Random walks on graphene: generating functions, state probabilities and asymptotic behavior

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Abstract

We consider a discrete-time random walk on the nodes of a graphene-like graph, i.e. an unbounded hexagonal lattice. We determine the probability generating functions, the transition probabilities and the relevant moments. The convergence of the stochastic process to a 2-dimensional Brownian motion is also discussed. Finally, we obtain some results on its asymptotic behavior making use of large deviation theory.

Keywords: Random walk; Hexagonal lattice; Probability generating function; Large deviations; Moderate deviations.

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1 Introduction

Graphene is a possible form of carbon, in which each atom constitutes the vertex of a two-dimensional honeycomb-shaped graph. Recently it has attracted large attention due to its remarkable properties. Stimulated by its potential applications in many fields of science and engineering, in this paper we aim to study a discrete-time random walk on the nodes of a graphene-like graph. We recall that some general results on discrete-time random walks on a lattice, such as the multi-dimensional integer lattice $\mathbb{Z}^d$, are described in the book by Lawler and Limic [12].

Our attention is placed on some mathematical properties of such stochastic process, where the underlying lattice state-space is viewed as a general honeycomb structure (the hexagonal lattice). Specifically, we give emphasis to the transient distribution of the random walk. We also study its asymptotic behavior making use of the theory of large deviations.

Two-dimensional random walk models on honeycomb structures deserve interest in various applied fields. For instance we recall the following:

Applications to Physics. Two-dimensional random walks on the hexagonal lattice are employed to study: the behavior of cracks between frozen regions in a dimer model (cf. Boutillier

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the representation of the correlation functions in valence-bond solid models (cf. Kennedy et al. [10]), the light transport in a honeycomb structure (cf. Miri and Stark [13]), electronic properties of deformed carbon nanotubes (cf. Schuyler et al. [16]), and the incoherent energy transfer due to long range interactions in two-dimensional regular systems (cf. Zumofen and Blumen [18]).

– **Chemical models.** A mathematical model based on a three-axes description of the honeycomb lattice has been proposed by Cotfas [4], where the movement of an excitation (or a vacancy) on a quasicrystal is regarded as a suitable random walk. A random-walk model of absorption of an isolated polymer chain on various lattice models, including the hexagonal one, is investigated in Rubin [15]. Moreover, as a model of polymer dynamics, Sokolov et al. [17] analyzed the continuous-time motion of a rigid equilateral triangle in the plane, where the center of mass of the triangle performs a random walk on the hexagonal lattice.

– **Cellular networks.** The movement of mobile users in Personal Communications Services networks, such as the honeycomb Poisson-Voronoi access cellular network model, may be captured by random walks models on the hexagonal lattice (cf. Akyildiz et al. [1], Baccelli and Blaszczyszyn [2]).

– **Biomathematics.** A correlated random walk on an hexagonal lattice has been used by Prasad and Borges [14] in order to determine the optimal movement strategy of an animal searching for resources upon a network of patches.

Our study is first finalized to obtain a closed-form result of the probability generating function and of the probability distribution of the random walk on the hexagonal lattice. This is performed by considering a partition of the state space into two sets, i.e. the states visited at even and odd times. Then, the iterative equations of the relevant probabilities for the two sets are expressed in a suitable way. A similar approach has been used by Di Crescenzo et al. [7] for the analysis of random walks in continuous time characterized by alternating rates. Some auxiliary results are also obtained, such as certain symmetry properties of the state probabilities and the relevant moments, including the covariance. The validity of a customary convergence to a 2-dimensional Brownian motion is also shown. Differently from previous investigations oriented to computing numerical quantities of interest, such as critical exponents (see de Forcrand et al. [5], for instance), our approach is mainly theoretical. Indeed, we remark that our study leads to closed-form results even in the general case of non-constant one-step transition probabilities.

Our second aim is to investigate two different forms of asymptotic behavior of the random walk on the hexagonal lattice, by making use of some applications of the Gärtner Ellis Theorem. About this topic we recall the text by Feng and Kurtz [9] for a wide study on sample path large deviations for general Markov processes.

This is the plan of the paper. The main definitions and the description of the process are given in Section 2. The probability distribution of the random walk, with the generating function and the main moments are obtained in Section 3. Finally, Section 4 is devoted to investigate the large and moderate deviations for the stochastic process under investigation.

## 2 The Random Walk

We consider the hexagonal structure of the graphene on a reference system of cartesian axes, taking match a vertex of a generic hexagon with the origin of the reference system, as shown in Fig. [1]. Since the graphene consists of hexagonal cells, with angles of $2\pi/3$, we can assume that the distance between adjacent vertices is a constant, say $a$. Hence, the coordinates
of the vertices are repeated regularly. We divide the vertices into two categories:

$$\mathcal{V}_i = \left\{ \left( \frac{3}{2} a j + i a; \frac{\sqrt{3}}{2} a j + \sqrt{3} a k \right); \ j, k \in \mathbb{Z} \right\}, \ i = 0, 1.$$  

(1)

Figure 1: Graphical representation of graphene, where the vertices of \( \mathcal{V}_0 (\mathcal{V}_1) \) are represented by white (black) circles.

Figure 2: One-step transition probabilities.

With reference to Fig. 1 we consider a random walk of a particle that starts at a vertex with coordinates \((x, y)\) and it moves to an adjacent vertex following an appropriate transition probability. In particular, as shown in Fig. 2 if the particle is located in a vertex of the set \( \mathcal{V}_0 \), it can reach the three adjacent positions with probabilities \( q_{0,0}, q_{0,1}, q_{0,2} \) and then the particle will occupy a vertex of \( \mathcal{V}_1 \). Similarly, if the particle is in a vertex of \( \mathcal{V}_1 \), in one step it reaches one of the three adjacent positions, belonging to \( \mathcal{V}_0 \), with probabilities \( q_{1,0}, q_{1,1}, q_{1,2} \) (see Fig. 2). Let \( \{(X_n, Y_n), n \in \mathbb{N}_0\} \) be the discrete-time random walk having state space \( \mathcal{V}_0 \cup \mathcal{V}_1 \) and representing the position of the particle at time \( n \). From the above assumptions, for \( i = 0, 1 \)
and \( r = 0, 1, 2 \) the one-step transition probabilities are expressed as
\[
g_{i,r} = P \left( \begin{array}{c} X_{n+1} \\ Y_{n+1} \end{array} \right) = \begin{pmatrix} x + a \cos \left( \frac{r}{3} \pi + i \pi \right) \\ y + a \sin \left( \frac{r}{3} \pi + i \pi \right) \end{pmatrix} \left| \begin{array}{c} X_n \\ Y_n \end{array} \right) = \begin{pmatrix} x \\ y \end{pmatrix},
\]
with
\[
\sum_{r=0}^{2} q_{i,r} = 1, \quad i = 0, 1.
\]

Let us now introduce the state probabilities at time \( n, n \in \mathbb{N}_0 \),
\[
p_{j,k}(n) := P \left( (X_n, Y_n) = \left( \frac{3}{2} aj + i_n a, \sqrt{\frac{3}{2}} aj + \sqrt{3} ak \right) \right), \quad j, k \in \mathbb{Z},
\]
where
\[
i_n = \frac{1}{2} (1 - (-1)^n).
\]

We assume that \( P[(X_0, Y_0) = (0, 0)] = 1 \), so that the initial condition reads
\[
p_{0,0}(0) = 1.
\]

Hence, from the previous assumptions, and noting that at even (odd) times the particle occupies states of set \( \mathcal{Y}_0 (\mathcal{Y}_1) \), the forward Kolmogorov equations for the state probabilities, for all \( n \in \mathbb{N}_0 \) are given by
\[
p_{j,k}(n + 1) = \begin{cases} p_{j,k}(n) q_{0,0} + p_{j+1,k}(n) q_{0,2} + p_{j+1,k-1}(n) q_{0,1}, & n \text{ even} \\ p_{j,k}(n) q_{1,0} + p_{j-1,k+1}(n) q_{1,1} + p_{j-1,k-1}(n) q_{1,2}, & n \text{ odd} \end{cases}
\]
with initial condition (5).

3 Probability Distribution

Now we focus on the probability generating function \( G(u, v; n) \) of \( (X_n, Y_n) \). Due to (3), it is defined as
\[
G(u, v; n) = \mathbb{E} \left[ u^{X_n} v^{Y_n} \right] = \sum_{j \in \mathbb{Z}} u^{\frac{3}{2} aj + i_n a} \sum_{k \in \mathbb{Z}} v^{\frac{3}{2} aj + \sqrt{3} ak} p_{j,k}(n),
\]
for \( u > 0 \) and \( v > 0 \).

**Proposition 1.** The explicit expression of the probability generating function \( G(u, v; n) \) of \( (X_n, Y_n) \), for \( n \in \mathbb{N}_0, u > 0 \) and \( v > 0 \) is:
\[
G(u, v; n) = F_{i_n}(\tilde{u}, \tilde{v}; n) u^{i_n a},
\]
where \( i_n \) is defined in (4), with
\[
\tilde{u} = u^{\frac{3}{2} a} e^{\frac{\sqrt{3} a}{2}}, \quad \tilde{v} = v^{\sqrt{3} a},
\]
and
\[
F_{i_n}(u, v; n) = \left( q_{1,0} + q_{1,2} u + q_{1,1} u \right)^{\frac{3}{2} - \frac{i_n}{2}} \left( q_{0,0} + q_{0,1} \frac{v}{u} + q_{0,2} \frac{1}{u} \right)^{\frac{3}{2} + \frac{1}{2} i_n}.
\]
Proof. For all \( n \in \mathbb{N}_0 \), let us define
\[
F_n(u, v; n) = \sum_{j=\infty}^{+\infty} u^j \sum_{k=-\infty}^{+\infty} v^k p_{j,k}(n),
\]
so that for \( n \) even (odd), \( F_0(u, v; n) \) (\( F_1(u, v; n) \)) is the probability generating function of \((X_n, Y_n)\) for the vertex set \( \mathcal{V}_0 (\mathcal{V}_1) \) defined in (1). Due to Eq. (6) we have
\[
\phi^{(n+1)} = M \phi^{(n)},
\]
where
\[
M = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix}, \quad \phi^{(n)} = \begin{pmatrix} F_0(u, v; n) \\ F_1(u, v; n) \end{pmatrix},
\]
with
\[
\alpha = \alpha(u, v) = q_{1,0} + q_{1,2} u + q_{1,1} \frac{v}{u}, \\
\beta = \beta(u, v) = q_{0,0} + q_{0,1} \frac{v}{u} + q_{0,2} \frac{1}{u}.
\]
Due to initial condition (5) we have \( \phi^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \), so that the system (12) has solution:
\[
\phi^{(n)} = M^n \phi^{(0)},
\]
where
\[
M^n = \begin{pmatrix} \alpha^{\frac{n}{2}} \beta^{\frac{n}{2}} & 0 \\ 0 & \alpha^{\frac{n}{2}} \beta^{\frac{n}{2}} \end{pmatrix}, \quad \text{if } n \text{ is even,}
\]
\[
M^n = \begin{pmatrix} 0 & \alpha^{\frac{n+1}{2}} \beta^{\frac{n+1}{2}} \\ \alpha^{\frac{n}{2}} \beta^{\frac{n}{2}} & 0 \end{pmatrix}, \quad \text{if } n \text{ is odd.}
\]
Recalling (13), we have the following explicit expressions:
\[
F_0(u, v; n) = \begin{cases} \alpha^{\frac{n}{2}} \beta^{\frac{n}{2}}, & n \text{ even } \\ 0, & n \text{ odd} \end{cases}, \quad F_1(u, v; n) = \begin{cases} 0, & n \text{ even } \\ \alpha^{\frac{n+1}{2}} \beta^{\frac{n+1}{2}}, & n \text{ odd.} \end{cases}
\]
Now, noting that the generating function (7) can be written, due to (11), as
\[
G(u, v; n) = \begin{cases} F_0(\tilde{u}, \tilde{v}; n), & n \text{ even } \\ F_1(\tilde{u}, \tilde{v}; n) u^{\alpha}, & n \text{ odd} \end{cases},
\]
by comparing this last expression with (11), (14), (15), and by taking into account (9), the thesis (8) follows. \( \square \)

Let us recall the Gauss hypergeometric function
\[
2F_1(a, b; c; z) = \sum_{n=0}^{+\infty} \frac{(a)_n(b)_n}{(c)_n} \frac{z^n}{n!},
\]
where \((a)_n\) is the Pochhammer symbol defined as \((a)_n = a(a+1) \ldots (a + n - 1)\) for \( n \in \mathbb{N} \) and \((a)_0 = 1\).

We now determine the state probabilities of \((X_n, Y_n)\).
Proposition 2. Let $m \in \mathbb{N}$, and
\[
\rho = \frac{q_{0,1} q_{1,1}}{q_{0,2} q_{1,2}}.
\] (17)

(i) For $0 \leq j \leq m$ and $-m \leq k \leq 0$,
\[
p_{j,k}(2m) = \sum_{t=0}^{m-j} \binom{m}{t} \binom{m}{j+t} \binom{m-t}{-k} q_{0,0}^{m-t} q_{1,0}^{m-j-t} q_{0,2}^t q_{1,2}^{j+k+t} q_{1,1}^{-k} \times 2F_1 \left( -j - k - t, -t; 1 - k; \rho \right).
\]

(ii) For $0 \leq j \leq m$ and $1 \leq k \leq m - j$,
\[
p_{j,k}(2m) = \sum_{t=-k}^{m-j} \binom{m}{t} \binom{m}{j+t} \binom{t}{k} q_{0,0}^{m-t} q_{1,0}^{m-j-t} q_{0,1}^k q_{0,2}^{-k+t} q_{1,2}^{-j-k} \times 2F_1 \left( -j - k - t, -t; 1 + k; \rho \right).
\]

(iii) For $-m \leq j \leq -1$ and $-m - j \leq k \leq -1$,
\[
p_{j,k}(2m) = \sum_{t=-k}^{m+j} \binom{m}{t} \binom{m}{j+t} \binom{t}{-k} q_{0,0}^{m+j-t} q_{1,0}^{m-j-t} q_{0,2}^k q_{1,2}^{-j-t} q_{1,1}^{-k} \times 2F_1 \left( j - t, -k - t; 1 - k; \rho \right).
\]

(iv) For $-m \leq j \leq -1$ and $0 \leq k \leq m$,
\[
p_{j,k}(2m) = \sum_{t=0}^{m+j} \binom{m}{t} \binom{m}{j+t} \binom{-j+t}{k} q_{0,0}^{m-t} q_{1,0}^{m+j-t} q_{0,1}^{-k} q_{0,2}^{-j-k+t} q_{1,2}^{i} \times 2F_1 \left( j + k - t, -t; 1 + k; \rho \right).
\]

Proof. By extracting the coefficients of $w^j$ and $v^k$ in Eq. (11) for $i = 0$, making use of definition (16) and recalling that
\[
(x)_n = \frac{(-1)^n}{(1-x)^n}, \quad n \in \mathbb{Z},
\]
the proof then follows after cumbersome calculations. \hfill \Box

Some plots of the distribution (3) are shown in Fig. 3. Symmetry properties of two-dimensional stochastic processes are often encountered in various applications (see, for instance, Proposition 2.1 of Di Crescenzo and Martinucci [8] for a family of two-dimensional continuous-time random walks). Hereafter we exploit various symmetry properties for the transition probabilities given in Proposition 2.

Corollary 1. From Proposition 2 the following symmetry properties hold for $m \in \mathbb{N}$.

(i) For $-m \leq j \leq m$ and $-m \leq k \leq m$ we have
\[
p_{j,k}(2m) = \xi^{2k+j} p_{j,-j-k}(2m), \quad \text{for} \quad \frac{q_{0,1}}{q_{0,2}} = \frac{q_{1,2}}{q_{1,1}} = \xi.
\]

(ii) For $-m \leq j \leq m$ and $-m \leq k \leq m$, if $q_{0,1} = q_{1,2}$ and $q_{1,1} = q_{0,2}$, we have
\[
p_{j,k}(2m) = \delta^{2k+j} p_{j,-j-k}(2m), \quad \text{for} \quad \frac{q_{0,1}}{q_{1,1}} = \frac{q_{1,2}}{q_{0,2}} = \delta.
\]

(iii) For $-m \leq j \leq m$ and $-m \leq k \leq m$, if $q_{0,1} = q_{1,2}$ and $q_{1,1} = q_{0,2}$, we have
\[
p_{j,k}(2m) = p_{-j,j+k}(2m).
\]
We remark that in all cases treated in Corollary 1 from (17) we have $\rho = 1$.

We point out that the state probabilities given in Proposition 2 can be evaluated for odd times making use of equation (6). Specifically, it is not hard to see that $p_{j,k}(2m+1) > 0$ for $0 \leq j \leq m$ and $-m \leq k \leq m-j$, and for $-m-1 \leq j \leq -1$ and $-m-j-1 \leq k \leq m+1$. Hence, Corollary 1 can be extended to the case of odd times.

Denoting by $X_i$ the amplitude of the $i$-th step on the $x$ axis and by $Y_i$ the amplitude of the $i$-th step on the $y$ axis, for $i = 1, 2, \ldots, n$, the random walk $(X_n, Y_n)$ can be expressed as

$$S_n := \begin{pmatrix} X_n \\ Y_n \end{pmatrix} = \begin{pmatrix} \tilde{X}_1 + \tilde{X}_2 + \ldots + \tilde{X}_n \\ \tilde{Y}_1 + \tilde{Y}_2 + \ldots + \tilde{Y}_n \end{pmatrix}, \quad n \in \mathbb{N},$$

(18)

the joint distribution of $(\tilde{X}_i, \tilde{Y}_i)$ being given by Eq. (2).

Let us now determine some moments of interest.

Figure 3: Plot of $10^2 p_{j,k}(n)$ for $q_{i,r} = 1/3$ for all $i, r$ (on the left), and $q_{i,0} = 1/2, q_{i,1} = q_{i,2} = 1/4$ for $i = 0, 1$ (on the right).
Proposition 3. For all $n \in \mathbb{N}$, for the random vector $S_n$ defined in (18) the vector mean is:

$$m_n := \left( \begin{array}{c} \mathbb{E}(X_n) \\ \mathbb{E}(Y_n) \end{array} \right) = \left( \begin{array}{c} \mu_1 n + \theta_1 i_n \\ \mu_2 n + \theta_2 i_n \end{array} \right),$$

(19)

where $i_n$ is defined in (4), and

$$\mu_1 = \frac{3}{4} a \left[ (q_{1,1} + q_{1,2}) - (q_{0,1} + q_{0,2}) \right], \quad \theta_1 = a - \frac{3}{4} a \left[ (q_{1,1} + q_{1,2}) + (q_{0,1} + q_{0,2}) \right],$$

$$\mu_2 = \frac{\sqrt{3}}{4} a \left[ (q_{0,1} - q_{0,2}) - (q_{1,1} - q_{1,2}) \right], \quad \theta_2 = \frac{\sqrt{3}}{4} a \left[ (q_{0,1} - q_{0,2}) + (q_{1,1} - q_{1,2}) \right].$$

The variance of $S_n$ is expressed as

$$\left( \begin{array}{c} \text{Var}(X_n) \\ \text{Var}(Y_n) \end{array} \right) = \left( \begin{array}{c} \sigma_1^2 n + \theta_3 i_n \\ \sigma_2^2 n + \theta_4 i_n \end{array} \right),$$

where

$$\sigma_1^2 = \frac{9}{8} a^2 \left[ (q_{0,1} + q_{0,2}) - (q_{0,1} + q_{0,2})^2 + (q_{1,1} + q_{1,2}) - (q_{1,1} + q_{1,2})^2 \right],$$

$$\theta_3 = \frac{9}{8} a^2 \left[ (q_{0,1} + q_{0,2}) - (q_{0,1} + q_{0,2})^2 - (q_{1,1} + q_{1,2}) + (q_{1,1} + q_{1,2})^2 \right],$$

$$\sigma_2^2 = \frac{3}{8} a^2 \left[ (q_{0,1} + q_{0,2}) - (q_{0,1} - q_{0,2})^2 + (q_{1,1} + q_{1,2}) - (q_{1,1} - q_{1,2})^2 \right],$$

$$\theta_4 = \frac{3}{8} a^2 \left[ (q_{0,1} + q_{0,2}) - (q_{0,1} - q_{0,2})^2 - (q_{1,1} + q_{1,2}) + (q_{1,1} - q_{1,2})^2 \right].$$

Finally, the expression of the covariance is

$$\text{Cov}(X_n, Y_n) = \sigma_{1,2} n + \theta_5 i_n,$$

where

$$\sigma_{1,2} = \frac{3 \sqrt{3}}{8} a^2 \left[ q_{0,1}(q_{0,1} - 1) + q_{0,2}(1 - q_{0,2}) - q_{1,1}(1 - q_{1,1}) + q_{1,2}(1 - q_{1,2}) \right],$$

$$\theta_5 = \frac{3 \sqrt{3}}{8} a^2 \left[ q_{0,1}(q_{0,1} - 1) + q_{0,2}(1 - q_{0,2}) + q_{1,1}(1 - q_{1,1}) - q_{1,2}(1 - q_{1,2}) \right].$$

Proof. The proof follows making use of the moment generating function obtained in Proposition 3.

We are now able to state a central limit theorem for the considered random walk.

Proposition 4. Let $S_n$ be the random vector defined in (18), and $m_n$ its mean given in (19). Then, as $n \to \infty$,

$$n^{-1/2}(S_n - m_n)$$

converges weakly to the centered bivariate normal distribution with covariance matrix $C$, where

$$C := \left( \begin{array}{cc} \sigma_1^2 & \sigma_{1,2} \\ \sigma_{1,2} & \sigma_2^2 \end{array} \right),$$

(20)

whose elements are expressed in Proposition 3.
Proof. The proof follows noting that $(\tilde{X}_i, \tilde{Y}_i)$, $i = 1, 2, \ldots$, are independent and $(\tilde{X}_{2i-1} + \tilde{X}_{2i}, \tilde{Y}_{2i-1} + \tilde{Y}_{2i})$, $i = 1, 2, \ldots$, are identically distributed. 

Hereafter we discuss another form of convergence to the bivariate normal distribution, which involves also a scaling of the hexagonal lattice, and a convergence to Brownian motion.

Remark 1. Let $\{S^*_k(t); t \geq 0\}_{k \in \mathbb{N}}$ be a sequence of continuous-time stochastic processes defined in terms of the random vector $(\mathbf{I}_k, \mathbf{S}_k)$, such that

$$S^*_k(t) = S_{[t]k}|_{a \equiv a/\sqrt{k}} = \frac{1}{\sqrt{k}} S_{[t]k}, \quad t \geq 0.$$ 

Hence, from Proposition 4 it follows that, as $k \to \infty$,

$$[t]^{-\frac{1}{2}} [S^*_k(t) - \mathbb{E}(S^*_k(t))]$$

converges weakly to the centered bivariate normal distribution with covariance matrix $[20]$.

Remark 2. As application of the multidimensional Donsker’s Theorem, and by Proposition 4 the normalized partial-sum process

$$S_n(t) := n^{-1/2}(S_{[nt]} - m_{[nt]}), \quad t \geq 0,$$

converges weakly to $BD$ (as $n \to \infty$), where $B$ is the standard 2-dimensional Brownian motion, and $D$ is a $2 \times 2$ matrix such that $D^T D = C$, with $C$ defined in (20). In other words we mean $BD \equiv \{B(t;0,C) : t \geq 0\}$, where $B(t;0,C)$ denotes the 2-dimensional Brownian motion with drift vector 0 and covariance matrix $C$.

4 Large and Moderate Deviations

We start this section by recalling some well-known basic definitions in large deviations (see [6] as a reference on this topic). A sequence of positive numbers $\{v_n : n \geq 1\}$ is called speed if $\lim_{n \to \infty} v_n = \infty$. Given a topological space $Z$, a lower semi-continuous function $I : Z \to [0, \infty]$ is called rate function; moreover, if the level sets $\{\{z \in Z : I(z) \leq \eta\} : \eta \geq 0\}$ are compact, the rate function $I$ is said to be good. Finally a sequence of random variables $\{Z_n : n \geq 1\}$, taking values on a topological space $Z$, satisfies the large deviation principle (LDP for short) with speed $v_n$ and rate function $I$ if

$$\liminf_{n \to \infty} \frac{1}{v_n} \log P(Z_n \in O) \geq - \inf_{z \in O} I(z)$$

for all open sets $O$ and

$$\limsup_{n \to \infty} \frac{1}{v_n} \log P(Z_n \in C) \leq - \inf_{z \in O} I(z)$$

for all closed sets $C$.

In this section we prove two results:

1. the LDP of $\{(\frac{X_n}{n}, \frac{Y_n}{n}) : n \geq 1\}$, with speed $v_n = n$;

2. for all sequences of positive numbers $\{a_n : n \geq 1\}$ such that $a_n \to 0$ and $na_n \to \infty$ (as $n \to \infty$),

$$\sqrt{na_n} \left(\frac{X_n - \mathbb{E}(X_n)}{n}, \frac{Y_n - \mathbb{E}(Y_n)}{n}\right) : n \geq 1,$$

the LDP of $\left\{\frac{X_n - \mathbb{E}(X_n)}{n}, \frac{Y_n - \mathbb{E}(Y_n)}{n} : n \geq 1\right\}$, with speed function $1/a_n$. 

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In both cases we prove the LDPs with an application of Gärtner Ellis Theorem (see e.g. Theorem 2.3.6 in [6]).

We start with the first result which allows to say that
\[
\left( \frac{X_n}{n}, \frac{Y_n}{n} \right) \to (\mu_1, \mu_2) \quad (\text{as } n \to \infty)
\]
(note that in particular we have
\[
\frac{E(X_n)}{n} \to \mu_1 \quad \text{and} \quad \frac{E(Y_n)}{n} \to \mu_2 \quad (\text{as } n \to \infty)
\]
by Proposition [3].

**Proposition 5.** The sequence \( \left\{ \left( \frac{X_n}{n}, \frac{Y_n}{n} \right) : n \geq 1 \right\} \) satisfies the LDP, with speed \( v_n = n \), and good rate function \( \Lambda^* \) defined by
\[
\Lambda^*(x, y) := \sup_{(\lambda_1, \lambda_2) \in \mathbb{R}^2} \left\{ \lambda_1 x + \lambda_2 y - \Lambda(\lambda_1, \lambda_2) \right\},
\]
where
\[
\Lambda(\lambda_1, \lambda_2) = \frac{1}{2} \log \left( g_0(\lambda_1, \lambda_2) g_1(\lambda_1, \lambda_2) \right),
\]
and
\[
g_i(\lambda_1, \lambda_2) = q_{i,0} + q_{i,1} e^{(-1)^i \sqrt{3} a \left( \frac{\sqrt{3}}{2} \lambda_1 + \frac{1}{2} \lambda_2 \right)} + q_{i,2} e^{(-1)^i \sqrt{3} a \left( \frac{\sqrt{3}}{2} \lambda_1 + \frac{1}{2} \lambda_2 \right)}, \quad i = 0, 1.
\]

**Proof.** We have to check that
\[
\lim_{n \to +\infty} \frac{1}{n} \log G(e^{\lambda_1}, e^{\lambda_2}; n) = \Lambda(\lambda_1, \lambda_2) \quad (\text{for all } (\lambda_1, \lambda_2) \in \mathbb{R}^2),
\]
where \( \Lambda \) is the function in (22). Then the LDP will follow from a straightforward application of Gärtner Ellis Theorem because the function \( \Lambda \) is finite and differentiable. In order to do that we remark that
\[
G(e^{\lambda_1}, e^{\lambda_2}; n) = \begin{cases} 
F_0(e^{\sqrt{3} a \left( \frac{\sqrt{3}}{2} \lambda_1 + \frac{1}{2} \lambda_2 \right)}, e^{\lambda_2 \sqrt{3} a}; n), & n \text{ even} \\
F_1(e^{\sqrt{3} a \left( \frac{\sqrt{3}}{2} \lambda_1 + \frac{1}{2} \lambda_2 \right)}, e^{\lambda_2 \sqrt{3} a}; n), & n \text{ odd}
\end{cases}
\]
by (8). Then, by recalling the expression of \( F_1 \) in (10), one has
\[
\frac{1}{n} \log G(e^{\lambda_1}, e^{\lambda_2}; n) = \begin{cases} 
\frac{1}{2} \log [g_0(\lambda_1, \lambda_2) g_1(\lambda_1, \lambda_2)], & n \text{ even} \\
\frac{1}{n} \lambda_1 a + \frac{1}{2} \log [g_0(\lambda_1, \lambda_2) g_1(\lambda_1, \lambda_2)] + \frac{1}{n} \log [g_1^{-1}(\lambda_1, \lambda_2) g_0(\lambda_1, \lambda_2)]^{1/2}, & n \text{ odd}
\end{cases}
\]
from which the thesis follows by taking the limit for \( n \to +\infty. \)
Remark 3. From (22) and (23), if \( q_{i,r} = \frac{1}{3} \) for all \( i = 0, 1 \) and \( r = 0, 1, 2 \), it results

\[
\Lambda(\lambda_1, \lambda_2) = \frac{1}{2} \log \left( \frac{1}{3} + \frac{2}{9} \left\{ \cosh \left[ \sqrt{3}a \left( \frac{\sqrt{3}}{2} \lambda_1 - \frac{1}{2} \lambda_2 \right) \right] + \cosh \left[ \sqrt{3}a \left( \frac{\sqrt{3}}{2} \lambda_1 + \frac{1}{2} \lambda_2 \right) \right] \right\} \right).
\]

The next result provides a class of LDPs for centered random variables which fill the gap between a convergence to zero and an asymptotic Normality result (here we mean the asymptotic Normality result in Proposition 4 above; see also Remark 5 below). The term used for this class of LDPs is moderate deviations.

**Proposition 6.** For all sequences of positive numbers \( \{a_n : n \geq 1\} \) such that (21) holds, the sequence \( \left\{ \sqrt{n/a_n} \left( X_n - \mathbb{E}(X_n), Y_n - \mathbb{E}(Y_n) \right) : n \geq 1 \right\} \) satisfies the LDP, with speed \( 1/a_n \), and good rate function \( \tilde{\Lambda}^* \) defined by

\[
\tilde{\Lambda}^*(x, y) := \sup_{(\lambda_1, \lambda_2) \in \mathbb{R}^2} \{ \lambda_1 x + \lambda_2 y - \tilde{\Lambda}(\lambda_1, \lambda_2) \}, \tag{24}
\]

where

\[
\tilde{\Lambda}(\lambda_1, \lambda_2) := \frac{1}{2} (\lambda_1, \lambda_2) C \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix}, \tag{25}
\]

and \( C \) is the matrix defined by (20), whose elements are expressed in Proposition 5.

**Proof.** We have to check that

\[
\lim_{n \to +\infty} \tilde{\Lambda}_n(\lambda_1, \lambda_2) = \tilde{\Lambda}(\lambda_1, \lambda_2) \text{ (for all } (\lambda_1, \lambda_2) \in \mathbb{R}^2 \text{)},
\]

where

\[
\tilde{\Lambda}_n(\lambda_1, \lambda_2) := a_n \left( \log G(e^{\lambda_1/\sqrt{n/a_n}}, e^{\lambda_2/\sqrt{n/a_n}}; n) - \frac{\lambda_1 \mathbb{E}(X_n) + \lambda_2 \mathbb{E}(Y_n)}{\sqrt{n/a_n}} \right)
\]

and \( \tilde{\Lambda} \) is the function in (25). Then the LDP will follow from a straightforward application of Gärtner-Ellis Theorem because the function \( \Lambda \) is finite and differentiable. In order to do that, by taking into account \( na_n \to \infty \) (by (21)), we consider the Mac Laurin formula of order 2 of

\[
\Psi_n(\lambda_1, \lambda_2) := \log G \left( e^{\lambda_1/\sqrt{n/a_n}}, e^{\lambda_2/\sqrt{n/a_n}}; n \right)
\]

namely

\[
\Psi_n(\lambda_1, \lambda_2) = \frac{\lambda_1 \mathbb{E}(X_n) + \lambda_2 \mathbb{E}(Y_n)}{\sqrt{n/a_n}} + \frac{1}{2} \left( \frac{\lambda_1^2}{na_n} \mathbb{V}ar(X_n) + \frac{\lambda_2^2}{na_n} \mathbb{V}ar(Y_n) + 2 \frac{\lambda_1 \lambda_2}{na_n} \mathbb{C}ov(X_n, Y_n) + o \left( \frac{1}{na_n} \right) \right).
\]

Then we obtain

\[
\tilde{\Lambda}_n(\lambda_1, \lambda_2) = a_n \left( \frac{1}{2} \left( \frac{\lambda_1^2}{na_n} \mathbb{V}ar(X_n) + \frac{\lambda_2^2}{na_n} \mathbb{V}ar(Y_n)
\right.
\]

\[
+ 2 \frac{\lambda_1 \lambda_2}{na_n} \mathbb{C}ov(X_n, Y_n) + o \left( \frac{1}{na_n} \right) \right)
\]

\[
= \frac{1}{2} \left( \frac{\lambda_1^2}{n} \mathbb{V}ar(X_n) + \frac{\lambda_2^2}{n} \mathbb{V}ar(Y_n) + 2 \frac{\lambda_1 \lambda_2}{n} \mathbb{C}ov(X_n, Y_n) + o \left( \frac{1}{n} \right) \right).
\]
We conclude noting that the desired limit holds because
\[
\frac{\text{Var}(X_n)}{n} \to \sigma_1^2, \quad \frac{\text{Var}(Y_n)}{n} \to \sigma_2^2, \quad \frac{\text{Cov}(X_n, Y_n)}{n} \to \sigma_{1,2} \quad \text{(as } n \to \infty)\
\]
by Proposition\[3\] and by taking into account the function \(\tilde{\Lambda}\) in \(25\).

**Remark 4.** If \(C\) is invertible, then the supremum in \(24\) is attained at \((\lambda_1, \lambda_2) = C^{-1}(x, y)\) and we get
\[
\tilde{\Lambda}^\ast(x, y) = \frac{1}{2}(x, y)C^{-1}(x, y) \quad \text{(for all } (x, y) \in \mathbb{R}^2)\).
\]

**Remark 5.** A close inspection of the proof of Proposition\[6\] reveals that all the computations for moderate deviations work well even if \(a_n = 1\); note that in such a case the first condition in \(27\) fails. Thus, for all \((\lambda_1, \lambda_2) \in \mathbb{R}^2,\)
\[
\lim_{n \to \infty} \log \mathbb{E} \left[ \exp \left( \frac{\lambda_1 X_n - \mathbb{E}(X_n)}{\sqrt{n}} + \frac{\lambda_2 Y_n - \mathbb{E}(Y_n)}{\sqrt{n}} \right) \right] = \frac{1}{2}(\lambda_1, \lambda_2)C(\lambda_1, \lambda_2),
\]
and therefore \(\left\{ \left( \frac{X_n - \mathbb{E}(X_n)}{\sqrt{n}}, \frac{Y_n - \mathbb{E}(Y_n)}{\sqrt{n}} \right) : n \geq 1 \right\}\) converges weakly (as \(n \to \infty\)) to the centered bivariate Normal distribution with covariance matrix \(C\) (cfr. Proposition\[7\]).

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