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constants for a random walk in a heterogeneous environment

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A Markov Chain Identity and Monotonicity of the Diffusion Constants for a Random Walk in a Heterogeneous Environment

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We consider a 2-D square lattice which is partitioned into a periodic array of rectangular cells, on which a nearest neighbor random walk with symmetric increments is defined whose transition probabilities only depend on the relative position within a cell. On the basis of a determinantal identity proved in this paper, we obtain a result for finite Markov chains which shows that the diffusion constants for the random walk are monotonic functions of the individual transition probabilities. We point out the similarity of this monotonicity property to Rayleigh's Monotonicity Law for electric networks or, equivalently, reversible random walks.

1980 Mathematics Subject Classification: 15A15, 15A51, 60J10, 60J15, 82A42

Keywords & Phrases: Random walk with symmetric increments, inhomogeneously periodic environment, anisotropic scatterers, determinantal identity, Markov chain identity, monotonicity of diffusion constants, Rayleigh's Monotonicity Law.

1. INTRODUCTION

Consider the following random walk on \mathbb{Z}^2 with site-dependent transition probabilities. Define a rectangular unit cell with N sites to be the subset $U = \{1, 2, \dots, m_1\} \times \{1, 2, \dots, m_2\} \subset \mathbb{Z}^2$, where m_1 and m_2 are integers denoting the width and height of the unit cell ($m_1 m_2 = N$). A so-called "inhomogeneously periodic" 2-D square lattice is obtained by repeating this unit cell periodically in two independent directions, such that the copies of the unit cell cover the grid \mathbb{Z}^2 without overlap, see Fig. 1. The translation vectors $\mathbf{a}_1 \in \mathbb{Z}^2$ and $\mathbf{a}_2 \in \mathbb{Z}^2$ defining the partition into cells are not necessarily orthogonal, see Fig. 2, where $\mathbf{a}_1 = 3\mathbf{e}_1 - \mathbf{e}_2$, $\mathbf{a}_2 = 3\mathbf{e}_2$, with \mathbf{e}_1 and \mathbf{e}_2 the standard unit vectors in \mathbb{Z}^2 . Any point \mathbf{r} on the lattice has a representation $\mathbf{r}(\ell, \alpha) = \ell_1 \mathbf{a}_1 + \ell_2 \mathbf{a}_2 + \alpha_1 \mathbf{e}_1 + \alpha_2 \mathbf{e}_2$, where the vector $\ell = (\ell_1, \ell_2) \in \mathbb{Z}^2$ serves to indicate the position of a translate of the unit cell and the vector $\alpha = (\alpha_1, \alpha_2) \in U$ denotes the relative position within a cell. To each site α in the unit cell assign a real variable p_α , $-1/4 < p_\alpha < 1/4$. A periodic environment with unit cell U is the map $e: \mathbb{Z}^2 \rightarrow \{p_\alpha: \alpha \in U\}$ given by

$$\begin{aligned} e(\mathbf{r}) &= e(\mathbf{r} + \ell_1 \mathbf{a}_1 + \ell_2 \mathbf{a}_2) & \mathbf{r} \in \mathbb{Z}^2, \\ e(\mathbf{r}) &= p_\alpha & \mathbf{r} \in U. \end{aligned}$$

Then a nearest neighbor random walk $X_j \in \mathbb{Z}^2$ with symmetric increments is defined by the transition probabilities

$$P\{X_{j+1} - X_j = \pm \mathbf{e}_1\} = 1/2 - P\{X_{j+1} - X_j = \pm \mathbf{e}_2\} = 1/4 + e(X_j).$$

In other words, to each site α in the unit cell is assigned a transition probability $h_\alpha = 1/4 + p_\alpha$ in the positive and negative x -direction, and $v_\alpha = 1/4 - p_\alpha$ in the positive and negative y -direction (see Fig. 3), and this assignment is repeated periodically. Sites with this type of transition probabilities have previously been termed *anisotropic scatterers* [6-9]. The site-symmetry in the positive and negative space directions causes the single-step averages of the horizontal and vertical displacements from every site to be zero. We call random walks with this property *locally unbiased*. Instead of infinite lattices we also consider finite lattices consisting of a single unit cell with periodic boundary conditions. In both cases we will speak of the "anisotropic scatterer model".

Report AM-R8917

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Figure 1. Construction of a 2-D lattice from a 3 by 3 unit cell with toroidal boundary conditions: $\mathbf{a}_1 = (3,0), \mathbf{a}_2 = (0,3)$.

•7 •8 •9	•7 •8 •9	
•4 •5 •6	•7 •8 •9	
•1 •2 •3	•4 •5 •6	•7 •8 •9
•7 •8 •9	•1 •2 •3	•4 •5 •6
•4 •5 •6	•7 •8 •9	•1 •2 •3
•1 •2 •3	•4 •5 •6	•7 •8 •9
	•1 •2 •3	•4 •5 •6
		•1 •2 •3

Figure 2. Construction of a 2-D lattice from a 3 by 3 unit cell with helical boundary conditions: $\mathbf{a}_1 = (3, -1), \mathbf{a}_2 = (0,3)$.

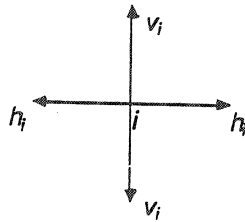


Figure 3. Transition probabilities of the anisotropic scatterer model.

In our previous work on the anisotropic scatterer model, we have paid special attention to the diffusion constants, as defined below, for this model [7-9]. Explicit computation of these constants is only feasible for small size N of the unit cell [7]. It is therefore of interest to establish qualitative properties of the diffusion constants, such as upper and lower bounds [9]. In this paper we will look at the dependence of the diffusion constants on the transition probabilities h_α and v_α . It appears to be “self-evident” that as the horizontal transition probability from one of the sites increases, diffusion in the horizontal direction increases as well. Our task will be to substantiate this intuition by mathematical proof.

We start by giving a definition of the diffusion constants. Both for the finite and the infinite lattice we define the total displacement $x(n)$ in the horizontal direction after n steps by

$$x(n) = \sum_{j=1}^n x_j,$$

where x_j is 1 or -1 if the j th step is in the positive or negative x -direction and zero otherwise. A similar definition holds for the total displacement $y(n)$ in the vertical direction. The horizontal and vertical diffusion constants of the random walk are defined by [6],

$$D_x := 1/2 \lim_{n \rightarrow \infty} \langle x^2(n) \rangle, \quad (1.1a)$$

$$D_y := 1/2 \lim_{n \rightarrow \infty} \langle y^2(n) \rangle, \quad (1.1b)$$

where the brackets denote an average over all realizations of the walk (notice that $\langle x(n) \rangle = \langle y(n) \rangle = 0$, since the walk is locally unbiased).

The calculation of the diffusion constants proceeds as follows [6,7]. For the finite lattice, let T be the N by N transition matrix of the associated finite Markov chain with N states. For the infinite inhomogeneously periodic lattice we define a similar matrix in the following way [6,7]. Let the position of the walker be indexed by (ℓ, α) , where ℓ denotes the cell occupied by the walker and α the relative position within the cell (“internal state”). Let the single-step transition probability from site (ℓ, γ) to site (ℓ, α) be denoted by $T_{\alpha\gamma}(\ell, \ell)$, which equals $T_{\alpha\gamma}(\ell - \ell)$ because of periodicity. Then an embedded (or lumped [2]) finite state Markov chain with N states is constructed by ignoring the cell the walker occupies and only taking his internal state into account. The corresponding transition matrix T has matrix elements^{*)}

$$T_{\alpha\gamma} = \sum_{\ell \in \mathbb{Z}^2} T_{\alpha\gamma}(\ell).$$

In the sequel T will always denote the transition matrix of the Markov chain on the finite lattice or, in the case of an infinite inhomogeneously periodic lattice, of the embedded Markov chain on the unit cell U . If the (embedded) Markov chain is ergodic there exists a unique stationary distribution vector π which is the normalized right eigenvector^{*)} of the matrix T corresponding to the eigenvalue $\lambda_0 = 1$. For the anisotropic scatterer problem as defined above ergodicity holds and the diffusion constants are given by [7],

$$D_x = \sum_{\alpha=1}^N h_\alpha \pi_\alpha = \frac{1}{4} + \sum_{\alpha=1}^N p_\alpha \pi_\alpha, \quad (1.2a)$$

$$D_y = \sum_{\alpha=1}^N v_\alpha \pi_\alpha = \frac{1}{4} - \sum_{\alpha=1}^N p_\alpha \pi_\alpha. \quad (1.2b)$$

To write down the transition matrix T for the geometry of Fig. 1, we label the sites in the unit cell by a double index (ij) , where i runs in the horizontal and j in the vertical direction

^{*)} We use column-stochastic matrices: $T_{\alpha\gamma}$ is the probability to go from state γ to state α , stationary distributions are right eigenvectors.

($i=1,2,\dots,m_1, j=1,2,\dots,m_2$). Denoting the matrix elements by $\langle ij|T|i'j'\rangle$, we have [7]

$$\langle ij|T|i'j'\rangle = (1/4+p_{i'j'})\{\delta_{i',i+1}+\delta_{i',i-1}\}\delta_{j,j'} + (1/4-p_{i'j'})\{\delta_{j',j+1}+\delta_{j',j-1}\}\delta_{i,i'}, \quad (1.3)$$

where i and j are counted mod(m_1) and mod(m_2), respectively, because of the toroidal boundary conditions. For the case of Fig. 2, where helical boundary conditions are employed, it is easier to use a single index i running from 1 to $N=m_1m_2$. In this case the matrix elements are,

$$\langle i|T|i'\rangle = (1/4+p_{i'})\{\delta_{i',i+1}+\delta_{i',i-1}\} + (1/4-p_{i'})\{\delta_{i',i+m_1}+\delta_{i',i-m_1}\}, \quad (1.4)$$

where now i is counted mod(N). Consider now the following

QUESTION: *If one of the horizontal transition probabilities is increased, does the horizontal diffusion constant D_x increase too?*

Remember that in the case of an inhomogeneously periodic lattice, increasing the transition probability at one site in the unit cell means increasing the transition probability at all the periodic translates of this site. On the basis of an explicit example we conjectured in [9] the validity of the following theorem, which we will prove in this paper:

THEOREM 1.1. *If any of the horizontal transition probabilities, say $h_\alpha=1/4+p_\alpha$, of the anisotropic scatterer model is increased, then the horizontal diffusion constant D_x increases too. More precisely, for any $\alpha \in U$,*

$$\frac{\partial D_x}{\partial p_\alpha} = N\pi_\alpha^2, \quad (1.5)$$

where π is the stationary distribution of the corresponding finite state Markov chain.

Since the horizontal and vertical stepping probabilities are nonzero, ergodicity holds and the r.h.s. of (1.5) is strictly positive, which is the monotonicity property alluded to above. From (1.2), $D_x + D_y = 1/2$, so the corresponding results for the vertical diffusion constant are immediate and do not require separate discussion.

The relation (1.5) is similar to Rayleigh's Monotonicity Law for electric networks, which says that *if the resistances of a circuit are increased, the effective resistance R_{EFF} between any two points can only increase; if they are decreased, it can only decrease* [1, p. 67]. More precisely, let R_{rs} be the resistance between sites r and s of the network, I_{rs} the current flowing from r to s and R_{EFF} the effective resistance between points a and b of the network. Under unit current flow, i.e. $I_a = -I_b = 1$, where I_c is defined as the sum of all currents leaving site c , it can be shown that [1, p. 77],

$$\frac{\partial}{\partial R_{rs}} R_{EFF} = I_{rs}^2.$$

We also note that Rayleigh's Monotonicity Law has an equivalent formulation in terms of escape probabilities for reversible random walks [1]. Both (1.5) and Rayleigh's Monotonicity Law establish a monotone dependence of macroscopic or "effective" parameters (effective resistance, escape probability, diffusion constant) on the microscopic parameters of the model.

The purpose of this paper is to show that the Monotonicity Law (1.5) is a consequence of a Markov chain identity (Theorem 3.2 below), which in turn is based on a certain determinantal identity (Theorem 3.1 below) underlying all the results of this paper. This theorem holds for a general class of matrices including those of the form $S = I - T$, with I the identity matrix and T a stochastic matrix satisfying certain conditions. We will show in section 3 that for the anisotropic scatterer problem with both types of boundary conditions used above, Theorem 3.2 is applicable and therefore (1.5) holds. Also certain types of waiting probabilities are allowed: one easily shows that the result (1.5) still holds if the transition probabilities are $a + bp_\alpha$ to jump horizontally from site α , $c + dp_\alpha$ to jump vertically,

and $1-2(a+c)-2(b+d)p_\alpha$ to stay at site α , $\alpha \in U$. Notice that all transitions from site α are described by a *single* parameter p_α (for an example with nonzero waiting probabilities where this condition is violated and (1.5) no longer holds, see [9]). It is straightforward to extend these results to higher dimensional lattices.

The monotonicity law (1.5) can be used to derive non-negativity of all derivatives of odd order of D_x w.r.t. p_α [9]. It can also be applied to the case of *random* arrangements of the anisotropic scatterers inside the unit cell, where this random arrangement is then periodically translated as before. When $h_\alpha = a$ with probability ρ and $h_\alpha = a'$ with probability $1-\rho$, independently for all sites in the unit cell, it can be deduced from (1.5) that the *average* horizontal diffusion constant is an increasing function of the density ρ when $a > a'$. This result can be extended to the completely random lattice (i.e. infinite unit cell) [9]. The existence of the diffusion constants for this case was proved by Lawler [3], who also obtained a rigorous low-density expansion [4].

The organization of the paper is as follows. Section 2 contains our notation and a summary of some prerequisites from the theory of determinants. In section 3 we present a proof of the Markov chain identity mentioned above and we show that the result (1.5) is a special case of this. The basic determinantal identity (Theorem 3.1) is proved in section 4.

2. NOTATION AND ELEMENTARY FACTS ABOUT DETERMINANTS.

In this section we establish our notation, mostly following Muir's treatise [5], and list some results about determinants. Matrices are denoted by capitals, A, B, C , etc.; matrix elements by lower case letters, e.g. a_{ij} is the ij -th element of the matrix A . The letter I is reserved for the identity matrix. The columns of an N by N matrix A are written in bold face, $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_N$. The transpose of a matrix A is denoted by A^T , with a similar notation in the case of row or column vectors. The determinant of A is denoted by $|A|$, so we will write

$$|A| = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \cdot & \cdot & \cdots & \cdot \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{vmatrix} = |\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_N|. \quad (2.1)$$

The determinant obtained from $|A|$ by deleting row k and column l is called a *first minor*, and denoted by A_{kl} . If $k=l$ we speak of a *principal* first minor. Minors in which the indices of the rows and columns taken to form the one are the same as the indices of the columns and rows taken to form the other are called *conjugate minors*. Multiplying the minor A_{kl} by the sign factor $(-1)^{k+l}$ one obtains a *first order (primary) cofactor* of the element a_{kl} in $|A|$, which is denoted by

$$\mathcal{Q}_{kl} = (-1)^{k+l} A_{kl}. \quad (2.2)$$

The following identity holds,

$$\delta_{ij} |A| = \sum_k a_{ik} \mathcal{Q}_{jk}. \quad (2.3)$$

If we regard the determinant as a function of N^2 independent variables $\{a_{ij}\}$, we can express the cofactors as derivatives,

$$\mathcal{Q}_{ij} = \frac{\partial |A|}{\partial a_{ij}}. \quad (2.4)$$

REMARK 2.1. In the sequel it will be tacitly understood that whenever derivatives of a determinant w.r.t. one or more of its elements occur, these elements are considered to be arbitrary (independent). Subsequently one may evaluate these derivatives for special values of the matrix elements, which then

* In [10] the cofactor \mathcal{Q}_{kl} is called a minor and denoted by A_{kl} .

need no longer be independent. \square

In the following we denote by e_i the i -th basis (column) vector of the standard basis in \mathbb{R}^N , $(e_i)_j = \delta_{ij}$. Also we write e for the column vector consisting entirely of one's,

$$e = (1, 1, \dots, 1)^T, \quad (2.5)$$

where the dimension of e will be clear from the context. Then we have the following alternative notation for the cofactor \mathcal{Q}_{ij} ,

$$\mathcal{Q}_{ij} = |a_1, \dots, a_{j-1}, e_i, a_{j+1}, \dots, a_N| \quad (2.6)$$

It will be tacitly understood that for $j=1$ the first column vector in expressions like (2.6) is e_i . Both notations (2.4) and (2.6) will be used in the sequel. For example, the second order cofactor of the pair of elements a_{ij}, a_{kl} in $|A|$, which is up to a sign factor equal to the determinant obtained from $|A|$ by deleting rows i, k and columns j, l , can be written as (assuming $j < l$)

$$\frac{\partial^2 |A|}{\partial a_{ij} \partial a_{kl}} = |a_1, \dots, a_{j-1}, e_i, a_{j+1}, \dots, a_{l-1}, e_k, a_{l+1}, \dots, a_N|.$$

Notice that this second derivative vanishes when $i = k$ or $j = l$.

Next we list a number of results which are needed below.

- (i) Let each column sum of A be zero, i.e. $\sum_i a_{ij} = 0, j = 1, 2, \dots, N$. Then

$$|A| = 0 \quad (2.7a)$$

$$\mathcal{Q}_{jn} = \mathcal{Q}_{nn} \text{ for all } j = 1, \dots, N, \quad (2.7b)$$

i.e. the cofactors do not depend on the first index.

PROOF: Adding all rows $2, \dots, N$ of $|A|$ to the first one, a row of zero's is obtained, hence $|A| = 0$. To prove (2.7b) differentiate (2.3) w.r.t. a_{mn} :

$$\delta_{ij} \frac{\partial |A|}{\partial a_{mn}} = \delta_{im} \mathcal{Q}_{jn} + \sum_k a_{ik} \frac{\partial \mathcal{Q}_{jk}}{\partial a_{mn}}. \quad (2.8)$$

Now sum (2.8) over i and use that A has zero column sums. Taking into account (2.4) one finds $\mathcal{Q}_{mn} = \mathcal{Q}_{jn}$, which proves (2.7b). \blacksquare

- (ii) If the matrix A is symmetric, i.e. $a_{ij} = a_{ji}$, conjugate minors are equal [5, p. 368], therefore

$$\mathcal{Q}_{ij} = \mathcal{Q}_{ji}. \quad (2.9)$$

- (iii) If A is both symmetric and has zero column sums then from (2.7) and (2.9),

$$\mathcal{Q}_{ij} = \mathcal{Q}_{kl}, \text{ all } i, j, k, l, \quad (2.10)$$

i.e. all primary cofactors are equal.

- (iv) The following identity between the determinant of A and its first and second order cofactors holds [5, p. 135],

$$|A| \frac{\partial^2 |A|}{\partial a_{ij} \partial a_{kl}} = \frac{\partial |A|}{\partial a_{ij}} \frac{\partial |A|}{\partial a_{kl}} - \frac{\partial |A|}{\partial a_{il}} \frac{\partial |A|}{\partial a_{kj}}. \quad (2.11)$$

- (v) Differentiation of the relation (2.11) w.r.t a_{mn} gives

$$\begin{aligned} \frac{\partial \Delta}{\partial a_{mn}} \frac{\partial^2 \Delta}{\partial a_{ij} \partial a_{kl}} + \Delta \frac{\partial^3 \Delta}{\partial a_{mn} \partial a_{ij} \partial a_{kl}} &= \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{ij}} \frac{\partial \Delta}{\partial a_{kl}} + \frac{\partial \Delta}{\partial a_{ij}} \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{kl}} \\ &\quad - \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{il}} \frac{\partial \Delta}{\partial a_{kj}} - \frac{\partial \Delta}{\partial a_{il}} \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{kj}}, \end{aligned} \quad (2.12)$$

where we have put $\Delta = |A|$. If A has zero column sums then from (2.7) this relation can be

simplified to

$$\begin{aligned} \frac{\partial \Delta}{\partial a_{nn}} \frac{\partial^2 \Delta}{\partial a_{ij} \partial a_{kl}} - \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{ij}} \frac{\partial \Delta}{\partial a_{ll}} &= \frac{\partial \Delta}{\partial a_{jj}} \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{kl}} - \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{il}} \frac{\partial \Delta}{\partial a_{jj}} \\ &\quad - \frac{\partial \Delta}{\partial a_{ll}} \frac{\partial^2 \Delta}{\partial a_{mn} \partial a_{kj}}. \end{aligned} \quad (2.13)$$

3. THE MAIN RESULT

The transition matrices (1.3), (1.4) of the (embedded) Markov chain associated to the anisotropic scatterer model have the form $T = A' + B'P$. Here A' and B' are symmetric, cyclic matrices and the column sums of A' and B' are unity and zero, respectively, whereas P is a diagonal matrix having the variables $\{p_\alpha\}$ appearing in Theorem 1.1 on its diagonal. Motivated by this, we prove in section 4 the following theorem, from which all the results of this paper are immediate consequences. Notice that the theorem does not require the matrices involved to be cyclic.

THEOREM 3.1. *Let S be an $N \times N$ matrix of the form $S = A(I + CP)$, where I is the $N \times N$ identity matrix, A and C are symmetric $N \times N$ matrices with column sums equal to zero, and P is a diagonal matrix, $(P)_{ij} = \delta_{ij}p_j$, where p_1, \dots, p_N are indeterminates. Let S_{kk} , $k = 1, 2, \dots, N$, be the principal first minors of $|S|$, and define*

$$Q = \sum_{k=1}^N S_{kk}, \quad R = \sum_{k=1}^N p_k S_{kk}. \quad (3.1)$$

Then,

$$\left(\frac{\partial R}{\partial p_i}\right)Q - R\left(\frac{\partial Q}{\partial p_i}\right) = NS_{ii}^2, \quad i = 1, 2, \dots, N. \quad (3.2)$$

REMARK 3.1. The quantities S_{kk}, Q, R occurring in this theorem are multilinear functions in the unspecified or formal variables $\{p_i\}$. The expression (3.2) therefore may be regarded as a succinct way of summarizing the set of identities between certain subdeterminants of $|S|$, which arise after expansion of (3.2) with respect to the variables $\{p_i\}$. \square

As an immediate corollary of Theorem 3.1 we have the following Markov chain identity.

THEOREM 3.2. *Let T be the (column-stochastic) transition matrix of a Markov chain with N states, and let $S := I - T$, where I is the $N \times N$ identity matrix. Assume that*

(i) *S has the form $S = A(I + CP)$, where A and C are symmetric $N \times N$ matrices with column sums equal to zero, and P is a diagonal matrix, $(P)_{ij} = \delta_{ij}p_j$, where p_1, \dots, p_N are real variables defined on a domain \mathcal{X} in \mathbb{R}^N ;*

(ii) *$\lambda_0 = 1$ is a simple root of T for all values of p_1, \dots, p_N in \mathcal{X} .*

Let π be the stationary probability vector of the Markov chain, i.e. the right eigenvector of T corresponding to the maximal root $\lambda_0 = 1$, and define $\mathfrak{D} := \sum_{k=1}^N p_k \pi_k$. Then for all values of p_1, \dots, p_N in \mathcal{X} ,

$$\frac{\partial \mathfrak{D}}{\partial p_i} = N\pi_i^2, \quad i = 1, 2, \dots, N. \quad (3.3)$$

REMARK 3.2. Suppose that S is as in Theorems 3.1/3.2, with the exception that the column sums of C are equal to some constant K , not necessarily zero. Then define a modified matrix C^* by $c_{ij}^* = c_{ij} - K/N$. Clearly C^* is symmetric, has zero column sums and satisfies $AC^* = AC$, since

$$(AC^*)_{ij} = \sum_k a_{ik} c_{kj} - \frac{K}{N} \sum_k a_{ik} = (AC)_{ij},$$

where we have used that the matrix A has zero row sums. So if S has the form as in Theorems 3.1/3.2 where the matrix C has constant column sums, then the results still hold. \square

REMARK 3.3. Condition (ii) is satisfied for *ergodic* chains, where the states form a single ergodic set (every state can be reached from every other state of the set [2, p. 37]). In this case all components of π are strictly positive. It is also satisfied when in addition to a single ergodic set there are transient states. Then the components π_α are positive for the ergodic and zero for the transient states. \square

PROOF OF THEOREM 3.2. If $\lambda_0 = 1$ is a simple root of T , the components $\{\pi_k\}$ of the stationary vector π can be expressed as,

$$\pi_k = \frac{S_{kk}}{Q}, \quad (3.4)$$

where $S = I - T$. Here S_{kk} , $k = 1, \dots, N$, are the principal first minors of $|S|$, which are non-negative and not all zero [10, p. 21], and Q is their sum. Therefore \mathcal{Q} can be written as $\mathcal{Q} = R/Q$, where R and Q are defined in (3.1). Since

$$\frac{\partial \mathcal{Q}}{\partial p_i} = \frac{(\frac{\partial R}{\partial p_i})Q - R(\frac{\partial Q}{\partial p_i})}{Q^2}, \quad (3.5)$$

and S satisfies the conditions of Theorem 3.1, we find from (3.2),

$$\frac{\partial \mathcal{Q}}{\partial p_i} = N \frac{S_{ii}^2}{Q^2} = N \pi_i^2. \quad \blacksquare \quad (3.6)$$

PROOF OF THEOREM 1.1. In the remainder of this section we will show that the anisotropic scatterer problem satisfies the conditions of Theorem 3.2 so that (3.6) and therefore (1.5) holds. Since the random walk is ergodic, condition (ii) of Theorem 3.2 is satisfied (see remark 3.3) and we only have to demonstrate that the matrix $S = I - T$ with T defined by (1.3) or (1.4) can be written in the form required by condition (i) in Theorem 3.2.

First consider (1.4). We have that $S = A + BP$, where the matrices A and B are given by

$$\langle i | A | i' \rangle = \delta_{i,i'} - 1/4 \{ \delta_{i',i+1} + \delta_{i',i-1} \} - 1/4 \{ \delta_{i',i+m_1} + \delta_{i',i-m_1} \}, \quad (3.7)$$

$$\langle i | B | i' \rangle = - \{ \delta_{i',i+1} + \delta_{i',i-1} \} + \{ \delta_{i',i+m_1} + \delta_{i',i-m_1} \}. \quad (3.8)$$

It is clear that the matrices A and B are symmetric with zero column sums. So we only have to show that $B = AC$ for some symmetric matrix C with constant column sums (see remark 3.2).

Since the first minors of A are nonzero (when all p_k 's are zero, the walk is still ergodic), any set of $N-1$ columns of A forms a basis for the space of N -dimensional vectors with zero column sums. So in particular, any column \mathbf{b}_i of B can be uniquely written as a linear combination of the columns \mathbf{a}_k , $k \neq i$, of A ,

$$\mathbf{b}_i = \sum_{k \neq i} c_{ik} \mathbf{a}_k. \quad (3.9)$$

We will show that the matrix C occurring in (3.9) is symmetric with constant column sums (the diagonal elements of C are undetermined; for definiteness we set $c_{ii} = 0$). First we observe that the matrices A and B are cyclic. Hence, if we denote by W the permutation matrix which cyclically shifts every entry of a vector one position down, we can write

$$\mathbf{a}_k = W^{k-1} \mathbf{a}_1, \quad \mathbf{b}_k = W^{k-1} \mathbf{b}_1, \quad k = 1, 2, \dots, N, \quad (3.10)$$

with $W^N = I$. From (3.9) there exist coefficients α_k , $k = 2, 3, \dots, N$, such that

$$\mathbf{b}_1 = \sum_{k=2}^N \alpha_k \mathbf{a}_k, \quad (3.11)$$

hence by using (3.10) we find

$$\mathbf{b}_i = \sum_{k=2}^N \alpha_k (W^{i-1} \mathbf{a}_k) = \sum_{k=2}^N \alpha_k \mathbf{a}_{k+i-1} = \sum_{k \neq i} \alpha_{k-i+1} \mathbf{a}_k, \quad (3.12)$$

where here and below indices are to be counted mod(N). So the matrix C has elements

$$c_{ik} = \alpha_{k-i+1}, \quad (3.13)$$

where we put $\alpha_1 := 0$. Clearly C is a cyclic matrix, hence has constant column sums. To show that C is symmetric we invoke the site-symmetry of the anisotropic scatterer model in the horizontal and vertical directions, to which is associated the following symmetry operation. Let U denote the matrix corresponding to the permutation $1 \rightarrow 1, 2 \rightarrow N, 3 \rightarrow N-1, \dots, N \rightarrow 2$. Under this permutation $\mathbf{a}_1, \mathbf{b}_1$ are invariant, while $\mathbf{a}_k \rightarrow \mathbf{a}_{2-k}, \mathbf{b}_k \rightarrow \mathbf{b}_{2-k}$ (indices modulo N). Application of U to (3.11) yields

$$U\mathbf{b}_1 = \sum_{k=2}^N \alpha_k U\mathbf{a}_k = \sum_{k=2}^N \alpha_k \mathbf{a}_{2-k} = \sum_{k=2}^N \alpha_{2-k} \mathbf{a}_k. \quad (3.14)$$

Since $U\mathbf{b}_1 = \mathbf{b}_1$ and the vectors $\mathbf{a}_2, \dots, \mathbf{a}_N$ are independent, a comparison of (3.11) and (3.14) gives $\alpha_k = \alpha_{2-k}$, so

$$c_{ik} = \alpha_{k-i+1} = \alpha_{-k+i+1} = c_{ki}, \quad (3.15)$$

i.e. C is symmetric. By Remark 3.2, Theorem 3.2 is applicable, so that from (1.2a),

$$\frac{\partial D_x}{\partial p_i} = \frac{\partial \mathcal{D}}{\partial p_i} = N\pi_i^2, \quad (3.16)$$

where \mathcal{D} is as in Theorem 3.2.

In the case of torus-geometry, Eq. (1.3), one shows in the same way that the matrix C is a symmetric cyclic block matrix, where the blocks are themselves symmetric and cyclic. Hence C is again symmetric with constant column sums. This completes the proof of the monotonicity law for the anisotropic scatterer problem. ■

4. PROOF OF THEOREM 3.1.

The proof of Theorem 3.1 is broken down into several steps, where the class of matrices involved is successively narrowed down. We start with the following lemma.

LEMMA 4.1. *Let S be an $N \times N$ matrix of the form $S = A + BP$, where the matrices A and B have zero column sums, and P is a diagonal matrix, $(P)_{ij} = \delta_{ij}p_j$, $i, j = 1, \dots, N$. Let $\Xi^{(\alpha)}$ be defined as*

$$\Xi^{(\alpha)} = \left(\frac{\partial R}{\partial p_\alpha}\right)Q - R\left(\frac{\partial Q}{\partial p_\alpha}\right), \quad (4.1)$$

where Q and R are given by (3.1) and $\alpha \in \{1, 2, \dots, N\}$. Then,

$$\Xi^{(\alpha)} = S_{\alpha\alpha} \left\{ \sum_k S_{kk} - \sum_{k,l,i} p_k b_{i\alpha} \frac{\partial^2 |S|}{\partial s_{ll} \partial s_{ik}} \right\}. \quad (4.2)$$

REMARK 4.1. The quantity $\Xi^{(\alpha)}$ is independent of p_α . To see this notice that any first minor S_{kk} is obviously independent of p_k and (multi)linear in the other variables $p_\beta, \beta \neq k$. So,

$$R' = S_{\alpha\alpha} + \sum_{k \neq \alpha} p_k S'_{kk}, \quad R'' = 0,$$

$$Q' = \sum_{k \neq \alpha} S'_{kk}, \quad Q'' = 0,$$

where (double) primes denote (double) differentiation w.r.t. p_α . Therefore, $\Xi^{(\alpha)'} = R''Q - RQ'' = 0$.

Since $S_{\alpha\alpha}$ is itself independent of p_α , the same is true for the quantity between braces in (4.2). \square

PROOF OF LEMMA 4.1. From the definition of Q and R we have

$$\Xi^{(\alpha)} = S_{\alpha\alpha} \sum_l S_{ll} + \sum_{k,l} p_k \gamma_{kl}, \quad (4.3)$$

with

$$\gamma_{kl} = S'_{kk} S_{ll} - S_{kk} S'_{ll}. \quad (4.4)$$

Since

$$\frac{\partial}{\partial p_\alpha} = \sum_i b_{i\alpha} \frac{\partial}{\partial s_{i\alpha}}, \quad S_{kk} = \frac{\partial |S|}{\partial s_{kk}},$$

we have,

$$\gamma_{kl} = \sum_i b_{i\alpha} \left\{ \frac{\partial^2 |S|}{\partial s_{i\alpha} \partial s_{kk}} \frac{\partial |S|}{\partial s_{ll}} - \frac{\partial^2 |S|}{\partial s_{i\alpha} \partial s_{ll}} \frac{\partial |S|}{\partial s_{kk}} \right\}. \quad (4.5)$$

Applying relation (2.13) to the matrix S , with $m = n \rightarrow l, j \rightarrow \alpha, l \rightarrow k$, we find

$$\begin{aligned} \gamma_{kl} &= \sum_i b_{i\alpha} \left\{ S_{\alpha\alpha} \frac{\partial^2 |S|}{\partial s_{ll} \partial s_{kk}} - S_{\alpha\alpha} \frac{\partial^2 |S|}{\partial s_{ll} \partial s_{ik}} - S_{kk} \frac{\partial^2 |S|}{\partial s_{ll} \partial s_{k\alpha}} \right\} \\ &= - \sum_i b_{i\alpha} S_{\alpha\alpha} \frac{\partial^2 |S|}{\partial s_{ll} \partial s_{ik}}, \end{aligned} \quad (4.6)$$

where the second equality follows from the fact that B has zero column sums. A combination of (4.3) with (4.6) completes the proof. \blacksquare

To prove Theorem 3.1 we have to show that the quantity $\Xi^{(\alpha)}$ as defined by (4.1) is equal to $NS_{\alpha\alpha}^2$. By applying the above lemma, which is clearly applicable in the setting of theorem 3.1, it remains to be shown that $\Xi^{(\alpha)} = NS_{\alpha\alpha}$, where

$$\Xi^{(\alpha)} = \sum_k S_{kk} - \sum_{k,l,i} p_k b_{i\alpha} \frac{\partial^2 |S|}{\partial s_{ll} \partial s_{ik}}, \quad (4.7)$$

is the quantity in braces in (4.2).

Our next step is to show that the dependence of $\Xi^{(\alpha)}$ on the matrix A can be completely factored out. We first prove a simple lemma.

LEMMA 4.2. *Let S be an $N \times N$ matrix of the form $S = AF$, where A and F are both $N \times N$ matrices and each row sum of A is zero. Then the following relation between the first order cofactors of the matrices S , A and F exists:*

$$S_{kk} = A_{kk} \sum_m \frac{\partial |F|}{\partial f_{mk}}. \quad (4.8)$$

PROOF. In the notation introduced in (2.6) the right hand side of (4.8) can be written as the product

$$|a_1, \dots, a_{k-1}, e_k, a_{k+1}, \dots, a_N| |f_1, \dots, f_{k-1}, e, f_{k+1}, \dots, f_N|, \quad (4.9)$$

where e is defined in (2.5). First we notice that, without affecting its value, we can replace the first factor in (4.9), which is the determinant of A with the k -th column replaced by e_k , by the determinant which arises by replacing the k -th row of $|A|$ by the transposed basis vector e_k^T . Next we use the multiplication property of determinants to write (4.9) as a single determinant, say $|M|$, where M is the product of the matrices involved in each of the factors. We find, using that $S = AF$ and A has zero row sums that

$$m_{ij} = \sum_l a_{il} f_{lj} = s_{ij}, \quad i \neq k, j \neq k; \quad (4.10a)$$

$$m_{kj} = f_{kj}, \quad j \neq k; \quad (4.10b)$$

$$m_{ik} = \sum_l a_{il} = 0, \quad i \neq k; \quad (4.10c)$$

$$m_{kk} = 1. \quad (4.10d)$$

We thus see that $|M|$ has the form

$$|M| = |s_1^*, \dots, s_{k-1}^*, e_k, s_{k+1}^*, \dots, s_N^*|,$$

where s_j^* equals s_j except for the k -th entry. Since the k -th column of M equals e_k , $|M|$ is clearly independent of the non-diagonal entries in the k -th row and therefore equals the minor S_{kk} of S , which proves (4.8). ■

We now apply this lemma to the terms in $\Xi^{(\alpha)}$, eq. (4.7), under additional conditions on the matrices A and B which are in accordance with the assumptions of Theorem 3.1.

LEMMA 4.3. *Let S be an $N \times N$ matrix satisfying the conditions of lemma 4.1, with the additional assumptions that A is symmetric and $B = AC$ for some $N \times N$ matrix C . Define the matrix D by $D := I + CP$. Then the quantity $\Xi^{(\alpha)}$ in eq. (4.7) satisfies the identity*

$$\Xi^{(\alpha)} = \beta \Xi_2^{(\alpha)}, \quad (4.11)$$

where β is the k -independent value of the first order cofactors A_{kk} of A , and

$$\Xi_2^{(\alpha)} = \sum_k D_k - \sum_{k,l,i,m} p_k c_{i\alpha} \frac{\partial^2 |D|}{\partial d_{ml} \partial d_{ik}}, \quad (4.12)$$

with

$$D_k = \sum_m \frac{\partial |D|}{\partial d_{mk}} = |d_1, \dots, d_{k-1}, e, d_{k+1}, \dots, d_N|. \quad (4.13)$$

PROOF. First, under the stated conditions, the matrix S has the form $S = AD$, where A is symmetric and has zero column sums, therefore also zero row sums. Applying lemma 4.2 one finds

$$S_{kk} = \beta D_k, \quad (4.14)$$

where D_k is given by (4.13) and we have put $A_{kk} = \beta$, since the first order cofactors of A do not depend on k , see (2.10). Next consider the second term in (4.7):

$$\sum_i b_{i\alpha} \frac{\partial^2 |S|}{\partial s_{il} \partial s_{ik}} = |s_1, \dots, s_{k-1}, b_\alpha, s_{k+1}, \dots, s_{l-1}, e_l, s_{l+1}, \dots, s_N|.$$

Since $S = AD$ and $B = AC$, this expression equals the minor S_{ll}^* of the matrix $S^* = AD^*$, where D^* is obtained from D by replacing the k -th column by c_α . So we can again apply lemma 4.2 to find

$$\begin{aligned} \sum_i b_{i\alpha} \frac{\partial^2 |S|}{\partial s_{il} \partial s_{ik}} &= \beta |d_1, \dots, d_{k-1}, c_\alpha, d_{k+1}, \dots, d_{l-1}, e, d_{l+1}, \dots, d_N| \\ &= \beta \sum_{i,m} c_{i\alpha} \frac{\partial^2 |D|}{\partial d_{ml} \partial d_{ik}}. \end{aligned} \quad (4.15)$$

Substitution of (4.14) and (4.15) in (4.7) completes the proof. ■

As our final step in the proof of Theorem 3.1 we have to show that $\Xi_2^{(\alpha)}$ equals ND_α . This leads us to our last lemma.

LEMMA 4.4. Let C be a symmetric $N \times N$ matrix with zero column sums, and let D be the matrix $D = I + CP$, where I is the unit matrix and P is a diagonal matrix, $(P)_{ij} = \delta_{ij}p_j, i, j = 1, \dots, N$. Define

$$\Xi_2^{(\alpha)} = \sum_k D_k - \sum_{k,l,i,m} p_k c_{i\alpha} \frac{\partial^2 |D|}{\partial d_{ml} \partial d_{ik}}, \quad (4.16)$$

with D_k given by (4.13). Then,

$$\Xi_2^{(\alpha)} = ND_\alpha. \quad (4.17)$$

REMARK 4.2. By Remark 4.1 the quantity $\Xi_1^{(\alpha)}$ in (4.7) or (4.11) is independent of p_α . Since β is a constant, (4.11) shows that the quantity $\Xi_2^{(\alpha)}$ in (4.16) is independent of p_α as well. \square

REMARK 4.3. Without loss of generality we can take $\alpha=1$, for we can always perform a permutation such that the α -th row and column of all the matrices involved become the first row and column. Under such a permutation the right hand side of (4.16) transforms to an expression of exactly the same form with α replaced by 1 and C, P and D replaced by matrices C^*, P^* and D^* , having the same properties (symmetry etc.) as C, P and D . \square

PROOF OF LEMMA 4.4. We first show that

$$\sum_k D_k = N|D|. \quad (4.18)$$

To see this first notice that the sum in the l.h.s. of (4.18) can be written as a single $(N+1)$ -dimensional determinant,

$$\sum_k D_k = \sum_k |\mathbf{d}_1, \dots, \mathbf{d}_{k-1}, \mathbf{e}, \mathbf{d}_{k+1}, \dots, \mathbf{d}_N| = |\bar{D}|, \quad (4.19)$$

where

$$|\bar{D}| = - \left| \begin{bmatrix} 0 \\ \mathbf{e} \end{bmatrix}, \begin{bmatrix} 1 \\ \mathbf{d}_1 \end{bmatrix}, \dots, \begin{bmatrix} 1 \\ \mathbf{d}_N \end{bmatrix} \right|. \quad (4.20)$$

This is easily checked by expanding $|\bar{D}|$ after its first row. Now subtract from the first row of $|\bar{D}|$ the sum of all the remaining rows, taking into account that under the assumptions of lemma 4.4 the column sum of any \mathbf{d}_i equals unity. The result is

$$|\bar{D}| = - \left| \begin{bmatrix} -N \\ \mathbf{e} \end{bmatrix}, \begin{bmatrix} 0 \\ \mathbf{d}_1 \end{bmatrix}, \dots, \begin{bmatrix} 0 \\ \mathbf{d}_N \end{bmatrix} \right| = N|\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_N|, \quad (4.21)$$

as was to be shown.

Applying the same reasoning to the second term in (4.16), using in addition that the column sum of c_α is zero, one obtains

$$\begin{aligned} \sum_{l,i,m} c_{i\alpha} \frac{\partial^2 |D|}{\partial d_{ml} \partial d_{ik}} &= \sum_{l \neq k} |\mathbf{d}_1, \dots, \mathbf{d}_{k-1}, \mathbf{c}_\alpha, \mathbf{d}_{k+1}, \dots, \mathbf{d}_{l-1}, \mathbf{e}, \mathbf{d}_{l+1}, \dots, \mathbf{d}_N| \\ &= - \left| \begin{bmatrix} 0 \\ \mathbf{e} \end{bmatrix}, \begin{bmatrix} 1 \\ \mathbf{d}_1 \end{bmatrix}, \dots, \begin{bmatrix} 1 \\ \mathbf{d}_{k-1} \end{bmatrix}, \begin{bmatrix} 0 \\ \mathbf{c}_\alpha \end{bmatrix}, \begin{bmatrix} 1 \\ \mathbf{d}_{k+1} \end{bmatrix}, \dots, \begin{bmatrix} 1 \\ \mathbf{d}_N \end{bmatrix} \right| \\ &= N|\mathbf{d}_1, \dots, \mathbf{d}_{k-1}, \mathbf{c}_\alpha, \mathbf{d}_{k+1}, \dots, \mathbf{d}_N|. \end{aligned} \quad (4.22)$$

So we arrive at the result

$$\Xi_2^{(\alpha)} = N\Xi_3^{(\alpha)}, \quad (4.23)$$

where

$$\Xi_3^{(\alpha)} = |\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_N| - \sum_{k=1}^N p_k |\mathbf{d}_1, \dots, \mathbf{d}_{k-1}, \mathbf{c}_\alpha, \mathbf{d}_{k+1}, \dots, \mathbf{d}_N|. \quad (4.24)$$

The final step in the proof of lemma 4.4 is to show that $\Xi_3^{(\alpha)}$ equals D_α . By remark 4.2 $\Xi_3^{(\alpha)}$ is independent of p_α , so we are allowed to put $p_\alpha = 0$ in (4.24), and by remark 4.3 it is sufficient to give the proof for $\alpha = 1$. Therefore consider

$$\Xi_3^{(1)} = |\mathbf{e}_1, \mathbf{d}_2, \dots, \mathbf{d}_N| + \mathfrak{S}, \quad (4.25)$$

where

$$\mathfrak{S} = - \sum_{k=2}^N p_k |\mathbf{e}_1, \mathbf{d}_2, \dots, \mathbf{d}_{k-1}, \mathbf{c}_1, \mathbf{d}_{k+1}, \dots, \mathbf{d}_N|. \quad (4.26)$$

Now introduce the following notation for the column vector consisting of all except the first entry of \mathbf{d}_i ,

$$\mathbf{d}_i^\# = (d_{2i}, d_{3i}, \dots, d_{Ni})^T$$

and similarly for \mathbf{c}_i etc. Also write $C^\#$ for the matrix obtained from C by deleting the first row and column, and similarly $I^\#$ for the corresponding truncation of the identity matrix I . Then one easily obtains

$$\begin{aligned} \mathfrak{S} &= - \sum_{k=2}^N p_k |\mathbf{d}_2^\#, \dots, \mathbf{d}_{k-1}^\#, \mathbf{c}_1^\#, \mathbf{d}_{k+1}^\#, \dots, \mathbf{d}_N^\#| \\ &= \left| \begin{bmatrix} 0 \\ \mathbf{c}_1^\# \end{bmatrix}, \begin{bmatrix} p_2 \\ \mathbf{d}_2^\# \end{bmatrix}, \dots, \begin{bmatrix} p_N \\ \mathbf{d}_N^\# \end{bmatrix} \right| = |I_1 + C_1 P_1|, \end{aligned} \quad (4.27)$$

where I_1, C_1 and P_1 are the partitioned matrices,

$$I_1 = \begin{bmatrix} 0 & \\ & I^\# \end{bmatrix}, C_1 = \begin{bmatrix} 0 & (\mathbf{c}_1^\#)^T \\ \mathbf{c}_1^\# & C^\# \end{bmatrix}, P_1 = \begin{bmatrix} 1 & \\ & P^\# \end{bmatrix}. \quad (4.28)$$

Now multiply in the last expression of (4.27) from the left by the determinant $|P_1|$ and from the right by $|P_1^{-1}|$ (since the variables p_2, \dots, p_N have only a formal meaning, we can assume without loss of generality that P_1^{-1} exists). Then we obtain

$$\mathfrak{S} = |I_1 + P_1 C_1|. \quad (4.29)$$

Next we use the invariance of a determinant under transposition to obtain

$$\begin{aligned} \mathfrak{S} &= |I_1 + C_1^T P_1| = \\ &= \left| \begin{bmatrix} 0 & \\ & I^\# \end{bmatrix} + \begin{bmatrix} 0 & (\mathbf{c}_1^\#)^T \\ \mathbf{e}^\# & (C^\#)^T \end{bmatrix} \begin{bmatrix} 1 & \\ & P^\# \end{bmatrix} \right|. \end{aligned} \quad (4.30)$$

Finally we invoke the symmetry of the matrix C :

$$(C^\#)^T = C^\#, (\mathbf{c}_1^\#)^T = (c_{21}, \dots, c_{N1}) = (c_{12}, \dots, c_{1N}). \quad (4.31)$$

Substituting this in (4.30) yields

$$\mathfrak{S} = \left| \begin{bmatrix} 0 \\ \mathbf{e}^\# \end{bmatrix}, \begin{bmatrix} d_{12} \\ \mathbf{d}_2^\# \end{bmatrix}, \dots, \begin{bmatrix} d_{1N} \\ \mathbf{d}_N^\# \end{bmatrix} \right| = |\mathbf{e} - \mathbf{e}_1, \mathbf{d}_2, \dots, \mathbf{d}_N|. \quad (4.32)$$

To end the proof, insert (4.32) in (4.25) to find

$$\Xi_3^{(1)} = |\mathbf{e}_1, \mathbf{d}_2, \dots, \mathbf{d}_N| + |\mathbf{e} - \mathbf{e}_1, \mathbf{d}_2, \dots, \mathbf{d}_N| = |\mathbf{e}, \mathbf{d}_2, \dots, \mathbf{d}_N| = D_1. \quad (4.33)$$

So we conclude that $\Xi_3^{(\alpha)} = D_\alpha$ for all α and therefore, by (4.23), $\Xi_2^{(\alpha)} = ND_\alpha$, as was to be shown. ■

Summarizing, by successive application of (4.2), (4.11) and (4.17) we find

$$\Xi^{(\alpha)} = S_{\alpha\alpha}\Xi_1^{(\alpha)} = S_{\alpha\alpha}\beta\Xi_2^{(\alpha)} = S_{\alpha\alpha}\beta ND_\alpha = NS_{\alpha\alpha}^2,$$

since $S_{\alpha\alpha} = \beta D_\alpha$ by (4.14). This proves the theorem.

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