Spanning Trees on Hypercubic Lattices and Non-orientable Surfaces

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Abstract

We consider the problem of enumerating spanning trees on lattices. Closed-form expressions are obtained for the spanning tree generating function for a hypercubic lattice of size $N_1 \times N_2 \times \cdots \times N_d$ in d dimensions under free, periodic, and a combination of free and periodic boundary conditions. Results are also obtained for a simple quartic net embedded on two non-orientable surfaces, a Möbius strip and the Klein bottle. Our results are based on the use of a formula expressing the spanning tree generating function in terms of the eigenvalues of an associated tree matrix. An elementary derivation of this formula is given.

Key words: Spanning trees, Hypercubic lattices, Möbius strip, Klein bottle.

1 INTRODUCTION

The problem of enumerating spanning trees on a graph was first considered by Kirchhoff [1] in his analysis of electrical networks. Consider a graph $G = \{V, E\}$ consisting of a vertex set V and an edge set E. We shall assume that G is connected. A subset of edges $T \subset E$ is a spanning tree if it has $|V| - 1$ edges with at least one edge incident at each vertex. Therefore T has no cycles. In ensuing discussions we shall use T to also denote the spanning tree.

Number the vertices from 1 to $|V|$ and associate to the edge e_{ij} connecting vertices i and j a weight x_{ij}, with the convention of $x_{ii} = 0$. The enumeration of spanning trees concerns with the evaluation of the tree generating function

$$T(G; \{x_{ij}\}) = \sum_{T \subseteq E} \prod_{e_{ij} \in T} x_{ij}, \tag{1}$$

where the summation is taken over all spanning trees T. Particularly, the number of spanning trees on G is obtained by setting $x_{ij} = 1$ as

$$N_{SPT}(G) = T(G; 1). \tag{2}$$

Considerations of spanning tree also arise in statistical physics [2] in the enumeration of close-packed dimers (perfect matchings) [3]. Using a similar consideration, for example, one of us [4] has evaluated the number of spanning trees for the simple quartic, triangular and honeycomb lattices in the limit of $|V| \to \infty$. In this *Letter* we report new results on the evaluation of the generating function Eq. (1) for *finite* hypercubic lattices in arbitrary dimensions. Results are also obtained for a simple quartic net embedded on two non-orientable surfaces, the Möbius strip and the Klein bottle. As the main formula used in this Letter is a relation expressing the tree generating function in terms of the eigenvalues of an associated tree matrix, for completeness we give an elementary derivation of this formula.

2 THE TREE MATRIX

For a given graph $G = \{V, E\}$ consider a $|V| \times |V|$ matrix $\mathbf{M}(G)$ with elements

$$M_{ij}(G) = \begin{cases} \sum_{k=1}^{|V|} x_{ik}, & i = j = 1, 2, \cdots, |V| \\ -x_{ij}, & \text{if vertices } i,\ j,\ i \neq j, \text{ are connected by an edge} \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

We shall refer to $\mathbf{M}(G)$ simply as the tree matrix. It is well-known [5, 6] that the tree generating function, Eq. (1), is given by the cofactor of any element of the tree matrix, and that the cofactor is the same for all elements. Namely, we have the identity

$$T(G; \{x_{ij}\}) = \text{the cofactor of } \textit{any} \text{ element of the matrix } \mathbf{M}(\mathrm{G}). \tag{4}$$

The tree generating function can also be expressed in terms of the eigenvalues of the tree matrix $\mathbf{M}(G)$. We give here an elementary derivation of this result which we use in subsequent sections.

Let $\mathbf{M}(G)$ be the tree matrix of a graph $G = \{V, E\}$. Since the sum of all elements in a row of $\mathbf{M}(G)$ equals to zero, $\mathbf{M}(G)$ has 0 as an eigenvalue and, by definition, we have

$$\det |M_{ij}(G) - \lambda\delta_{ij}| = -\lambda F(\lambda) \tag{5}$$

where

$$F(\lambda) = \prod_{i=2}^{|V|} (\lambda_i - \lambda), \tag{6}$$

$\lambda_2, \lambda_3, \ldots, \lambda_{|V|}$ being the remaining eigenvalues.

Now the sum of all elements in a row of the determinant $|M_{ij}(G) - \lambda\delta_{ij}|$ is $-\lambda$. This permits us to replace the first column of $\det|M_{ij}(G) - \lambda\delta_{ij}|$ by a column of elements $-\lambda$ without affecting its value. Next we carry out a Laplace expansion of the resulting determinant along the modified column, obtaining

$$\det|M_{ij}(G) - \lambda\delta_{ij}| = -\lambda \sum_{i=1}^{|V|} C_{i1}(\lambda), \tag{7}$$

where $C_{i1}(\lambda)$ is the cofactor of the $(i1)$-th element of the determinant. Combining Eqs. (5)-(7), we are led to the identity

$$F(\lambda) = \sum_{i=1}^{|V|} C_{i1}(\lambda). \tag{8}$$

Now, $C_{i1}(0)$ is precisely the cofactor of the $(i1)$-th element of $\mathbf{M}(G)$ which, by Eq. (4), is equal to the tree generating function $T(G;\{x_{ij}\})$. It follows that, after setting $\lambda = 0$ in Eq. (8), we obtain an expression giving the tree generating function in terms of the eigenvalues of the tree matrix [7, p. 39]

$$T(G;\{x_{ij}\}) = \frac{1}{|V|}\prod_{i=2}^{|V|}\lambda_i. \tag{9}$$

This result can also be deduced by considering the tree matrix of a graph obtained from G by adding an auxiliary vertex connected to all vertices with edges of weight x, followed by taking the limit of $x \to 0$ [8].

3 HYPERCUBIC LATTICES

We now deduce the closed-form expression for the tree generating function for a hypercubic lattice in d dimensions under various boundary conditions.

3.1. Free boundary conditions

THEOREM 1. *Let $\mathbf{Z}_d$ be a d-dimensional hypercubic lattice of size $N_1 \times N_2 \times \cdots \times N_d$ with edge weights x_i along the ith direction, $i = 1, 2, \ldots, d$. The tree generating function for $\mathbf{Z}_d$ is*

$$\begin{aligned} T(\mathbf{Z}_d;\{x_i\}) \quad &= \quad \frac{2^{\mathcal{N}-1}}{\mathcal{N}}\prod_{n_1=0}^{N_1-1}\cdots\prod_{n_d=0}^{N_d-1}\left[\sum_{i=1}^{d} x_i\left(1-\cos\frac{n_i\pi}{N_i}\right)\right], \\ &\qquad\qquad (n_1,\ldots,n_d) \neq (0,\ldots,0), \end{aligned} \tag{10}$$

where $\mathcal{N} = N_1N_2\cdots N_d$.

PROOF.

The tree matrix of $\mathbf{Z}_d$ assumes the form of a linear combination of direct products of smaller matrices,

$$\begin{aligned} \mathbf{M}(\mathbf{Z}_d) \quad &= \quad \sum_{i=1}^{d} x_i[2I_{N_1}\otimes I_{N_2}\otimes\cdots\otimes I_{N_d} \\ &- \quad I_{N_1}\otimes\cdots\otimes I_{N_{i-1}}\otimes H_{N_i}\otimes I_{N_{i+1}}\otimes\cdots\otimes I_{N_d}], \end{aligned} \tag{11}$$

where I_N is an $N \times N$ identity matrix and H_N is the $N \times N$ tri-diagonal matrix

$$H_N = \begin{pmatrix} 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 \end{pmatrix}. \tag{12}$$

It is readily verified that H_N is diagonalized by the similarity transformation

$$S_N H_N S_N^{-1} = \Lambda_N, \tag{13}$$

where S_N and S_N^{-1} are $N\times N$ matrices with elements

$$\begin{aligned}(S_N)_{mn} &= \left(S_N^{-1}\right)_{nm} = \sqrt{\frac{2}{N}}\cos\left[(2n+1)\left(\frac{m\pi}{2N}\right)\right] + \left(\sqrt{\frac{1}{N}}-\sqrt{\frac{2}{N}}\right)\delta_{m,0},\\ & \qquad m,n=0,1,\ldots,N-1, \end{aligned} \tag{14}$$

and Λ_N is an $N\times N$ diagonal matrix with diagonal elements

$$\lambda_n = 2\cos\frac{n\pi}{N}, \quad n=0,1,\ldots,N-1. \tag{15}$$

Here $\delta_{m,n}$ is the Kronecker delta. It follows that $\mathbf{M}(\mathbf{Z}_d)$ is diagonalized by the similarity transformation

$$\mathbf{S}_{\mathcal{N}}\mathbf{M}(\mathbf{Z}_d)\mathbf{S}_{\mathcal{N}}^{-1} = \Lambda_{\mathcal{N}}, \tag{16}$$

where

$$\mathbf{S}_{\mathcal{N}} = S_{N_1}\otimes S_{N_2}\otimes\cdots\otimes S_{N_d}, \tag{17}$$

and $\Lambda_{\mathcal{N}}$ is an $\mathcal{N}\times\mathcal{N}$ diagonal matrix with diagonal elements

$$\lambda_{n_1,\ldots,n_d} = 2\sum_{i=1}^{d} x_i\left[1-\cos\frac{n_i\pi}{N_i}\right], \quad n_i=0,1,\ldots,N_i-1. \tag{18}$$

Now, we have $\lambda_{n_1,\ldots,n_d}=0$ for $n_1=n_2=\cdots=n_d=0$. This establishes Theorem 1 after using Eq. (9). Q.E.D.

REMARK. *The result Eq. (18) generalizes the* $d=2$ *eigenvalues of* $\mathbf{M}(\mathbf{Z}_2)$ *for* $x_i=1$ *reported in* [7, p. 74].

3.2. Periodic boundary conditions

In applications in physics one often requires periodic boundary conditions depicted by the condition that two "boundary" vertices at coordinates $(\ldots,n_i=1,\ldots)$ and $(\ldots,n_i=N_i,\ldots)$, $i=1,2,\ldots,d$, are connected by an extra edge. This leads to a lattice $\mathbf{Z}_d^{\rm Per}$ which is a regular graph with degree $2d$ at all vertices. For $d=2$, for example, $\mathbf{Z}_2^{\rm Per}$ can be regarded as being embedded on the surface of a torus.

THEOREM 2. *Let* $\mathbf{Z}_d^{\rm Per}$ *be a hypercubic lattice in* d *dimensions of size* $N_1\times N_2\times\cdots\times N_d$ *with edge weights* x_i *along the* i*th direction,* $i=1,2,...,d$ *with periodic boundary conditions. The tree generating function for* $\mathbf{Z}_d^{\rm Per}$ *is*

$$\begin{aligned}T(\mathbf{Z}_d^{\rm Per};\{x_i\}) &= \frac{2^{\mathcal{N}-1}}{\mathcal{N}}\prod_{n_1=0}^{N_1-1}\cdots\prod_{n_d=0}^{N_d-1}\left[\sum_{i=1}^{d} x_i\left(1-\cos\frac{2n_i\pi}{N_i}\right)\right],\\ &\qquad\qquad (n_1,\ldots,n_d)\neq(0,\ldots,0). \end{aligned} \tag{19}$$

PROOF.

The tree matrix assumes the form

$$\begin{aligned}\mathbf{M}(\mathbf{Z}_d^{\rm Per}) &= \sum_{i=1}^{d} x_i[2I_{N_1}\otimes I_{N_2}\otimes\cdots\otimes I_{N_d}\\ &- I_{N_1}\otimes\cdots\otimes I_{N_{i-1}}\otimes G_{N_i}\otimes I_{N_{i+1}}\otimes\cdots\otimes I_{N_d}], \end{aligned} \tag{20}$$

where G_N is the $N \times N$ cyclic matrix

$$G_N = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}. \tag{21}$$

As in Eq. (16), the matrix $\mathbf{M}(\mathbf{Z}_d^{\mathrm{Per}})$ can be diagonalized by a similarity transformation generated by

$$\mathbf{R}_{\mathcal{N}} = R_{N_1} \otimes R_{N_2} \otimes \cdots \otimes R_{N_d}, \tag{22}$$

where R_N is an $N \times N$ matrix with elements

$$(R_N)_{nj} = \left(R_N^{-1}\right)^*_{jn} = N^{-1/2} e^{i2\pi jn/N}, \tag{23}$$

where * denotes the complex conjugate, yielding eigenvalues of G_N as

$$\lambda_n = 2\cos\frac{2n\pi}{N}, \quad n = 0, 1, \ldots, N-1. \tag{24}$$

This establishes Theorem 2 after using Eq. (9). Q.E.D.

3.3. Periodic boundary conditions along $m \le d$ directions

COROLLARY. *Let $\mathbf{Z}_d^{\mathrm{Per}(m)}$ be a hypercubic lattice in d dimensions of size $N_1 \times N_2 \times \cdots \times N_d$ with periodic boundary conditions in directions $1, 2, \ldots, m \le d$ and free boundaries in the remaining $d - m$ directions. The tree generating function is*

$$T(\mathbf{Z}_d^{\mathrm{Per}(m)}; \{x_i\}) = \frac{2^{\mathcal{N}-1}}{\mathcal{N}} \prod_{n_1=0}^{N_1-1} \cdots \prod_{n_d=0}^{N_d-1} \left[\sum_{i=1}^{m} x_i \left(1 - \cos\frac{2n_i\pi}{N_i}\right) \right.$$
$$\left. + \sum_{i=m+1}^{d} x_i \left(1 - \cos\frac{n_i\pi}{N_i}\right)\right], \qquad (n_1, \ldots, n_d) \ne (0, \ldots, 0). \tag{25}$$

4 THE MÖBIUS STRIP AND THE KLEIN BOTTLE

Due to the interplay with the conformal field theory [9], it is of current interest in statistical physics to study lattice systems on non-orientable surfaces [10, 11]. Here, we consider two such surfaces, the Möbius strip and the Klein bottle, and obtain the respective tree generating functions.

4.1. The Möbius strip

THEOREM 3. *Let $\mathbf{Z}_2^{\mathrm{Mob}}$ be an $M \times N$ simple quartic net embedded on a Möbius strip forming a Möbius net of width M and twisted in the direction N, with edge weights x_1 and*

x_2 along directions M and N respectively. The tree generating function for $\mathbf{Z}_2^{\text{Mob}}$ is

$$
\begin{aligned}
T(\mathbf{Z}_2^{\text{Mob}}; \{x_1, x_2\}) = \frac{2^{MN-1}}{MN} \prod_{m=0}^{M-1} \prod_{n=0}^{N-1} \Bigg[x_1 \left(1 - \cos\frac{m\pi}{M}\right) \\
- x_2 \left(1 - \cos\frac{4n-3-(-1)^m}{2N}\pi\right)\Bigg], \quad (m,n) \neq (0,0). \qquad (26)
\end{aligned}
$$

PROOF.

Specifically, let the the two vertices at coordinates $\{m, 1\}$ and $\{M-m, N\}, m = 1, 2, \cdots, M$ be connected with a lattice edge of weight x_2. Then the tree matrix assumes the form

$$
\mathbf{M}(\mathbf{Z}_2^{\text{Mob}}) = 2(x_1 + x_2) I_M \otimes I_N - x_1 H_M \otimes I_N - x_2 [I_M \otimes F_N + J_M \otimes K_N], \qquad (27)
$$

where

$$
F_N = \begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0
\end{pmatrix}, \quad
J_M = \begin{pmatrix}
0 & 0 & \cdots & 0 & 0 & 1 \\
0 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & \cdots & 1 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 1 & \cdots & 0 & 0 & 0 \\
1 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix},
$$

$$
K_N = \begin{pmatrix}
0 & 0 & 0 & \cdots & 0 & 1 \\
0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 \\
1 & 0 & 0 & \cdots & 0 & 0
\end{pmatrix}.
$$

Since H_M and J_M commute, they can be simultaneously diagonalized by applying the similarity transformation Eq. (13). The transformed matrix $\mathbf{S}_{\mathcal{N}} \mathbf{M}(\mathbf{Z}_2^{\text{Mob}}) \mathbf{S}_{\mathcal{N}}^{-1}$ is "block diagonal" with $N \times N$ blocks

$$
2\left(x_1 - x_1 \cos\frac{m\pi}{M} + x_2\right) I_N - x_2 \left(F_N + (-1)^m K_N\right), \quad m = 0, 1, \ldots, M-1. \qquad (28)
$$

Now, the eigenvalues of $G_N = F_N + K_N$ and $F_N - K_N$ are, respectively, $2\cos[2(n+1)\pi/N]$ and $2\cos[(2n+1)\pi/N], n = 0, 1, ..., N-1$. Theorem 3 is established by combining these results with Eq. (9). Q.E.D.

REMARK. *For $M = 2$ and $x_1 = x_2 = 1$, Eq. (26) gives the number of spanning trees on a $2 \times N$ Möbius ladder as*

$$
\begin{aligned}
N_{SPT} &= \frac{1}{2N} \prod_{j=1}^{2N-1} \left[3 - (-1)^j - 2\cos\frac{j\pi}{N}\right] \\
&= \frac{N}{2}\left[2 + (2+\sqrt{3})^N + (2-\sqrt{3})^N\right]. \qquad (29)
\end{aligned}
$$

These two equivalent expressions have previously been given by [7, p.218] and by Guy and Harary [12], respectively.

4.2. The Klein bottle

The embedding of an $M \times N$ simple quartic net on a Klein bottle is accomplished by further imposing a periodic boundary condition to $\mathbf{Z}_2^{\rm Mob}$ in the M direction, namely, by connecting vertices of $\mathbf{Z}_2^{\rm Mob}$ at coordinates $\{1, n\}$ and $\{M, n\}$, $n = 1, 2, \ldots, N$ with an edge of weight x_1. This leads to a lattice $\mathbf{Z}_2^{\rm Klein}$ of the topology of a Klein bottle.

THEOREM 4 *The tree generating function for* $\mathbf{Z}_2^{\rm Klein}$ *(described in the above) is*

$$\begin{aligned} T(\mathbf{Z}_2^{\rm Klein}; \{x_1, x_2\}) &= \frac{2^{MN-1}}{MN} \left[\prod_{n=1}^{N-1} 2x_2 \left(1 - \cos\frac{2n\pi}{N}\right) \right] \\ &\times \prod_{m=1}^{\left[\frac{M-1}{2}\right]} \prod_{n=0}^{2N-1} \left[2x_1 \left(1 - \cos\frac{2m\pi}{M}\right) + 2x_2 \left(1 - \cos\frac{n\pi}{N}\right) \right] \\ &\times \begin{cases} \prod_{n=0}^{N-1} \left[4z_1 - 2z_2 \left(1 - \cos\frac{(2n+1)\pi}{N}\right) \right], & \text{for } M \text{ even} \\ 1, & \text{for } M \text{ odd,} \end{cases} \end{aligned} \qquad (30)$$

where $[n]$ *is the integral part of* n.

PROOF.

The tree matrix of $\mathbf{Z}_2^{\rm Klein}$ assumes the form

$$\mathbf{M}(\mathbf{Z}_2^{\rm Klein}) = 2(x_1 + x_2) I_M \otimes I_N - x_1 G_M \otimes I_N - x_2 [I_M \otimes F_N + J_M \otimes K_N]. \qquad (31)$$

To obtain its eigenvalues, we first apply the similarity transformation generated by R_M in the M subspace. While this diagonalizes G_M with eigenvalues $2\cos(2m\pi/M)$, $m = 0, 1, \ldots, M-1$, it transforms the matrix J_M into

$$R_M J_M R_M^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \omega \\ 0 & 0 & 0 & \cdots & 0 & \omega^2 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \omega^{M-2} & \cdots & 0 & 0 & 0 \\ 0 & \omega^{M-1} & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}, \qquad (32)$$

where $\omega = e^{i2\pi/M}$, and thus $\mathbf{M}(\mathbf{Z}_2^{\rm Klein})$ into

$$\begin{pmatrix} A_0 + B_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & A_1 & 0 & \cdots & 0 & 0 & B_1 \\ 0 & 0 & A_2 & \cdots & 0 & B_2 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\ 0 & 0 & B_{M-2} & \cdots & 0 & A_{M-2} & 0 \\ 0 & B_{M-1} & 0 & \cdots & 0 & 0 & A_{M-1} \end{pmatrix}, \qquad (33)$$

where A_m and B_m are $N \times N$ matrices given by

$$\begin{aligned} A_m &= 2\left[x_1 + x_2 - x_1 \cos\frac{2m\pi}{M} \right] I_N - x_2 F_N, \\ B_m &= -\omega^m x_2 K_N, \qquad m = 0, 1, \ldots, M-1. \end{aligned} \qquad (34)$$

The matrix Eq. (33) is block diagonal with blocks

$$\begin{aligned} U_N(0) &= A_0 + B_0 = x_2(2I_N - G_N) \\ U_{2N}(m) &= \begin{pmatrix} A_m & B_m \\ B_{M-m} & A_{M-m} \end{pmatrix}, \quad m = 1, 2, \cdots, \left[\frac{M-1}{2}\right] \end{aligned} \tag{35}$$

and for $M =$ even,

$$\begin{aligned} U_N(M/2) &= A_{M/2} + B_{M/2}, \\ &= 2(2x_1 + x_2)I_N - x_2(F_N - K_N), \end{aligned} \tag{36}$$

where the subscripts of the U matrices denote the matrix dimensions. It follows that we need only to find the eigenvalues of the U matrices.

Eigenvalues of $U_N(0)$ and $U_N(M/2)$ can be deduced from those of G_N and $F_N - K_N$. Furthermore, eigenvalues of $U_{2N}(m)$ are obtained from those of G_N after applying the similarity transformation

$$T_{2N}(m)U_{2N}(m)T_{2N}^{-1}(m) = 2\left(x_1 + x_2 - x_1 \cos\frac{2m\pi}{m}\right) I_{2N} - x_2 G_{2N} \tag{37}$$

where

$$T_{2N}(m) = \begin{pmatrix} I_N & 0 \\ 0 & \omega^{-m} I_N \end{pmatrix}. \tag{38}$$

Combining these results with Eq. (9), we are led to Eq. (30) and the theorem. Q.E.D.

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