mathcal{V}_n)$ be the vector space of all the functions $\psi : \mathcal{V}_n \longrightarrow \mathbb{C}$, and let us consider the linear operator of Schrödinger type [5, 31]

$$H : \mathcal{F}(\mathcal{V}_n) \longrightarrow \mathcal{F}(\mathcal{V}_n) \qquad (H\psi)(x) = \alpha\psi(x) + \sum_{j=1}^{n} \beta_j \psi(x^j) \tag{32}$$

where $\alpha,\ \beta_1,\ \beta_2, \ldots,\ \beta_n$ are fixed real numbers.

Theorem 4. *The numbers*

$$E_{1,2}(k) = \alpha \pm \left(\sum_{j=1}^{n} \beta_j^2 + \sum_{j \neq l} \beta_j \beta_l \cos(k_j - k_l) \right)^{1/2} \tag{33}$$

belong to the spectrum of H *for all* $k = (k_1, k_2, \ldots, k_n) \in \mathbb{R}^n$.

Proof. The bounded function $\psi_k : \mathcal{V}_n \longrightarrow \mathbb{C}$

$$\psi_k(x) = \begin{cases} a\mathrm{e}^{\mathrm{i}(k_1 x_1 + k_2 x_2 + \cdots + k_n x_n)} & \text{if} \quad \varepsilon(x) = 1 \\ b\mathrm{e}^{\mathrm{i}(k_1 x_1 + k_2 x_2 + \cdots + k_n x_n)} & \text{if} \quad \varepsilon(x) = -1 \end{cases} \tag{34}$$

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

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

This system has non-trivial solutions if and only if

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

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

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

Using the relation $\mathrm{e}^{\mathrm{i}k_j} = \cos k_j + \mathrm{i} \sin k_j$ we get (33). □

If $\beta_1 = \beta_2 = \cdots = \beta_n = \beta$ then we get $E_{1,2}(k) = \alpha \pm \beta\big(n + \sum_{j \neq l} \cos(k_j - k_l)\big)^{1/2}$. The relation $(g\psi)(x) = \psi(g^{-1}x)$ defines a unitary representation of G_n in the Hilbert space $l^2(\mathcal{V}_n)$. The restriction of H to $l^2(\mathcal{V}_n)$ is a G_n-invariant self-adjoint operator [2].

Let $\mathcal{F}(\mathcal{V}_{n,c})$ (resp. $\mathcal{F}(\mathcal{V}_{n,m})$) be the vector space of all the functions $\psi : \mathcal{V}_{n,c} \longrightarrow \mathbb{C}$ (resp. $\psi : \mathcal{V}_{n,m} \longrightarrow \mathbb{C}$).

Theorem 5. *(a) If $k \in \mathbb{R}^n$ and $k_1c_1+k_2c_2+\cdots+k_nc_n \in 2\pi\mathbb{Z}$ then the numbers $E_{1,2}(k)$ defined by (33) belong to the spectrum of the linear operator*

$$H : \mathcal{F}(\mathcal{V}_{n,c}) \longrightarrow \mathcal{F}(\mathcal{V}_{n,c}) \qquad (H\psi)[x] = \alpha\psi[x] + \sum_{j=1}^{n} \beta_j \psi[x^j]. \tag{35}$$

(b) If $k_1, k_2, \ldots, k_n \in \left\{ 2\pi \frac{l}{m} \middle| \; l \in \{0, 1, \ldots, m-1\} \right\}$ then the numbers $E_{1,2}(k)$ defined by (33) belong to the spectrum of the linear operator

$$H : \mathcal{F}(\mathcal{V}_{n,m}) \longrightarrow \mathcal{F}(\mathcal{V}_{n,m}) \qquad (H\psi)(\hat{x}) = \alpha\psi(\hat{x}) + \sum_{j=1}^{n} \beta_j \psi(\hat{x}^j). \tag{36}$$

Proof. If k satisfies the indicated conditions then the relation (34) defines a function $\psi_k : \mathcal{V}_{n,c} \longrightarrow \mathbb{C}$ (resp. $\psi_k : \mathcal{V}_{n,m} \longrightarrow \mathbb{C}$) such that $H\psi_k = E_{1,2}(k)\,\psi_k$. □

Our results are in good agreement with those presented in [17, 18, 28, 32].

3. Random walks

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 to the coefficient of $Z_1^{n_1} Z_2^{n_2}$ in the expression $(Z_1+Z_1^{-1}+Z_2+Z_2^{-1})^k$. Since

$$\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}m\varphi}\, \mathrm{d}\varphi = \begin{cases} 0 & \text{for} \quad m \neq 0 \\ 2\pi & \text{for} \quad m = 0 \end{cases} \tag{37}$$

the number $\mathcal{N}_k$ is given by the formula [19]

$$\mathcal{N}_k = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left(\mathrm{e}^{\mathrm{i}\varphi_1} + \mathrm{e}^{-\mathrm{i}\varphi_1} + \mathrm{e}^{\mathrm{i}\varphi_2} + \mathrm{e}^{-\mathrm{i}\varphi_2} \right)^k \mathrm{e}^{-\mathrm{i}(n_1\varphi_1+n_2\varphi_2)}\, \mathrm{d}\varphi_1\, \mathrm{d}\varphi_2. \tag{38}$$

Let $\varrho_1,\ \varrho_2, \ldots, \varrho_n$ be n complex numbers. We associate the weight ϱ_j to the edge $\{x, x^j\} \in \mathcal{E}_n$ and the weight $\varrho_{i_1}\varrho_{i_2}\ldots\varrho_{i_k}$ to a walk $(x, i_1 i_2 \ldots i_k)$. The formula for the sum $w_k(a, x)$ of the weights of all the k-step walks from a to x we obtain in this section is useful, for example, in a microscopic approach of the diffusion. If we use a discrete time and assume that in one timestep a particle can only pass from a point y to one of its nearest neighbours $y^1,\ y^2,\ \ldots,\ y^n$ with the probabilities $\varrho_1,\ \varrho_2, \ldots,\ \varrho_n \in [0, 1]$, then $w_k(a, x)$ is the probability to find a particle at point x after k timesteps given that it was initially at point a.

Theorem 6. *We have*

$$w_k(o, x) = \begin{cases} \left\langle \left(\sum_{j=1}^{n} \varrho_j \mathrm{e}^{\mathrm{i}\varphi_j} \right)^{k/2} \left(\sum_{j=1}^{n} \varrho_j \mathrm{e}^{-\mathrm{i}\varphi_j} \right)^{k/2} \mathrm{e}^{-\mathrm{i}x\varphi} \right\rangle & \text{if} \quad k \text{ is even} \\ \left\langle \left(\sum_{j=1}^{n} \varrho_j \mathrm{e}^{\mathrm{i}\varphi_j} \right)^{(k+1)/2} \left(\sum_{j=1}^{n} \varrho_j \mathrm{e}^{-\mathrm{i}\varphi_j} \right)^{(k-1)/2} \mathrm{e}^{-\mathrm{i}x\varphi} \right\rangle & \text{if} \quad k \text{ is odd} \end{cases} \tag{39}$$

where $x\varphi = x_1\varphi_1 + x_2\varphi_2 + \cdots + x_n\varphi_n$, and

$$\langle f(\varphi) \rangle = \frac{1}{(2\pi)^n} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \ldots \int_{-\pi}^{\pi} f(\varphi)\, \mathrm{d}\varphi_1\, \mathrm{d}\varphi_2\, \ldots\, \mathrm{d}\varphi_n. \tag{40}$$

Proof. The number $\mathcal{N}_k(o, x)$ of k-step walks from o to $x = (x_1, x_2, \ldots, x_n)$ corresponds to the number of possibilities to express x in the form

$$e_{i_1} - e_{i_2} + e_{i_3} - e_{i_4} + \cdots + (-1)^{k+1} e_{i_k} = (x_1, x_2, \ldots, x_n).$$

If k is even, $k = 2m$, then $w_k(o, x)$ is the coefficient of $Z_1^{x_1} Z_2^{x_2} \dots Z_n^{x_n}$ in

$$((\varrho_1 Z_1 + \varrho_2 Z_2 + \dots + \varrho_n Z_n)\,(\varrho_1 Z_1^{-1} + \varrho_2 Z_2^{-1} + \dots + \varrho_n Z_n^{-1}))^m$$

and if k is odd, $k = 2m + 1$, then $w_k(o, x)$ is the coefficient of $Z_1^{x_1} Z_2^{x_2} \dots Z_n^{x_n}$ in

$$(\varrho_1 Z_1 + \varrho_2 Z_2 + \dots + \varrho_n Z_n)^{m+1}\,(\varrho_1 Z_1^{-1} + \varrho_2 Z_2^{-1} + \dots + \varrho_n Z_n^{-1})^m.$$

If $\varrho_1 = \varrho_2 = \dots = \varrho_n = 1$ then $w_k(o, x) = \mathcal{N}_k(o, x)$. □

Since, for each $a \in \mathcal{V}_n$, the transformation

$$g : \mathcal{V}_n \longrightarrow \mathcal{V}_n \qquad gx = \begin{cases} x - a & \text{if} \quad a \in \mathcal{V}'_n \\ -x + a & \text{if} \quad a \in \mathcal{V}''_n \end{cases} \tag{41}$$

belongs to G_n and $ga = o$, we have $w_k(a, x) = w_k(o, gx)$.

Taking into account the definitions of the graphs $\mathcal{V}_{n,c}$ and $\mathcal{V}_{n,m}$ one can remark [4] that the walks on $\mathcal{V}_{n,c}$ and $\mathcal{V}_{n,m}$ are related to some classes of walks on $\mathcal{V}_n$, and (a finite number of terms are non-zero)

$$w_k([o], [x]) = \sum_{j \in \mathbb{Z}} w_k(o, x + jc) \tag{42}$$

$$w_k(\hat{o}, \hat{x}) = \sum_{j_1, j_2, \dots, j_n \in \mathbb{Z}} w_k(o, (x_1 + j_1 m, x_2 + j_2 m, \dots, x_n + j_n m)). \tag{43}$$

Starting from the graph $\mathcal{G}_n = (\mathcal{V}_n, \mathcal{E}_n)$ we can obtain the graph $\mathcal{G}'_n = (\mathcal{V}_n, \mathcal{E}'_n)$, where $\mathcal{E}'_n = \mathcal{E}_n \cup \{\{x\} | x \in \mathcal{V}_n\}$, by adding a loop $\{x\}$ for each $x \in \mathcal{V}_n$. The walks on $\mathcal{G}'_n$ allow us to describe the discrete trajectories of a particle which in one step time can either keep its position or move to a nearest-neighbour position, and they are related to the walks on $\mathcal{G}_n$. For $k > j$, starting from any j-step walk on $\mathcal{G}_n$ we can generate some k-step walks on $\mathcal{G}'_n$ by inserting $k - j$ timesteps in which the particle does not change its position. Any walk on $\mathcal{G}'_n$ can be obtained in this way, and the number of the k-step walks on $\mathcal{G}'_n$ obtained by starting from a fixed j-step walk on $\mathcal{G}_n$ coincides with the number of strictly increasing functions $f : \{1, 2, \dots, j\} \longrightarrow \{1, 2, \dots, k\}$, and it is $k!/(j!(k - j)!)$. If we associate the weight ϱ_0 to a loop $\{x\} \in \mathcal{E}_n$, then one can remark that the sum $w'_k(o, x)$ of the weights of the k-step walks from o to x on $\mathcal{G}'_n$ is

$$w'_k(o, x) = \sum_{j=0}^{k} \frac{k!}{j!(k - j)!} \varrho_0^{k-j} w_j(o, x). \tag{44}$$

4. Quantum random walks

In this section we present a possible application of the discrete quantum mechanics to diamond-type crystals and carbon nanotubes based on our graphs. Let us consider the set

$$\mathcal{S}_n = \mathcal{V}_n \times \mathcal{I}_n = \{(x, k) \mid x \in \mathcal{V}_n,\ k \in \mathcal{I}_n\} \tag{45}$$

interpreted as a set of 'states' that a quantum particle can occupy. Following Gudder [12,13,16], we can consider that a particle in state (x, k) is a particle lying in the vicinity of the point x and moving in the direction of x^k (that is, a particle with 'position' x and 'momentum' k).

Theorem 7. *If* $\alpha,\ \beta \in \mathbb{C}$ *satisfy the conditions*

$$\alpha + (n - 1)\beta = 1 \qquad |\alpha|^2 + (n - 1)|\beta|^2 = 1 \qquad |\alpha - \beta| = 1 \tag{46}$$

then the function $K_1 : \mathcal{S}_n \times \mathcal{S}_n \longrightarrow \mathbb{C}$

$$K_1((x,k),(y,l)) = \begin{cases} \alpha & \text{if} \quad y = x^k \text{ and } l = k \\ \beta & \text{if} \quad y = x^k \text{ and } l \neq k \\ 0 & \text{otherwise} \end{cases} \tag{47}$$

is a stochastic one-step transition amplitude.

Proof. The set of pairs $(\alpha, \beta) \in \mathbb{C}^2$ satisfying the relations (46) is not empty. Indeed, the complex numbers

$$\begin{aligned} \alpha &= \frac{1}{n} \pm \frac{1-n}{n}\sqrt{1-n^2\kappa^2} + (1-n)\kappa \mathrm{i} \\ \beta &= \frac{1}{n} \pm \frac{1}{n}\sqrt{1-n^2\kappa^2} + \kappa \mathrm{i} \end{aligned} \tag{48}$$

satisfy (46) for any $\kappa \in [-1/n, 1/n]$. Since $x = x^{kk} = x^{ll}$, for $s_1 = s_2 = (x,k)$ we get

$$\sum_s K_1(s_1,s)\,\overline{K}_1(s_2,s) = \sum_{l=1}^{n} |K_1((x,k),(x^k,l))|^2 = |\alpha|^2 + (n-1)|\beta|^2 = 1$$

$$\sum_s K_1(s,s_1)\,\overline{K}_1(s,s_2) = \sum_{l=1}^{n} |K_1((x^l,l),(x,x^k))|^2 = |\alpha|^2 + (n-1)|\beta|^2 = 1.$$

Since $x^k = x^{kll}$, for $s_1 = (x,k),\ s_2 = (x^{kl},l),\ k \neq l$, we obtain

$$\begin{aligned} \sum_s K_1(s_1,s)\,\overline{K}_1(s_2,s) &= \sum_{j=1}^{n} K_1((x,k),(x^k,j))\,\overline{K}_1((x^{kl},l),(x^k,j)) \\ &= \alpha\overline{\beta} + \beta\overline{\alpha} + (n-2)|\beta|^2 \\ &= |\alpha|^2 + (n-1)|\beta|^2 - |\alpha-\beta|^2 = 0 \end{aligned}$$

and for $s_1 = (x,k),\ s_2 = (x,l),\ k \neq l$, we get

$$\begin{aligned} \sum_s K_1(s,s_1)\,\overline{K}_1(s,s_2) &= \sum_{j=1}^{n} K_1((x^j,j),(x,k))\,\overline{K}_1((x^j,j),(x,x^l)) \\ &= \alpha\overline{\beta} + \beta\overline{\alpha} + (n-2)|\beta|^2 = 0. \end{aligned}$$

□

Let K_1 be a fixed stochastic one-step transition amplitude of the form (47), and let N be a fixed natural number. For $j \in \mathbb{N}$, a j-path is a $j+1$-tuple $(s_0, s_1, \ldots, s_j) \in \mathcal{S}_n^{j+1}$. Let $\mathcal{P}_j(\mathcal{S}_n)$ denote the set of j-paths in $\mathcal{S}_n$ and let us consider the sample space $\Omega_n = \mathcal{P}_N(\mathcal{S}_n)$. For $j = 0, 1, \ldots, N$ the map

$$X_j : \Omega_n \longrightarrow \mathcal{S}_n \qquad X_j(s_0, s_1, \ldots, s_N) = s_j \tag{49}$$

becomes a *measurement* if we consider on $\mathcal{S}_n$ and $X_j^{-1}(s)$ the counting measures [16].

Following the general formalism of discrete quantum mechanics, consider the maps $K_j : \mathcal{S}_n \times \mathcal{S}_n \longrightarrow \mathbb{C}$ defined by $K_0(s_0, s) = \delta_{s_0 s}$, and

$$K_j(s_0,s) = \Sigma\{K_1(s_0,s_1)K_1(s_1,s_2)\ldots K_1(s_{j-1},s) \mid (s_0,s_1,\ldots,s_{j-1},s) \in \mathcal{P}_j(\mathcal{S}_n)\} \tag{50}$$

for $j \in \{1, 2, \ldots, N\}$. The complex number $K_j(s_0, s)$ is interpreted as the conditional amplitude that a particle is at s at time j given that it was at s_0 at time 0. In the case of a stochastic one-step transition amplitude of the form (47), for $s_0 = (x,k)$ and $s = (y,l)$ we can have $K_1(s_0,s_1)K_1(s_1,s_2)\ldots K_1(s_{j-1},s) \neq 0$ only if there exist $i_0 = k,\ i_1,\ \ldots,\ i_{j-1} \in \{1, 2, \ldots, n\}$ such that $y = x^{i_0 i_1 \ldots i_{j-1}}$ and $s_m = (x^{i_0 i_1 \ldots i_{m-1}}, i_m)$, for all $m \in \{1, 2, \ldots, j-1\}$.

Our main objective is to determine the maps K_j which allow us to obtain the wavefunction for X_j

$$f_j : \mathcal{S}_n \longrightarrow \mathbb{C} \qquad f_j(s) = \sum_{s_0} f_0(s_0)\, K_j(s_0, s) \tag{51}$$

for any initial distribution $f_0 \in l^2(\mathcal{S}_n)$. Since the computation of $K_j((x,k),(y,l))$ in general appears to be quite difficult, we consider firstly a similar but more tractable problem [23]. The maps $Q_j : \Omega_n \longrightarrow \mathcal{V}_n$, $P_j : \Omega_n \longrightarrow \mathcal{I}_n$, where

$$Q_j(s_0, s_1, \ldots, s_N) = \pi_1(s_j) \qquad P_j(s_0, s_1, \ldots, s_N) = \pi_2(s_j) \tag{52}$$

defined by using the projectors $\pi_1(x,k) = x$, $\pi_2(x,k) = k$ correspond to a position measurement and respectively a momentum measurement at the discrete time $j \in \{0, 1, \ldots, N\}$. The number

$$\tilde{K}_j(k,l) = \sum_x K_j((o,k),(x,l)) \tag{53}$$

can be interpreted [23] as the amplitude that a particle moves in direction l after j timesteps given that it was initially moving in the direction k. The corresponding probability is $|\tilde{K}_j(k,l)|^2$.

Theorem 8. *Denoting $\alpha - \beta = \mathrm{e}^{\mathrm{i}\theta}$, for any $j \in \{1, 2, \ldots, N\}$ we get*

$$\tilde{K}_j(k,l) = \begin{cases} \dfrac{1}{n} + \dfrac{n-1}{n}\cos\, j\theta + \mathrm{i}\dfrac{n-1}{n}\sin\, j\theta & \text{if} \quad k = l \\ \dfrac{1}{n} - \dfrac{1}{n}\cos\, j\theta - \mathrm{i}\dfrac{1}{n}\sin\, j\theta & \text{if} \quad k \neq l. \end{cases} \tag{54}$$

Proof. Let us consider the $n \times n$ matrices $I_n = (\delta_{kl})$, $M = (M_{kl})$, $L = (L_{kl})$, where $M_{kl} = (\alpha - \beta)\delta_{kl} + \beta$, $L_{kl} = 1$ for all $k, l \in \{1, 2, \ldots, n\}$. We have

$K_1(k,l) = K_1((o,o^k),(o^k,o^{kl})) = M_{kl}$

$$K_2(k,l) = \sum_{i=1}^{n} K_1((o,o^k),(o^k,o^{ki}))\; K_1((o^k,o^{ki}),(o^{ki},o^{kil})) = \sum_{i=1}^{n} M_{ki}M_{il} = (M^2)_{kl}$$

and generally

$$K_j(k,l) = \sum_{i_1,i_2,\ldots,i_{j-1}=1}^{n} M_{ki_1}M_{i_1i_2}\ldots M_{i_{j-1}l} = (M^j)_{kl}. \tag{55}$$

Since $M = (\alpha - \beta)I_n + \beta L$, $I_n L = L I_n$ and $L^j = n^{j-1}L$, we get

$$M^j = [(\alpha - \beta)I_n + \beta L]^j = (\alpha - \beta)^j I_n + \frac{1}{n}\sum_{i=1}^{j} \frac{j!}{i!\,(j-i)!}(\alpha - \beta)^{j-i}(n\beta)^i L$$

whence relation (54). □

The sum (55) contains terms corresponding to all the j-paths with initial element (o,k). If instead of the matrix M we use the matrix $\mathcal{M}(\varphi)$ with entries $\mathcal{M}_{kl}(\varphi) = M_{kl}\mathrm{e}^{\mathrm{i}\varphi_k}$, and if we replace the sum (55) by

$$\sum_{i_1,i_2,\ldots,i_{j-1}=1}^{n} \mathcal{M}_{ki_1}(\varphi)\mathcal{M}_{i_1i_2}(-\varphi)\mathcal{M}_{i_2i_3}(\varphi)\mathcal{M}_{i_3i_4}(-\varphi)\ldots\mathcal{M}_{i_{j-1}l}((-1)^{j-1}\varphi) \tag{56}$$

then we can select the terms corresponding to the j-paths with final element (x,l) by using the method from section 3. We get the following result.

Table 1. Time dependence of K_j in the case $n = 3$, $\kappa = \frac{1}{3}$ ($o = (0, 0, 0)$, $o^1 = (1, 0, 0)$).

j	$K_j((o,1),(o,1))$	$K_j((o,1),(o,2))$	$K_j((o,1),(o^1,1))$	$K_j((o,1),(o^1,2))$
1	0	0	$\frac{1}{3} - \frac{2}{3}\mathrm{i}$	$\frac{1}{3} + \frac{1}{3}\mathrm{i}$
2	$-\frac{1}{3} - \frac{4}{9}\mathrm{i}$	$\frac{1}{3} - \frac{1}{9}\mathrm{i}$	0	0
3	0	0	$-\frac{1}{9} + \frac{2}{9}\mathrm{i}$	$\frac{2}{9} - \frac{4}{9}\mathrm{i}$
4	$\frac{25}{81}$	$-\frac{14}{81} - \frac{4}{27}\mathrm{i}$	0	0
5	0	0	$\frac{7}{81} - \frac{34}{81}\mathrm{i}$	$-\frac{5}{81} + \frac{5}{81}\mathrm{i}$
6	$-\frac{1}{3} - \frac{140}{729}\mathrm{i}$	$\frac{37}{243} - \frac{35}{729}\mathrm{i}$	0	0
7	0	0	$-\frac{77}{729} + \frac{166}{729}\mathrm{i}$	$\frac{28}{729} - \frac{188}{729}\mathrm{i}$
8	$\frac{395}{2187}$	$-\frac{448}{2187} - \frac{32}{729}\mathrm{i}$	0	0
9	0	0	$-\frac{103}{2187} - \frac{626}{2187}\mathrm{i}$	$-\frac{199}{2187} + \frac{217}{2187}\mathrm{i}$
10	$-\frac{1}{3} + \frac{1892}{19683}\mathrm{i}$	$\frac{1103}{6561} + \frac{473}{19683}\mathrm{i}$	0	0
11	0	0	$\frac{965}{19683} + \frac{7526}{19683}\mathrm{i}$	$-\frac{454}{19683} - \frac{2344}{19683}\mathrm{i}$
12	$\frac{248377}{531441}$	$-\frac{70766}{531441} - \frac{4780}{177145}\mathrm{i}$	0	0
13	0	0	$\frac{45175}{531441} - \frac{222322}{531441}\mathrm{i}$	$\frac{30835}{531441} + \frac{96821}{531441}\mathrm{i}$
14	$-\frac{1}{3} - \frac{80764}{531441}\mathrm{i}$	$\frac{31921}{177147} - \frac{20191}{531441}\mathrm{i}$	0	0

Theorem 9. *We have*

$$K_j((o,k),(x,l)) = \begin{cases} \langle((\mathcal{M}(\varphi)\mathcal{M}(-\varphi))^{j/2})_{kl}\mathrm{e}^{-\mathrm{i}x\varphi}\rangle & \text{if} \quad j \text{ is even} \\ \langle((\mathcal{M}(\varphi)\mathcal{M}(-\varphi))^{(j-1)/2}\mathcal{M}(\varphi))_{kl}\mathrm{e}^{-\mathrm{i}x\varphi}\rangle & \text{if} \quad j \text{ is odd} \end{cases} \tag{57}$$

where $\langle f(\varphi)\rangle$ is defined by (40).

For any $a \in \mathcal{V}_n$, using the symmetry transformation (41) we get $K_j((a,k),(x,l)) = K_j((o,k),(gx,l))$. We can interpret $P_j((a,k),(x,l)) = |K_j((a,k),(x,l))|^2$ as the probability that a particle arrives at x and moves in the direction l after j timesteps given that it was initially at a moving in direction k.

For example, in the case $n = 3$ and $\kappa = \frac{1}{3}$ we get $\alpha = \frac{1}{3} - \frac{2}{3}\mathrm{i}$, $\beta = \frac{1}{3} + \frac{1}{3}\mathrm{i}$, and

$$\mathcal{M}(\varphi_1,\varphi_2,\varphi_3) = \begin{pmatrix} \left(\frac{1}{3} - \frac{2}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_1} & \left(\frac{1}{3} + \frac{1}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_1} & \left(\frac{1}{3} + \frac{1}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_1} \\ \left(\frac{1}{3} + \frac{1}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_2} & \left(\frac{1}{3} - \frac{2}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_2} & \left(\frac{1}{3} + \frac{1}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_2} \\ \left(\frac{1}{3} + \frac{1}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_3} & \left(\frac{1}{3} + \frac{1}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_3} & \left(\frac{1}{3} - \frac{2}{3}\mathrm{i}\right)\mathrm{e}^{\mathrm{i}\varphi_3} \end{pmatrix}. \tag{58}$$

The results presented in table 1, obtained by using (57), suggest that $K_j((o,k),(x,l))$ is an 'oscillating' function of discrete time parameter j.

Starting from $\mathcal{S}_{n,c} = \mathcal{V}_{n,c} \times \mathcal{I}_n$ instead of $\mathcal{S}_n$, we obtain a version of our model corresponding to the graph $\mathcal{G}_{n,c}$. To each transition amplitude on $\mathcal{S}_n$ of form (47) we associate the stochastic one-step transition amplitude on $\mathcal{S}_{n,c}$ defined by $K_1(([x],k),([y],l)) = K_1((x,k),(y,l))$, and we get the formula

$$K_j(([o],k),([x],l)) = \sum_{i\in\mathbb{Z}} K_j((o,k),(x+ic,l)). \tag{59}$$

For $n = 3$ this model may be useful in the description of the physical phenomena occurring in carbon nanotubes of chirality c.

A finite version [3] of our model useful in some applications concerning diamond-type crystals can be obtained by starting from $\mathcal{S}_{n,m} = \mathcal{V}_{n,m} \times \mathcal{I}_n$ instead of $\mathcal{S}_n$. In this case, the relation $K_1((\hat{x},k),(\hat{y},l)) = K_1((x,k),(y,l))$ defines a stochastic one-step transition amplitude on $\mathcal{S}_{n,m}$, and

$$K_j((\hat{o},k),(\hat{x},l)) = \sum_{i_1,\ldots,i_n\in\mathbb{Z}} K_j((o,k),((x_1+i_1m,\ldots,x_n+i_nm),l)). \tag{60}$$

A normalization to unity is necessary in the case of (59) and (60) in order to keep our probabilistic interpretation.

5. Concluding remarks

It is well known that some models existing in crystal physics are based on the path integral [8, 9, 21]. Even if we do not take into consideration the temperature of the crystal or the presence of an external field the description of the evolution of a particle inside a crystal is a very difficult problem. The particle interacts with the surrounding crystal and determines a local distortion, usually described as a cloud of phonons, which moves with the particle. Some quite drastic simplifications are needed in order to study such a physical system. Since the reduction to a simpler idealized problem is not unique, some very different path integral approaches may exist. In this paper we analyse some details concerning the possibility to use a discrete version of the path integral method.

Discrete versions of the path integral are usually obtained by time-slicing the path integral, replacing the differentials by some finite differences, using a lattice approximation to the Lagrangian, or some perturbative expansions [21]. But, there also exists the possibility to directly construct a discrete version by starting from the fundamental principles [7, 8], as in the case of the field theory on a lattice [27]. This is the method we use in this paper.

We start from a tight-binding approximation of the crystal [11, 20]. In this approach the particle may, with some probability, be located near any atom. Particle exchange between any two atoms of the crystal takes place by way of a chain of nearest-neighbour exchanges. It moves 'freely' through the crystal jumping from one atom to another by the exchange process [20]. We regard these sequences of jumps between neighbouring atoms as the 'classical' trajectories of the particle. More than that, in the discrete version of path integral we use in this paper, we restrict the class of all the paths to the class of these classical paths. The main question is whether after this drastic reduction the usual physical interpretation can be kept. We think that the answer may be in the affirmative, and a model obtained in this way may attain the accuracy of a model based on the tight-binding approximation.

It is well known that only the paths in the vicinity of classical trajectories bring significant contribution to the path integral, and no path really needs to be considered if the neighbouring path has a different action [8, p 29]. It is known that the amplitude for an event is the sum of the amplitudes for the various alternative ways that the event can occur. 'This permits the amplitude to be analysed in many different ways depending on the different classes into which the alternatives can be divided' [8, p 20]. We consider only the paths in the vicinity of the classical trajectories, and then we divide them into classes by putting into the same class the paths corresponding to the same classical trajectory. In order to make this partition intuitive, following the method of conceptual experiments presented in the book of Feynman and Hibbs, one can imagine a crystal as a very complicated network of screens which allow a particle only to jump between neighbouring atoms, and lead to only a discrete set of alternatives. On the other hand, in many cases a path integral may be reduced by using a quantum action instead of the classical action to a sum over classical paths only [22].

The discrete version of path integral we consider is a particular case for the discrete quantum mechanics [16]. It is known that this general formalism based on the fundamental principles of quantum mechanics leads in certain cases to results in good agreement with classical path integral and quantum mechanics [12, 14, 15]. We think that the same situation may occur in the case of our model for an adequate choice of the stochastic one-step transition amplitude. Formula (54) and the numerical data presented for $K_j((o,k),(x,l))$ show that these maps have the expected behaviour. In our description each 'state' (x,k) of the particle

is described by a position parameter x and an additional parameter $k \in \{1, 2, \ldots, n\}$. This description is in agreement with the description used by Ord and Deakin [25, 26] in their attempt to find a microscopic model for the Schrödinger equation.

The existing direct comparison of the discrete quantum mechanics with Schrödinger equation concern some simple quantum systems. It seems to be very difficult to obtain such a result in the case of a diamond-type crystal or a carbon nanotube described using an additional axis. The use of a nonholonomic mapping and the general theory of path integral in spaces with curvature and torsion [21] may be useful in such an attempt. We think that the application of discrete quantum mechanics to crystal physics considered in this paper is at least a useful toy model. Improved variants of this model can be obtained by using the results from [12–16].

References

[1] Birman J L 1982 Lattice dynamics-phonon symmetry and selection rules *Handbook on Semiconductors* vol 1 ed T S Moss (Amsterdam: North-Holland) pp 40–8

[2] Cotfas N 1991 Diamond structure in a natural description *J. Phys.: Condens. Matter* **3** 9279–96

[3] Cotfas N 1995 A mathematical model for diamond-type crystals *J. Phys. A: Math. Gen.* **28** 1371–9

[4] Cotfas N 2000 Random walks on carbon nanotubes and quasicrystals *J. Phys. A: Math. Gen.* **33** 2917–27

[5] Cycon H L, Froese R G, Kirsch W and Simon B 1987 *Schrödinger Operators with Application to Quantum Mechanics and Global Geometry* (Berlin: Springer) pp 164–5

[6] Damnjanović M, Milošević I, Vuković T and Sredanović R 1999 Symmetry and lattices of single-wall nanotubes *J. Phys. A: Math. Gen.* **32** 4097–104

[7] Feynman R P 1948 Space-time approach to non-relativistic quantum mechanics *Rev. Mod. Phys.* **20** 367–87

[8] Feynman R P and Hibbs R A 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)

[9] Feynman R P 1955 Slow electrons in a polar crystal *Phys. Rev.* **97** 660–5

[10] Ghatak A K and Kothari L S 1972 *An Introduction to Lattice Dynamics* (London: Addison-Wesley) pp 219–26

[11] Goringe C M, Bowler D R and Hernández E 1997 Tight-binding modelling of materials *Rep. Prog. Phys.* **60** 1447–512

[12] Gudder S 1988 *Quantum Probability* (Boston: Academic)

[13] Gudder S P 1986 Discrete quantum mechanics *J. Math. Phys.* **27** 1782–90

[14] Gudder S P 1988 A theory of amplitudes *J. Math. Phys.* **29** 2020–35

[15] Gudder S P 1992 Schrödinger and Dirac quantum random walks *Int. J. Theor. Phys.* **31** 1973–91

[16] Gudder S and Schindler C 1992 Quasi-discrete quantum Markov processes *Ann. Inst. Henri Poincaré* **56** 123–42

[17] Hamada N, Sawada S and Oshiyama 1992 New one-dimensional conductors: graphitic microtubules *Phys. Rev. Lett.* **68** 1579–81

[18] Jishi R A, Dresselhaus M S and Dresselhaus G 1993 Symmetry properties of chiral carbon nanotubes *Phys. Rev.* B **47** 16671–4

[19] Kasteleyn P W 1967 Graph theory and crystal physics *Graph Theory and Theoretical Physics* ed A Harary (London: Academic) pp 43–110

[20] Kireev P S 1974 *Semiconductor Physics* (Moscow: Mir) pp 103–16

[21] Kleinert H 1995 *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics* (Singapore: World Scientific)

[22] Jirari H, Kröger H, Luo X Q, Moriarty K J M and Rubin S G 2001 Closed paths integrals and the quantum action *Phys. Rev. Lett.* **86** 187–91

[23] Marbeau J and Gudder S 1989 A quantum random walk *Ann. Fond. Louis Broglie* **14** 439–59

[24] Mariot L 1959 *Groupes Finis de Symétrie et Recherche de Solutions de l'Équation de Schrödinger* (Paris: Dunod)

[25] Ord G N and Deakin A S 1996 Random walks, continuum limits, and Schrödinger equation *Phys. Rev.* A **54** 3772–8

[26] Ord G N and Deakin A S 1997 Random walks and Schrödinger's equation in (2 + 1) dimensions *J. Phys. A: Math. Gen.* **30** 819–30

[27] Roepstorff G 1994 *Path Integral Approach to Quantum Physics. An Introduction* (Berlin: Springer)

[28] Saito R, Dresselhaus G and Dresselhaus M S 2000 Trigonal wraping effect of carbon nanotubes *Phys. Rev.* B **61** 2981–90

[29] Sirotin Yu I and Shaskolskaya M P 1982 *Fundamentals of Crystal Physics* (Moscow: Mir) pp 98–101
Sirotin Yu I and Shaskolskaya M P 1982 *Fundamentals of Crystal Physics* (Moscow: Mir) pp 109–14

Sirotin Yu I and Shaskolskaya M P 1982 *Fundamentals of Crystal Physics* (Moscow: Mir) pp 129–30
[30] Streitwolf H W 1971 *Group Theory in Solid-State Physics* (London: Macdonald) pp 68–74
[31] Sütő A 1995 Schrödinger difference equation with deterministic ergodic potentials *Beyond Quasicrystals* ed F Axel and D Gratias (New York: Springer) pp 481–549
[32] White C T, Robertson D H and Mintmire J W 1993 Helical and rotational symmetries of nanoscale graphitic tubules *Phys. Rev.* B **47** 5485–8