

## Counting the exponents of single transfer matrices

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The eigenvalue equation of a band or a block tridiagonal matrix, the tight binding model for a crystal, a molecule, or a particle in a lattice with random potential or hopping amplitudes, and other problems lead to three-term recursive relations for (multicomponent) amplitudes. Amplitudes  $n$  steps apart are linearly related by a transfer matrix, which is the product of  $n$  matrices. Its exponents describe the decay lengths of the amplitudes. A formula is obtained for the counting function of the exponents, based on a duality relation and the Argument Principle for the zeros of analytic functions. It involves the corner blocks of the inverse of the associated Hamiltonian matrix. As an illustration, numerical evaluations of the counting function of quasi 1D Anderson model are shown. © 2011 American Institute of Physics. [doi:[10.1063/1.3594654](https://doi.org/10.1063/1.3594654)]

### I. INTRODUCTION

Consider the equation

$$C_n u_{n-1} + A_n u_n + B_n u_{n+1} = E u_n, \quad n \in \mathbb{Z}, \quad (1)$$

where  $A_n$ ,  $B_n$ , and  $C_n$  are given complex non-singular square matrices of size  $m$ ,  $E$  is a parameter, and the vectors  $u_n \in \mathbb{C}^m$  are unknown.

The case  $A_n = A_n^\dagger$ ,  $C_n = B_{n-1}^\dagger$  will be referred to as the *Hermitian case*, and is common occurrence in physics: it describes a chain of  $m$ -level *atoms* with Hamiltonians  $A_n$  and couplings  $B_n$  between neighboring atoms. In a lattice model for transport or in a model for a crystal, the atoms may be thought of as sections of the lattice or crystal, each containing  $m$  sites. In linear algebra, if off diagonal blocks are triangular the equation represents the eigenvalue equation for a band matrix of bandwidth  $2m + 1$ .

At each  $n$  the equation provides  $u_{n+1}$  in terms of  $u_n$  and  $u_{n-1}$ , and an iterative evaluation of them can be started from initial conditions  $u_0, u_1$ . The process can be formulated via a  $2m \times 2m$  transfer matrix:

$$\begin{bmatrix} u_{n+1} \\ u_n \end{bmatrix} = T(E) \begin{bmatrix} u_1 \\ u_0 \end{bmatrix}. \quad (2)$$

The  $n$ -step transfer matrix  $T(E)$  is the product  $t_n(E)t_{n-1}(E) \cdots t_1(E)$  of 1-step transfer matrices with the block structure ( $I_m$  is the unit matrix of size  $m$ )

$$t_k(E) = \begin{bmatrix} B_k^{-1}(E - A_k) & -B_k^{-1}C_k^\dagger \\ I_m & 0 \end{bmatrix}. \quad (3)$$

We are concerned with the  $2m$  exponents of the transfer matrix  $T(E)$ ,

$$\xi_a = \frac{1}{n} \log |z_a|, \quad (4)$$

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and their (normalized) counting function:

$$\mathcal{N}(\xi) = \frac{1}{2m} \{ \# \xi_a : \xi_a < \xi \} = \frac{1}{2m} \sum_{a=1}^{2m} \theta(\xi - \xi_a). \quad (5)$$

An operative approach to the numerical evaluation of the exponents is found in Ref. 17. In several cases of interest, the exponents have definite large  $n$  limits (Lyapunov exponents) and describe the exponential rates of growth or decay in  $n$  of the eigenvalues  $z_a$  and of the solutions  $u_n$  of the recursive Eq. (1). They are important, especially the largest or the (positive) smallest, in the study of dynamical systems, stability, localization problems, and wave transmission in layered structures.<sup>3</sup> Analytic expressions for the distribution of Lyapunov exponents are known only for few cases and such cases do not originate from a Hamiltonian, i.e., a recursion equation such as Eq. (1).<sup>2,6,10</sup> Most of the results where an Hamiltonian is given first were obtained numerically<sup>9,12,18</sup> or via some expansion.<sup>1,4</sup>

The main result of the paper is the following exact formula, valid for a *single* transfer matrix of type (2):

*Proposition 1.1* (Counting function):

$$\mathcal{N}(\xi) = \frac{1}{2} + \left( \frac{2\pi}{n} \right)^{-1} \int_0^{\frac{2\pi}{n}} d\varphi \frac{1}{2m} \text{tr} \left[ z G^B(E, z)_{1n} B_n - \frac{1}{z} G^B(E, z)_{n1} C_1 \right], \quad (6)$$

$$z = e^{\xi + i\varphi}$$

$G^B(E, z)_{ab}$  are the blocks of size  $m$  of the resolvent  $G^B(E, z) = [H^B(z) - E]^{-1}$ , and  $H^B(z)$  is the block tridiagonal matrix of size  $mn$  with corners

$$H^B(z) = \begin{bmatrix} A_1 & zB_1 & & C_1/z \\ C_2/z & \ddots & \ddots & \\ & \ddots & \ddots & zB_{n-1} \\ zB_n & & C_n/z & A_n \end{bmatrix}. \quad (7)$$

The suffix  $B$  stands for “balanced,” as this matrix is more tractable in numerical calculations than the Hamiltonian matrix  $H(z)$ , to be introduced next.

Notes: (1) the integral will be shown to be a *contour* integral, and cancels all  $z$  dependent terms of the Laurent expansion. Therefore, one cannot remove the integral in the large  $n$  limit. (2) The imaginary part of the integral is zero.

An expression of the counting function where the dependence on  $z$  is made “explicit” will be given in the Appendix, Proposition (A.1).

## II. A SPECTRAL DUALITY

According to the *Argument principle* of complex analysis, the zeros of an analytic function  $f(z)$  contained in the disk  $|z| < R$  (inside the domain of analyticity) are enumerated by the following complex integral on a circle of radius  $R$ :

$$n(R) = \oint_{|z|=R} \frac{dz}{2\pi i} \frac{f'(z)}{f(z)}. \quad (8)$$

We are interested in the zeros of  $f(z) = \det[T(E) - z]$  and their distribution  $\mathcal{N}(\xi) = (1/2m)n(e^{n\xi})$ . The result for the counting function rests on a remarkable duality that relates  $f(z)$  to the characteristic polynomial of a Hamiltonian matrix  $H(z)$ , which naturally arises from the problem (1) restricted to  $n$  steps in a ring topology, but with generalized boundary conditions specified by a complex

parameter  $z$ :

$$H(z) = \begin{bmatrix} A_1 & B_1 & & C_1/z \\ C_2 & \ddots & \ddots & \\ & \ddots & \ddots & B_{n-1} \\ zB_n & & C_n & A_n \end{bmatrix}. \quad (9)$$

The polynomial  $f(z) = \det[T(E) - z]$  has degree  $2m$  in the variable  $z$  and degree  $nm$  in the parameter  $E$ . Duality states that the polynomial is proportional to the characteristic polynomial of the matrix  $H(z)$ :

*Proposition 2.1* (Duality,<sup>13,14</sup>):

$$\det[T(E) - z] = (-z)^m \frac{\det[E - H(z)]}{\det[B_1 \cdots B_n]}. \quad (10)$$

It is a *duality relation* as it exchanges the roles of the parameters  $z$  and  $E$  among matrices: *whenever  $z$  is an eigenvalue of the transfer matrix evaluated at  $E$ , the value  $E$  is an eigenvalue of the block tridiagonal matrix  $H(z)$ .*

*Proposition 2.2:* The matrix  $H^B(z)$  is similar to  $H(z^n)$ :  $H(z^n) = S(z)H^B(z)S(z)^{-1}$ , where  $S(z)$  is the block diagonal matrix with blocks  $S(z)_{ab} = \delta_{ab}z^a I_m$ .

As a consequence the two matrices have the same eigenvalues. Another consequence is the property  $H^B(ze^{-i2\pi/n}) = S(e^{i2\pi/n})H^B(z)S(e^{-i2\pi/n})$ .

Before deriving the expression for the counting function, we quote interesting and related analytic consequences of duality. Duality and Jensen's formula of complex analysis provide an equation for the exponents  $\xi_a$  of the transfer matrix:

*Proposition 2.3* (Ref. 13):

$$\begin{aligned} & \frac{1}{2m} \sum_{a=1}^{2m} (|\xi_a - \xi| + \xi_a + \xi) - \xi \\ &= \frac{1}{mn} \int_0^{2\pi} \frac{d\varphi}{2\pi} \log |\det[H(e^{n\xi+i\varphi}) - E]| - \frac{1}{mn} \sum_{k=1}^n \log |\det B_k|. \end{aligned} \quad (11)$$

*Corollary 2.4:* For  $\xi = 0$ , the formula gives the sum of the positive exponents:

$$\begin{aligned} & \frac{1}{m} \sum_{a=1}^{2m} \xi_a \theta(\xi_a) \\ &= \frac{1}{mn} \int_0^{2\pi} \frac{d\varphi}{2\pi} \log |\det[H(e^{i\varphi}) - E]| - \frac{1}{mn} \sum_{k=1}^n \log |\det B_k|. \end{aligned} \quad (12)$$

*Remark 2.5:* The sum of all the exponents is  $\frac{1}{n} \log |\det T(E)|$ . Then

$$\sum_{a=1}^{2m} \xi_a = \frac{1}{n} \sum_{k=1}^n (\log |\det C_k| - \log |\det B_k|). \quad (13)$$

*Remark 2.6:* If the transfer matrix is symplectic, i.e., there is a matrix  $\Sigma$  such that  $T(E)^\dagger \Sigma T(E) = \Sigma$ , then the exponents come in opposite pairs.

*Proof:* If  $z$  is an eigenvalue of  $T(E)$  with eigenvector  $\theta$ , then  $\Sigma\theta$  is an eigenvector of  $T(E)^\dagger$  with eigenvalue  $1/\bar{z}$ . This means that  $1/\bar{z}$  is eigenvalue of  $T(E)$ . The corresponding exponents are either both zero or opposite real numbers.  $\square$

Equation (12) is exact and applies to any single transfer matrix. However, it is reminiscent of the formula for the sum of the Lyapunov exponents of an ensemble of random transfer matrices, obtained by Herbert, Jones, and Thouless for  $2 \times 2$  matrices, and by Kunz, Souillard, and Lacroix<sup>11</sup> for larger ones:

$$\frac{1}{m} \sum_a \lambda_a(E) = \int dE' \rho(E') \log |E - E'| + \text{const.}$$

This formula was obtained for the Hermitian case, but holds also in non-Hermitian tridiagonal problems.<sup>5,8</sup> In Eq. (12), the angular average on  $\varphi$  replaces the ensemble average, that produces the ensemble density of eigenvalues. It seems that an ergodic property is at play for such systems.

### III. THE COUNTING FUNCTION

The expression (7) for the counting function can be obtained straightforwardly from Eq. (11). Here, we give a direct proof based on the famous formula Eq. (8), the duality relation, and the simple formula

$$\frac{d}{dz} \det M(z) = \det M(z) \operatorname{tr} \left[ M(z)^{-1} \frac{d}{dz} M(z) \right].$$

*Proof:* Let  $G(E, z) = [H(z) - E]^{-1}$ ,  $f(z) = \det[T(E) - z]$ , and use duality

$$\begin{aligned} \frac{f'(z)}{f(z)} &= \frac{\frac{d}{dz} [z^m \det[H(z) - E]]}{z^m \det[H(z) - E]} = \frac{m}{z} + \operatorname{tr} \left[ G(E, z) \frac{d}{dz} H(z) \right] \\ &= \frac{m}{z} + \operatorname{tr} \left[ G(E, z)_{1n} B_n - \frac{1}{z^2} G(E, z)_{n1} C_1 \right]. \end{aligned}$$

The complex integral of the first term is  $m$ . Inclusion of the normalization factor gives

$$\begin{aligned} \mathcal{N}(\xi) &= \frac{1}{2} + \frac{1}{2m} \oint_{|z|=e^{n\xi}} \frac{dz}{2\pi i z} \operatorname{tr} \left[ z G(E, z)_{1n} B_n - \frac{1}{z} G(E, z)_{n1} C_1 \right] \\ &= \frac{1}{2} + \frac{1}{2m} \int_0^{2\pi} \frac{d\theta}{2\pi} \operatorname{tr} \left[ z G(E, z)_{1n} B_n - \frac{1}{z} G(E, z)_{n1} C_1 \right], \end{aligned}$$

where  $z = e^{n\xi + i\theta}$ . Next, we set  $\theta = n\varphi$ , then  $z = e^{n(\xi + i\varphi)}$ . We introduce the resolvent of  $H^B(z)$  and note that  $G(E, w^n)_{ab} = w^{a-b} G^B(E, w)_{ab}$  by virtue of the similarity; in particular it is

$$w^n G(E, w^n)_{1n} = w G^B(E, w)_{1n}, \quad \frac{1}{w^n} G(E, w^n)_{n1} = \frac{1}{w} G^B(E, w)_{n1}.$$

The final formula is obtained (after renaming  $w$  as  $z$ ). Since the counting function is real, only the real part of the integral is nonzero and

$$0 = \int_0^{\frac{2\pi}{n}} \frac{d\varphi}{2\pi} \operatorname{Im} \operatorname{tr} \left[ z G^B(E, z)_{1n} B_n - \frac{1}{z} G^B(E, z)_{n1} C_1 \right]. \quad (14)$$

$\square$

*Remark 3.1:* While the Argument Principle requires the circle radius to be  $e^{n\xi}$ , the use of the balanced matrix scales the radius to  $e^\xi$  and makes the formula for the counting function useful for numerical studies.

In numerical calculations, the angular integral is replaced by a sampling on different angles. As the circle of radius  $e^\xi$  crosses an eigenvalue  $e^{\xi_a + i\varphi_a}$ , the counting function jumps to a new plateau after strong oscillations due to close sampling points:

$$\frac{1}{e^{\xi + i\varphi} - e^{\xi_a + i\varphi_a}} \approx \frac{e^{\xi_a + i\varphi_a}}{(\xi - \xi_a)^2 + (\varphi - \varphi_a)^2} [(\xi - \xi_a) - i(\varphi - \varphi_a)].$$

The formula requires the inversion of the matrix  $H^B$ , and the explicit dependence on the interesting parameter  $z$  is lost. In the Appendix, we show that this dependence can be made more explicit by means of the resolvent equation for the matrix with corners removed.

#### IV. ANDERSON MODEL

As an illustration of the formula, consider the Anderson model for the motion of a particle in a cubic lattice with the shape of a bar, with a random potential. The particle may hop with equal amplitudes from a site  $\vec{k}$  to neighboring ones  $\vec{k} + \vec{e}$  and is subject to a site-potential  $\epsilon(\vec{k})$  (a random number uniformly distributed in the interval  $[-w/2, w/2]$ ):

$$\sum_{\vec{e}} \psi(\vec{k} + \vec{e}) + \epsilon(\vec{k})\psi(\vec{k}) = E\psi(\vec{k}).$$

If the bar is sliced perpendicularly to the long direction ( $k = k_z$ ), each slice is a square 2D lattice, with  $m$  sites. Accordingly, the Hamiltonian gains a block structure, with diagonal blocks  $A_k$  describing slices, and blocks  $B_k = C_k = I_m$  describing hopping among neighboring slices. The Schrödinger equation is now written as in (1):  $u_{k+1} + u_{k-1} + A_k u_k = E u_k$ , where the  $m$  components of  $u_k$  are the amplitudes  $\psi(\vec{k})$  in the slice  $k$ .

Because of disorder, in the large  $n$  limit, eigenstates are exponentially localized (Anderson localization) on a distance given by the inverse of the smallest positive exponent. In the large  $n$  limit, all the exponents  $\pm\xi_a(E)$  exist and are independent of the realization of the disorder.

Figures 1 and 2 show the counting function for a single realization of disorder and a sample of length 80 (cross section  $2 \times 2$  or  $3 \times 3$ ).

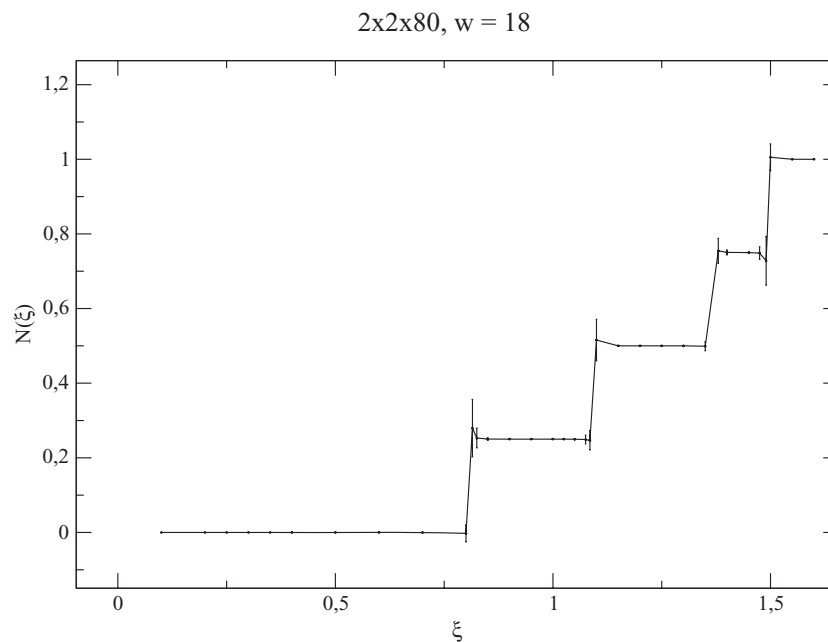


FIG. 1. The counting function  $\mathcal{N}(\xi)$  (a different normalization is used) for the Anderson model in a cubic lattice of dimensions  $2 \times 2 \times 80$ , with disorder strength  $w = 18$ , energy  $E = 0$ . Each discontinuity marks a positive exponent  $\xi_1, \dots, \xi_4$  (the negative exponents are just their opposites).

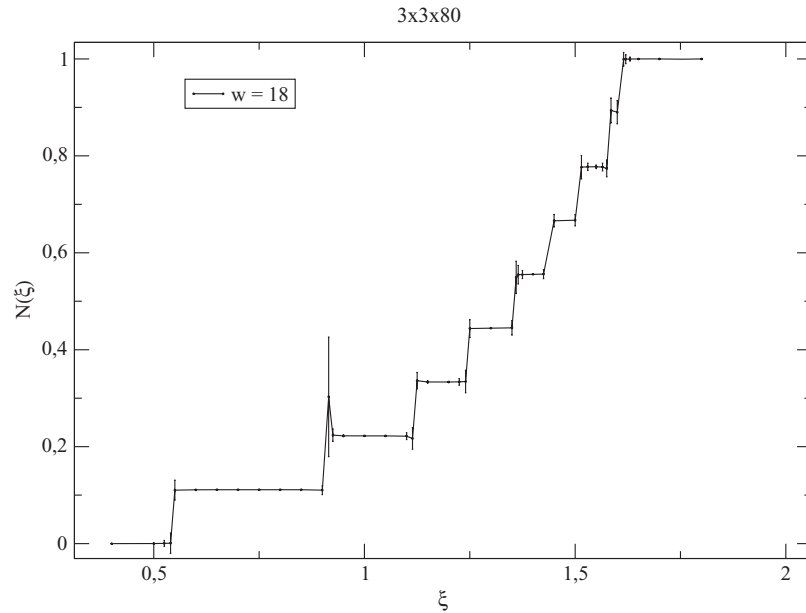


FIG. 2. The counting function  $\mathcal{N}(\xi)$  (a different normalization is used) for the Anderson model in a cubic lattice of dimensions  $3 \times 3 \times 80$ , with disorder strength  $w = 18$ , energy  $E = 0$ . Each discontinuity marks a positive exponent  $\xi_1, \dots, \xi_9$ .

The subject on Anderson localization is vast. A discussion of the spectral properties of Anderson matrices with non-Hermitian boundary conditions (the  $z$  and  $1/z$  dependence) is presented in Ref. 15. The one dimensional case was studied by Goldsheid and Khoruzhenko (Hermitian case)<sup>7</sup> and several others and by us in the non-Hermitian case.<sup>16</sup>

#### APPENDIX: RESOLVENT IDENTITY FOR EXPLICIT $z$ DEPENDENCE

Let  $h$  be the matrix  $H(z^n)$  with corners removed (then it is  $z$ -independent),

$$h = \begin{bmatrix} A_1 & B_1 & & \\ C_2 & \ddots & \ddots & \\ & \ddots & \ddots & B_{n-1} \\ & & C_n & A_n \end{bmatrix}, \quad (\text{A1})$$

and let  $g(E) = [h - E]^{-1}$  be the resolvent matrix, with blocks  $g_{ab}$ . Then

*Proposition A.1:*

$$\begin{aligned} & \text{tr} \left[ z G^B(E, z)_{1n} B_n - \frac{1}{z} G^B(E, z)_{n1} C_1 \right] \\ &= \text{tr} \begin{bmatrix} -z^n B_n g_{1n} - I_m & -z^n B_n g_{11} \\ \frac{1}{z^n} C_1 g_{nn} & \frac{1}{z^n} C_1 g_{n1} + I_m \end{bmatrix}^{-1}. \end{aligned} \quad (\text{A2})$$

*Proof:*  $\Delta(z^n) = H(z^n) - h$  is a matrix whose nonzero blocks are  $\Delta(z^n)_{1n} = z^{-n}C_1$  and  $\Delta(z^n)_{n1} = z^n B_n$ . The matrix equation for the resolvent is

$$G(E, z^n) = g(E) - g(E)\Delta(z^n)G(E, z^n). \quad (\text{A3})$$

The four equations for the blocks  $a, b = 1, n$  can be put in matrix form

$$\begin{bmatrix} G_{1n} & G_{11} \\ G_{nn} & G_{n1} \end{bmatrix} = \begin{bmatrix} g_{1n} & g_{11} \\ g_{nn} & g_{n1} \end{bmatrix} - \begin{bmatrix} g_{1n} & g_{11} \\ g_{nn} & g_{n1} \end{bmatrix} \begin{bmatrix} z^n B_n & 0 \\ 0 & C_1/z^n \end{bmatrix} \begin{bmatrix} G_{1n} & G_{11} \\ G_{nn} & G_{n1} \end{bmatrix}.$$

The blocks of  $G(E, z^n)$  are expressed in terms of the blocks of  $G^B(E, z)$ ,

$$\begin{bmatrix} G_{1n} & G_{11} \\ G_{nn} & G_{n1} \end{bmatrix} = \begin{bmatrix} 1/z^n & 0 \\ 0 & z^n \end{bmatrix} \begin{bmatrix} zG_{1n}^B & z^n G_{11}^B \\ G_{nn}^B/z^n & G_{n1}^B/z \end{bmatrix}.$$

Then

$$\begin{aligned} \begin{bmatrix} zG_{1n}^B & z^n G_{11}^B \\ G_{nn}^B/z^n & G_{n1}^B/z \end{bmatrix} &= \begin{bmatrix} z^n g_{1n} & z^n g_{11} \\ g_{nn}/z^n & g_{n1}/z^n \end{bmatrix} \\ &- \begin{bmatrix} z^n g_{1n} & z^n g_{11} \\ g_{nn}/z^n & g_{n1}/z^n \end{bmatrix} \begin{bmatrix} B_n & 0 \\ 0 & C_1 \end{bmatrix} \begin{bmatrix} zG_{1n}^B & z^n G_{11}^B \\ G_{nn}^B/z^n & G_{n1}^B/z \end{bmatrix}, \end{aligned}$$

with solution

$$\begin{bmatrix} zG_{1n}^B & z^n G_{11}^B \\ G_{nn}^B/z^n & G_{n1}^B/z \end{bmatrix} = \left( \begin{bmatrix} g_{1n} & g_{11} \\ g_{nn} & g_{n1} \end{bmatrix}^{-1} \begin{bmatrix} 1/z^n & 0 \\ 0 & z^n \end{bmatrix} + \begin{bmatrix} B_n & 0 \\ 0 & C_1 \end{bmatrix} \right)^{-1}.$$

Finally, left multiplication by the diagonal matrix with blocks  $B_n$  and  $-C_1$  gives

$$\begin{aligned} \begin{bmatrix} zB_n G_{1n}^B & z^n B_n G_{11}^B \\ -C_1 G_{nn}^B/z^n & -C_1 G_{n1}^B/z \end{bmatrix} \\ = \left( \begin{bmatrix} g_{1n} & g_{11} \\ g_{nn} & g_{n1} \end{bmatrix}^{-1} \begin{bmatrix} B_n^{-1}/z^n & 0 \\ 0 & -z^n C_1^{-1} \end{bmatrix} + \begin{bmatrix} I_m & 0 \\ 0 & -I_m \end{bmatrix} \right)^{-1}. \end{aligned}$$

The rhs is simplified by means of the following identity for invertible matrices  $A$  and  $B$ :  $(A^{-1} + B^{-1})^{-1} = A - A(A + B)^{-1}A$ ,

$$\begin{aligned} &= \begin{bmatrix} I_m & 0 \\ 0 & -I_m \end{bmatrix} - \begin{bmatrix} I_m & 0 \\ 0 & -I_m \end{bmatrix} \\ &\times \left( \begin{bmatrix} z^n B_n & 0 \\ 0 & -\frac{1}{z^n} C_1 \end{bmatrix} \begin{bmatrix} g_{1n} & g_{11} \\ g_{nn} & g_{n1} \end{bmatrix} + \begin{bmatrix} I_m & 0 \\ 0 & -I_m \end{bmatrix} \right)^{-1} \begin{bmatrix} I_m & 0 \\ 0 & -I_m \end{bmatrix}. \end{aligned}$$

The trace is then taken as

$$\text{tr} \left[ zB_n G_{1n}^B - \frac{1}{z} C_1 G_{n1}^B \right] = \text{tr} \begin{bmatrix} -z^n B_n g_{1n} - I_m & -z^n B_n g_{11} \\ \frac{1}{z^n} C_1 g_{nn} & \frac{1}{z^n} C_1 g_{n1} + I_m \end{bmatrix}^{-1}. \quad (\text{A4})$$

As a further step, one could perform the the block inversion of the matrix by Schur's formula. Since the trace is then taken, only the diagonal blocks are needed:

$$= -\text{tr} \left[ z^n B_n g_{1n} + I_m + B_n g_{11} \left( \frac{1}{z^n} C_1 g_{n1} + I_m \right)^{-1} C_1 g_{nn} \right]^{-1} \\ + \text{tr} \left[ \frac{1}{z^n} C_1 g_{n1} + I_m + C_1 g_{nn} (z^n B_n g_{1n} + I_m)^{-1} B_n g_{11} \right]^{-1}. \quad (\text{A5})$$

□

This final expression allows in principle the evaluation of the counting function with one single big matrix inversion to obtain the four  $z$ -independent corner blocks  $g_{ab}$  ( $a, b = 1, n$ ). Then, for each  $z$  value, only the inversion of two square  $m \times m$  matrices (A5) is required.

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