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Numerical estimation of the asymptotic behaviour of solid partitions of an integer

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Abstract
The number of solid partitions of a positive integer is an unsolved problem in combinatorial number theory. In this paper, solid partitions are studied numerically by the method of exact enumeration for integers up to 50 and by Monte Carlo simulations using Wang–Landau sampling method for integers up to 8000. It is shown that $\lim_{n\to\infty} \frac{\ln(p_3(n))}{n^{3/4}} = 1.79 \pm 0.01$, where $p_3(n)$ is the number of solid partitions of the integer n. This result strongly suggests that the MacMahon conjecture for solid partitions, though not exact, could still give the correct leading asymptotic behaviour.

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1. Introduction

Combinatorial enumeration problems arise naturally in many problems of statistical physics. The number of partitions of an integer (see [1, 2] for an introduction) is one such enumeration problem with a history dating back to Euler. Examples of applications to physical problems include the $q \to \infty$ Potts model [3], compact lattice animals [3, 4], crystal growth [5], lattice polygons [6], Bose–Einstein statistics [7, 8], dimer coverings [9] and rhombus tilings [10]. The solution to the integer partitioning problem is known for one-dimensional and two-dimensional partitions. However, not much is known about higher dimensional partitions. Numerical estimation of the asymptotic behaviour of these higher dimensional partitions could lead to theoretical insights. In this paper, we determine numerically the leading asymptotic behaviour of three-dimensional partitions by exact enumeration and Monte Carlo techniques.

A one-dimensional or linear partition of an integer is a decomposition into a sum of positive integers in which the summands are ordered from largest to smallest. A two-dimensional or plane partition of an integer is a decomposition into a sum of smaller positive integers which are arranged on a plane. The ordering property generalizes to the summands being non-increasing along both the rows and the columns. Generalization to d dimension is straightforward.

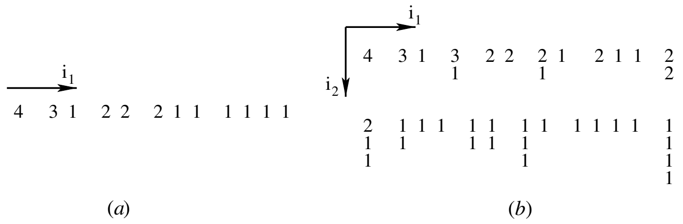

Figure 1. Partitions of the integer 4 in (*a*) one dimension and (*b*) two dimensions.

Consider a d-dimensional hyper cubic lattice with sites labelled by $\mathbf{i} = (i_1, i_2, \ldots, i_d)$, where $i_k = 1, 2, \ldots$. An integer height $h(\mathbf{i})$ (corresponding to a summand) is associated with site $\mathbf{i}$. A d-dimensional partition of a positive integer n is a configuration of heights such that

$$\begin{aligned} &h(\mathbf{i}) \geqslant 0 \\ &h(\mathbf{i}) \geqslant \max_{1\leqslant k\leqslant d} h(i_1, i_2, \ldots, i_k + 1, \ldots, i_d) \\ &\sum_{\mathbf{i}} h(\mathbf{i}) = n. \end{aligned} \tag{1}$$

The second condition in equation (1) means that the heights $h(\mathbf{i})$ are non-increasing in each of the d lattice directions. As an illustration, the linear and plane partitions of 4 are shown in figures 1(*a*) and (*b*) respectively.

Let $p_d(n)$ denote the number of partitions of n in d dimensions. The generating function $G_d(q)$ is then defined as

$$G_d(q) = \sum_{n=0}^{\infty} p_d(n) q^n \tag{2}$$

where $p_d(0) \equiv 1$. The generating function for linear partitions is due to Euler and is

$$G_1(q) = \prod_{k=1}^{\infty} (1 - q^k)^{-1} \tag{3}$$

and $p_1(n)$ for large n varies as [11]

$$p_1(n) \sim \frac{1}{4n\sqrt{3}} \exp\left(\pi \sqrt{\frac{2n}{3}}\right) \qquad n \gg 1. \tag{4}$$

The corresponding formulae for plane partitions are [12]

$$G_2(q) = \prod_{k=1}^{\infty} (1 - q^k)^{-k} \tag{5}$$

and

$$p_2(n) \sim \frac{c_2}{n^{25/36}} \exp(\alpha_2 n^{2/3}) \qquad n \gg 1 \tag{6}$$

where $c_2 = 0.400\,99\ldots$ and $\alpha_2 = 2.009\,45\ldots$ [13]. While the generating functions for three and higher dimensional partitions are not known, it is known that $\lim_{n\to\infty} \ln(p_d(n))/n^{d/(d+1)}$ has a finite non-zero limit [4]. We define α_d to be

$$\alpha_d = \lim_{n\to\infty} \frac{\ln(p_d(n))}{n^{d/(d+1)}}. \tag{7}$$

In this paper, we numerically estimate α_3 for solid (three-dimensional) partitions to be

$$\alpha_3 = 1.79 \pm 0.01. \tag{8}$$

Generalizing the results for linear and plane partitions to higher dimensions, MacMahon suggested that the generating function for d-dimensional partitions could be [12]

$$G_d^{(m)}(q) = \prod_{k=1}^{\infty}(1-q^k)^{-\binom{k+d-2}{d-1}}. \tag{9}$$

Equation (9) is usually known as the MacMahon conjecture. Clearly, $G_d^{(m)}(q)$ is the correct result for $d = 1, 2$. However, it is known that $G_d^{(m)}(q)$ is different from $G_d(q)$ for all $d \geqslant 3$ [14, 15]. In particular, in three dimensions

$$G_3^{(m)}(q) = \prod_{k=1}^{\infty}(1-q^k)^{-k(k+1)/2} \tag{10}$$

gives the wrong answer for the number of solid partitions of 6, 7, 8, ...

Let $p_d^{(m)}(n)$ denote the coefficient of q^n in $G_d^{(m)}(q)$. The asymptotic behaviour of $p_3^{(m)}(n)$ for large n can be determined from equation (10) by the method of steepest descent. In the appendix, we present a heuristic derivation of the large n behaviour of the coefficient of q^n in the expansion of the infinite product

$$F(q) = \prod_{k=1}^{\infty}(1-q^k)^{-a_1k^2-a_2k-a_3}. \tag{11}$$

Substituting $a_1 = 1/2$, $a_2 = 1/2$ and $a_3 = 0$ in equation (A5), we obtain

$$p_3^{(m)}(n) \sim \frac{c_3^{(m)}}{n^{61/96}} \exp\left(\alpha_3^{(m)} n^{3/4} + \beta_3^{(m)} n^{1/2} + \gamma_3^{(m)} n^{1/4}\right) \tag{12}$$

where $c_3^{(m)}$ is a constant and

$$\alpha_3^{(m)} = \frac{2^{7/4}\pi}{15^{1/4}3} = 1.7898\ldots \tag{13}$$

$$\beta_3^{(m)} = \frac{\sqrt{15}\zeta(3)}{\sqrt{2}\pi^2} = 0.3335\ldots \tag{14}$$

$$\gamma_3^{(m)} = -\frac{15^{5/4}\zeta(3)^2}{2^{7/4}\pi^5} = -0.0414\ldots. \tag{15}$$

Comparing the values for $\alpha_3^{(m)}$ in equation (8) and α_3 in equation (13), we conclude that the MacMahon conjecture, though not exact, could still give the correct leading asymptotic behaviour for solid partitions. The value of $\alpha_3^{(m)}$ is a function of only a_1 in equation (11). Thus, if we assume that the asymptotic behaviour for solid partitions is correctly captured by a product form as in equation (11), then it should have the form $\prod_k(1-q^k)^{-(1/2\pm0.012)k^2}$.

The rest of the paper is organized as follows. In section 2, we present the results of the exact enumeration study. In section 3, we describe the Monte Carlo algorithm and the simulation results for plane and solid partitions. Finally, we conclude with a summary and conclusions in section 4.

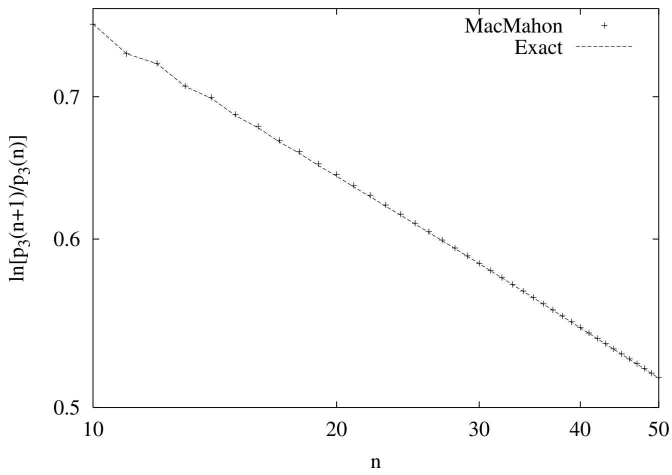

Figure 2. The results from exact enumeration are compared with $p_3^{(m)}$ obtained from the MacMahon conjecture.

Table 1. Solid partitions for $n = 26$ to $n = 50$.

n	$p_3(n)$	n	$p_3(n)$
29	714 399 381	40	352 245 710 866
30	1 281 403 841	41	605 538 866 862
31	2 287 986 987	42	1 037 668 522 922
32	4 067 428 375	43	1 772 700 955 975
33	7 200 210 523	44	3 019 333 854 177
34	12 693 890 803	45	5 127 694 484 375
35	22 290 727 268	46	8 683 676 638 832
36	38 993 410 516	47	14 665 233 966 068
37	67 959 010 130	48	24 700 752 691 832
38	118 016 656 268	49	41 495 176 877 972
39	204 233 654 229	50	69 531 305 679 518

2. Exact enumeration

Previous attempts at studying solid partitions on the computer have been based on exact enumeration [14, 16–18]. Tables of $p_3(n)$ exist for n up to 28 [16]. The table is extended up to $n = 50$ in this paper by using the standard back tracking algorithm [19]. The algorithm is made faster by the following. Partitions that are related to each other by symmetry operations are counted only once and multiplied by the corresponding symmetry factor. Also, parts of the partition that are restricted to planes are generated by using the known generating functions for plane partitions. In table 1, we list the solid partitions from $n = 29$ to $n = 50$. For solid partitions up to $n = 28$, we refer to [16].

We compare the exact enumeration results with the answer predicted by the MacMahon conjecture. In figure 2, we show the variation of $\ln[p_3(n+1)/p_3(n)]$ with n for both $p_3(n)$ as well as $p_3^{(m)}(n)$. While there seems to be a good agreement, we are unable to determine the precise asymptotic behaviour of $p_3(n)$ from these 50 numbers. Standard techniques such as ratio test, partial differential approximants and algebraic approximants (see [20, 21] for a review) fail to converge, possibly due to the presence of an essential singularity in the generating function. It is difficult to further extend the table of solid partitions due to the large computing times involved. One possible method of probing larger values of n is to use Monte Carlo simulations. These are described in section 3.

3. Monte Carlo simulation

3.1. Algorithm

We use an algorithm proposed recently by Wang and Landau for measuring density of states in spin systems [22]. The algorithm is described below. Consider a $N_x \times N_y \times N_z$ lattice with initial height $h(\mathbf{i})$ assigned to each lattice point in such a way that the configuration is a valid solid partition. With each positive integer n is associated a histogram $H(n)$ and the number of solid partitions $p_3(n)$. The histogram $H(n)$ keeps track of the number of times solid partitions of n have been visited during the simulations. The algorithm is based upon the fact that if the probability of transition to a solid partition n is proportional to $[p_3(n)]^{-1}$, then a flat distribution is generated for the histogram $H(n)$. At the start of the program $H(n) = 0$ and $p_3(n) = 1$.

A site is chosen randomly and as a trial move the height $h(\mathbf{i})$ is increased or decreased by 1 with equal probability, provided that the new state is an allowed partition. If the new state is an allowed partition, then the move is accepted with probability

$$\mathrm{Prob}(n_{\mathrm{old}} \to n_{\mathrm{new}}) = \min\left[\frac{p_3(n_{\mathrm{old}})}{p_3(n_{\mathrm{new}})}, 1\right] \tag{16}$$

where n_{old} and n_{new} are the sum of heights for the old and new states respectively, i.e., $n_{\mathrm{new}} = n_{\mathrm{old}} + 1$, $n_{\mathrm{old}} - 1$ or n_{old} depending on whether the height increased by 1, decreased by 1 or remained the same. The histogram $H(n)$ and $p_3(n)$ are updated as

$$H(n_{\mathrm{new}}) = H(n_{\mathrm{new}}) + 1 \tag{17}$$

$$p_3(n_{\mathrm{new}}) = f_i\, p_3(n_{\mathrm{new}}) \tag{18}$$

where f_i is a modification factor greater than 1.

These steps are repeated until a flat histogram is created; in practice, this means that $H(n)_{\mathrm{min}} > cH(n)_{\mathrm{ave}}$, where c is a flatness criterion typically between 0.75 and 0.9 while $H(n)_{\mathrm{min}}$ is the minimum of the $H(n)$ and $H(n)_{\mathrm{ave}}$ is the average of the $H(n)$. When the histogram becomes flat, the modification factor f_i is changed to

$$f_{i+1} = f_i^a \tag{19}$$

and the histogram is reset to zero. The exponent a is less than 1 and defines the smoothness of the iteration. The program runs until f is less than a pre-determined value f_{final}.

Note that the algorithm does not obey detailed balance during the simulations. However, in the limit $f_i \to 1$ when $p_3(n)$ takes its correct value, the system does obey detailed balance with the weight of a solid partition of n being proportional to $[p_3(n)]^{-1}$.

The algorithm can be made faster by adopting certain ideas from the N-fold method [23, 24]. In this modification, sites which cannot undergo a valid move are never chosen. To do so, we define four classes. (i) c1: sites at which the height can only increase. (ii) c2: sites at which the height can either increase or decrease. (iii) c3: sites at which the height can only decrease. (iv) c4: an auxiliary class to help implementation of detailed balance.

First, we update the histogram $H(n)$ and $p_3(n)$ by Δ times with $\mathrm{Prob}(\Delta = k) = p'^k(1 - p')$, where $p' = (|c_4| + |c_1|/2 + |c_3|/2)/(|c_1| + |c_2| + |c_3| + |c_4|)$ and $|c_k|$ denotes

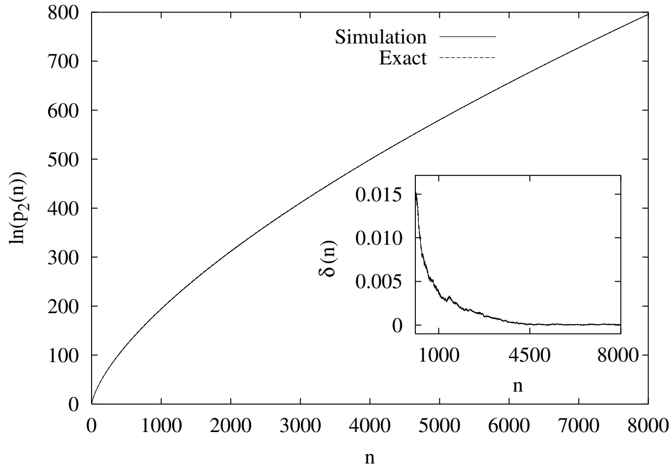

Figure 3. The simulation results for plane partitions are compared with the exact answer. In the inset, the variation of the relative error with n is shown.

the number of elements in the class c_k. We then choose one of the classes c1, c2, c3 with probabilities $|c_1|/(|c_1| + 2|c_2| + |c_3|)$, $2|c_2|/(|c_1| + 2|c_2| + |c_3|)$ and $|c_3|/(|c_1| + 2|c_2| + |c_3|)$ respectively. A site is picked up randomly from the chosen class and a trial move is decided, for example if site $\mathbf{i}$ from class c1 is chosen, the trial move is $h(\mathbf{i}) = h(\mathbf{i}) + 1$, while in the case of class c2 the height increases or decreases with equal probability. Finally, we either accept or reject the trial move according to equation (16) and update the histogram and $p_3(n)$ according to equations (17) and (18). With this construction, only valid trial moves are chosen at each time step and the algorithm becomes considerably faster. The role of the class c4 is to make the algorithm obey detailed balance asymptotically, i.e. when $f_i \to 1$. We define $|c4| = C - (|c_1| + |c_2| + |c_3|)$, where C is some large enough constant.

Further speeding up can be done by dividing the interval 1–8000 to smaller slightly overlapping intervals (14 in our case) and the simulation is done for each interval. After the simulations are over, these intervals can be joined together to produce $p_3(n)$. The distribution is finally normalized by setting $p_3(1) = 1$.

The parameters we have used for the simulations are $c = 0.85, a = 1.0/1.4, C = 2000$, $f_0 = 2.5$ and $f_{\text{final}} = 1.000\,009\,9$ (corresponding to 35 iterations). Changing these parameters slightly does not change the final outcome of the simulation. The lattice sizes used for plane and solid partitions were $100 \times 100 \times 1$ and $50 \times 50 \times 50$ respectively. Random numbers were generated using standard RANMAR algorithm. With this set-up, a typical run producing one $p_3(n)$ for n between 1–8000 takes about 12 h with a Pentium 4 processor. For statistics we performed 20 runs for plane partitions and 24 runs for solid partitions using different random number sequences. Since $p_3(n)$ is typically a very large number, the quantity that we keep track of in the simulations is $\ln(p_3(n))$.

3.2. Simulation results for plane partitions

We first test the algorithm against the known case of plane partitions. In figure 3, we compare the simulation results with the exact answer. The two curves are almost indistinguishable.

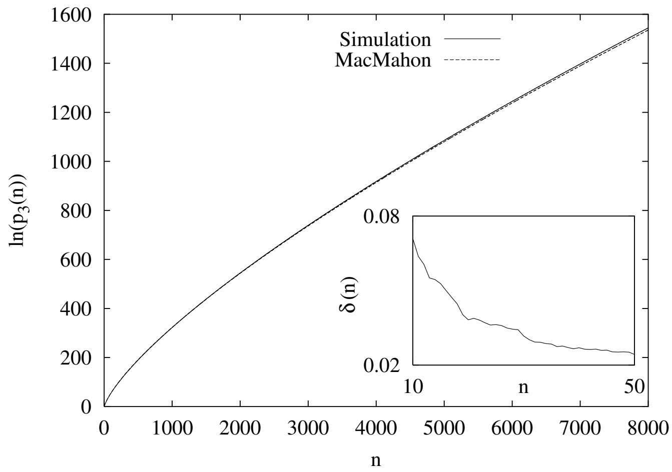

Figure 4. Simulation results for solid partitions are compared with $p_3^{(m)}$ obtained from the MacMahon conjecture. In the inset, we show the relative error with respect to the answer obtained from exact enumeration.

Table 2. The results obtained from the least square fit are shown. α_2, $\alpha_2^{(s)}$, $\alpha_3^{(m)}$ and $\alpha_3^{(s)}$ correspond to $p_{(2,3)}(n)$ obtained from the exact results for plane partitions equation (5), Monte Carlo results for plane partitions, MacMahon conjecture for solid partitions equation (10) and Monte Carlo results for solid partitions respectively.

α_2	$\alpha_2^{(s)}$	$\alpha_3^{(m)}$	$\alpha_3^{(s)}$
2.010 ± 0.002	2.01 ± 0.01	1.789 ± 0.002	1.79 ± 0.01

Consider the relative error defined by

$$\delta(n) = \frac{\left| \ln\left(p_2^{(s)}(n)\right) - \ln(p_2(n))\right|}{\ln(p_2(n))} \tag{20}$$

where $p_2^{(s)}(n)$ is the value obtained from simulations. We show the variation of $\delta(n)$ with n in the inset of figure 3. The relative error goes to zero for large n. Thus, we conclude that the algorithm does give the correct leading asymptotic behaviour. In principle, the simulations can be made arbitrarily precise, and the correction terms can be determined. However, in our case, the statistical errors are not small enough to allow a reliable determination of the correction terms to the leading asymptotic behaviour.

3.3. Simulation results for solid partitions

For solid partitions, we calculated $p_3(n)$ numerically by averaging over 24 different runs. In figure 4, we show the results from simulation while in the inset of figure 4, we show the relative error. We estimate the asymptotic behaviour by fitting the data to an assumed form by the method of least square fit. We fit $\ln\left[p_3^{(s)}(n+1)\big/p_3^{(s)}(n)\right]$ in the range 20–8000 to the form $0.75\alpha_3 n^{-1/4} + 0.5\beta_3 n^{-1/2} + 0.25\gamma_3 n^{-3/4} + d_3 n^{-1}$, where $p_3^{(s)}(n)$ is the value for solid partitions obtained from simulations. We choose this form since the MacMahon conjecture has the same functional form. As a test for the fitting routine, we test it against the simulation results as well as against the exact results for plane partitions using the fitting form $0.667\alpha_2 n^{-1/3} + 0.333\beta_2 n^{-2/3} + d_2 n^{-1}$. The results for $\alpha_{(2,3)}$ are presented in table 2.

For plane partitions, the value of α_2 obtained from the fitting routine is in excellent agreement with the exact answer 2.009 45 . . . [13]. Agreement with the correct answer is also seen for $\alpha_3^{(m)}$ (see equation (13)). Hence, we conclude that $\alpha_3 = 1.79 \pm 0.01$.

4. Summary and conclusions

In summary, we studied numerically the problem of solid partitions of an integer. Using exact enumeration methods, we extended the table of solid partitions for integers up to 50. However, we were unable to determine the precise asymptotic behaviour of solid partitions from these 50 numbers. Solid partitions for larger values of n were studied using Monte Carlo simulations. From these simulations, we showed that $\lim_{n\to\infty} n^{-3/4}\ln(p_3(n)) = 1.79 \pm 0.01$. This value is consistent with the MacMahon value for solid partitions. Thus, if we assume that the asymptotic behaviour for solid partitions is correctly captured by a product form as in equation (11), then it should have the form $\prod_k (1-q^k)^{-(1/2\pm 0.012)k^2}$.

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Appendix. Asymptotics for the MacMahon conjecture

In this appendix, we present a heuristic derivation of the asymptotic behaviour of the coefficient of q^n in the expansion of the product

$$F(q) = \prod_{k=1}^{\infty} (1-q^k)^{-a_1k^2-a_2k-a_3}. \tag{A1}$$

where $a_1 > 0$. Let $q = \mathrm{e}^{-\epsilon}$. Taking logarithms on both sides of equation (A1) and converting the resulting summation into an integral by using the Euler–Maclaurin summation formula (for example, see [25]), we obtain

$$\ln(F(\mathrm{e}^{-\epsilon})) = \frac{2a_1\zeta(4)}{\epsilon^3} + \frac{a_2\zeta(3)}{\epsilon^2} + \frac{a_3\zeta(2)}{\epsilon} + \frac{a_2+6a_3}{12}\ln(\epsilon) + O(\epsilon^0) \tag{A2}$$

where $\zeta(n)$ is the Riemann zeta function. Let the coefficient of q^n in $F(q)$ be denoted by $c(n)$. Then

$$c(n) = \frac{1}{2\pi\mathrm{i}}\oint \frac{F(q)}{q^{n+1}}. \tag{A3}$$

For large n, we evaluate $c(n)$ by the method of steepest descent. The saddle point is the maximum of $\epsilon n + \ln(F(\epsilon))$. This occurs at ϵ_0, where

$$\epsilon_0 = \frac{a_1^{1/4}\pi}{15^{1/4}}n^{-1/4} + \frac{\sqrt{15}a_2\zeta(3)}{2\sqrt{a_1}\pi^2}n^{-1/2} + \frac{15^{1/4}\left(a_1a_3\pi^6 - 45a_2^2\zeta(3)^2\right)}{24a_1^{5/4}\pi^5}n^{-3/4} + O(n^{-1}). \tag{A4}$$

Evaluating the integral about this saddle point, we obtain

$$\ln[c(n)] = \frac{4a_1^{1/4}\pi}{15^{1/4}3}n^{3/4} + \frac{\sqrt{15}a_2\zeta(3)}{\sqrt{a_1}\pi^2}n^{1/2} + \frac{5^{1/4}\left(a_1a_3\pi^6 - 45a_2^2\zeta(3)^2\right)}{2a_1^{5/4}3^{3/4}\pi^5}n^{1/4} - \left(\frac{5}{8} + \frac{a_2}{48} + \frac{a_3}{8}\right)\ln(n) + O(n^0). \tag{A5}$$

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