

Numerical Estimation of the Asymptotic Behaviour of Solid Partitions of an Integer

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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 $\lim_{n \rightarrow \infty} \frac{\ln(p_3(n))}{n^{3/4}} = 1.79 \pm 0.01$, 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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I. 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 $q \rightarrow \infty$ Potts model [3], compact lattice animals [3, 4], crystal growth [5], lattice polygons [6], Bose-Einstein statistics [7, 8] and dimer coverings [9]. The solution to the integer partitioning problem is known for 1-dimensional and 2-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 3-dimensional partitions by exact enumeration and Monte Carlo techniques.

A 1-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 2-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 generalises to the summands being non-increasing along both the rows and the columns. Generalisation to d -dimension is straightforward. Consider a d -dimensional hyper cubic lattice with sites labelled by $\mathbf{i} = (i_1, i_2, \dots, i_d)$, where $i_k = 1, 2, \dots$. 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

$$\begin{aligned} h(\mathbf{i}) &\geq 0, \\ h(\mathbf{i}) &\geq \max_{1 \leq k \leq d} h(i_1, i_2, \dots, i_k + 1, \dots, i_d), \\ \sum_{\mathbf{i}} h(\mathbf{i}) &= n. \end{aligned} \quad (1)$$

The second condition in Eq. (1) means that the heights $h(\mathbf{i})$ are non-increasing in each of the d lattice directions.

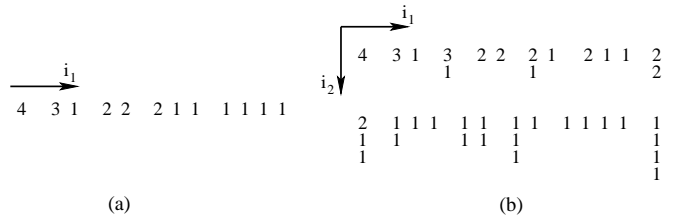


FIG. 1: Partitions of the integer 4 in (a) one dimension and (b) two dimensions.

As an illustration, the linear and plane partitions of 4 are shown in Fig. 1(a) and 1(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

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

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

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

and $p_1(n)$ for large n varies as [10]

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

The corresponding formulae for plane partitions are [11]

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

and

$$p_2(n) \sim \frac{c_2}{n^{25/36}} \exp\left(\alpha_2 n^{2/3}\right), \quad n \gg 1, \quad (6)$$

where $c_2 = 0.40099\dots$ and $\alpha_2 = 2.00945\dots$ [12]. While the generating functions for three and higher dimensional partitions are not known, it is known that $\lim_{n \rightarrow \infty} \ln(p_d(n))/n^{d/(d+1)}$ has a finite non-zero limit [4]. We define α_d to be

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

In this paper, we numerically estimate α_3 for solid (3-dimensional) partitions to be

$$\alpha_3 = 1.79 \pm 0.01. \quad (8)$$

Generalising the results for linear and plane partitions to higher dimensions, MacMahon suggested that the generating function for d -dimensional partitions could be [11]

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

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 $d \geq 3$ [13, 14]. In particular, in 3-dimensions

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

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

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 Eq. (10) by the method of steepest descent. In Appendix A, we present a heuristic derivation of the large n behaviour of the coefficient of q^n in the expansion of the infinite product

$$F(q) = \prod_{k=1}^{\infty} (1 - q^k)^{-a_1 k^2 - a_2 k - a_3}. \quad (11)$$

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

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

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

$$\alpha_3^{(m)} = \frac{27^{7/4}\pi}{15^{1/4}3} = 1.7898\dots, \quad (13)$$

$$\beta_3^{(m)} = \frac{\sqrt{15}\zeta(3)}{\sqrt{2}\pi^2} = 0.3335\dots, \quad (14)$$

$$\gamma_3^{(m)} = -\frac{15^{5/4}\zeta(3)^2}{27^{7/4}\pi^5} = -0.0414\dots \quad (15)$$

Comparing the values for $\alpha_3^{(m)}$ in Eq. (8) and α_3 in Eq. (13), we conclude that the MacMahon conjecture,

TABLE I: Solid partitions for $n = 26$ to $n = 50$.

n	$p_3(n)$	n	$p_3(n)$
29	714399381	40	352245710866
30	1281403841	41	605538866862
31	2287986987	42	1037668522922
32	4067428375	43	1772700955975
33	7200210523	44	3019333854177
34	12693890803	45	5127694484375
35	22290727268	46	8683676638832
36	38993410516	47	14665233966068
37	67959010130	48	24700752691832
38	118016656268	49	41495176877972
39	204233654229	50	69531305679518

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 Eq. (11). Thus, if we assume that the asymptotic behaviour for solid partitions is correctly captured by a product form as in Eq. (11), then it should have the form $\prod_k (1 - q^k)^{-(1/2 \pm 0.012)k^2}$.

The rest of the paper is organised as follows. In Sec. II, we present the results of the exact enumeration study. In Sec. III, we describe the Monte Carlo algorithm and the simulation results for plane and solid partitions. Finally, we conclude with a summary and conclusions in Sec. IV.

II. EXACT ENUMERATION

Previous attempts at studying solid partitions on the computer have been based on exact enumeration [13, 15, 16, 17]. Tables of $p_3(n)$ exist for n up to 28 [15]. The table is extended up to $n = 50$ in this paper by using the standard back tracking algorithm [18]. 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 I, we list the solid partitions from $n = 29$ to $n = 50$. For solid partitions up to $n = 28$, we refer to Ref. [15].

We compare the exact enumeration results with the answer predicted by the MacMahon conjecture. In Fig. 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. This is possibly due to the presence of strong corrections to the leading asymptotic behaviour. 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 Sec. III.

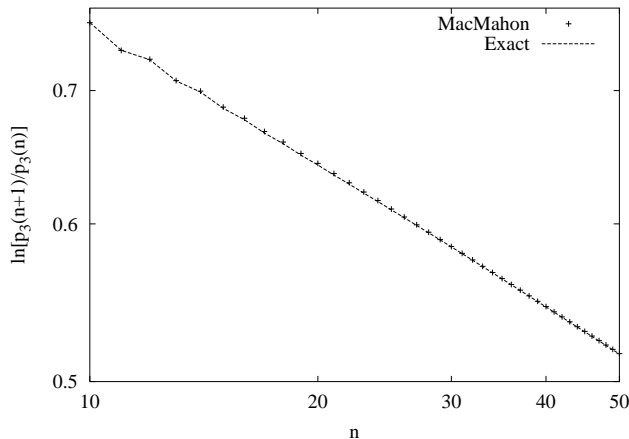


FIG. 2: The results from exact enumeration are compared with $p_3^{(m)}$ obtained from the MacMahon conjecture.

III. MONTE CARLO SIMULATION

A. Algorithm

We use an algorithm proposed recently by Wang and Landau for measuring density of states in spin systems [19]. 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. To 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 one 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

$$\text{Prob}(n_{old} \rightarrow n_{new}) = \min \left[\frac{p_3(n_{old})}{p_3(n_{new})}, 1 \right], \quad (16)$$

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

$$H(n_{new}) = H(n_{new}) + 1, \quad (17)$$

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

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 $H(n)_{min} > cH(n)_{ave}$,

where c is a flatness criteria typically between 0.75 and 0.9 while $H(n)_{min}$ is the minimum of the $H(n)$'s and $H(n)_{ave}$ is the average of the $H(n)$'s. When the histogram becomes flat, the modification factor f_i is changed to

$$f_{i+1} = f_i^a, \quad (19)$$

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 predetermined value f_{final} .

Note that the algorithm does not obey detailed balance during the simulations. However, in the limit $f_i \rightarrow 1$ 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 [20, 21]. 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 $\text{Prob}(\Delta = k) = p'^k (1 - p')$, where $p' = (|c_4| + |c_1|/2 + |c_3|/2)/(|c_1| + |c_2| + |c_3| + |c_4|)$ and $|c_k|$ denotes 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 Eq. (16) and update the histogram and $p_3(n)$ according to Eqs. (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 $f_i \rightarrow 1$. We define $|c_4| = C - (|c_1| + |c_2| + |c_3|)$, 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 normalised 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 $f_{final} = 1.0000099$ (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 setup, a typical run producing one $p_3(n)$ for n between 1–8000 takes about

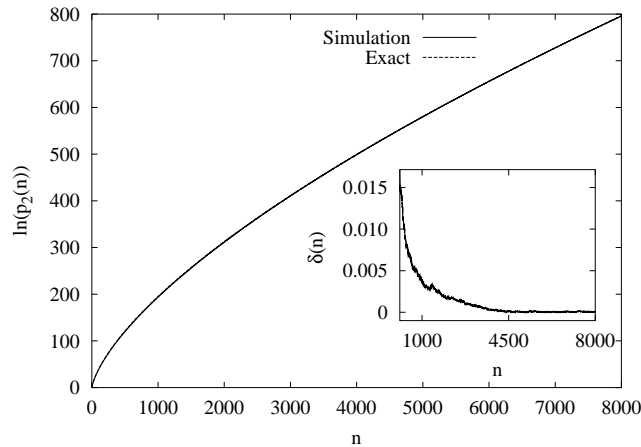


FIG. 3: The simulation results for plane partitions are compared with the exact answer. In the inset, the variation of the relative error with n is shown.

12 hours 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 $\ln(p_3(n))$.

B. Simulation results for plane partitions

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

$$\delta(n) = \frac{|\ln(p_2^{(s)}(n)) - \ln(p_2(n))|}{\ln(p_2(n))}, \quad (20)$$

where $p_2^{(s)}(n)$ is the value obtained from simulations. We show the variation of $\delta(n)$ with n in the inset of Fig. 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.

C. Simulation results for solid partitions

For solid partitions, we calculated $p_3(n)$ numerically by averaging over 24 different runs. In Fig. 4, we show the results from simulation while in the inset of Fig. 4, we show the relative error. We estimate the asymptotic behaviour by fitting the data to an assumed form by the method of least squares fit. We fit

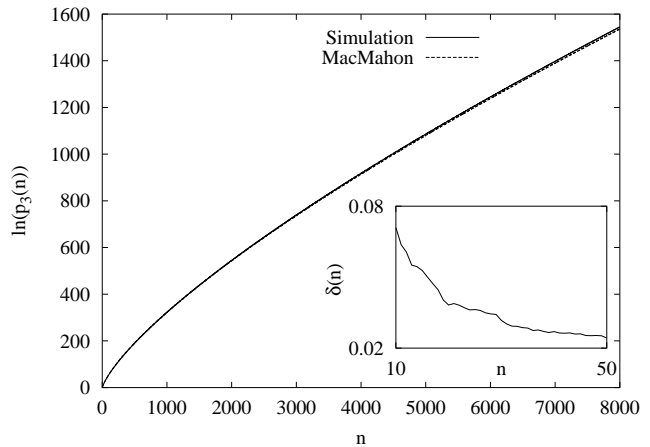


FIG. 4: Simulation results for solid partitions are compared with $p_3^{(m)}$ obtained from the MacMahon conjecture. In the inset, we show the relative error with respect to the answer obtained from exact enumeration.

TABLE II: 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 Eq. (5), Monte Carlo results for plane partitions, MacMahon conjecture for solid partitions Eq. (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

$\ln[p_3^{(s)}(n+1)/p_3^{(s)}(n)]$ 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. II.

For plane partitions, the value of α_2 obtained from the fitting routine is in excellent agreement with the exact answer 2.00945.. [12]. Agreement with the correct answer is also seen for $\alpha_3^{(m)}$ (see Eq. (13)). Hence, we conclude that $\alpha_3 = 1.79 \pm 0.01$.

IV. 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 $\lim_{n \rightarrow \infty} n^{-3/4} \ln(p_3(n)) = 1.79 \pm 0.01$. 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 Eq. (11), then it should have the form $\prod_k (1 - q^k)^{-(1/2 \pm 0.012)k^2}$.

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APPENDIX A: 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

$$F(q) = \prod_{k=1}^{\infty} (1 - q^k)^{-a_1 k^2 - a_2 k - a_3}. \quad (\text{A1})$$

Let $q = e^{-\epsilon}$. Taking logarithms on both sides of Eq. (A1) and converting the resulting summation into an integral by using the Euler-Maclaurin summation formula (for ex-

ample, see [22]), we obtain

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

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

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

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

$$\epsilon_0 = \frac{a_1^{1/4} \pi}{15^{1/4}} n^{-1/4} + \frac{\sqrt{15} a_2 \zeta(3)}{2\sqrt{a_1} \pi^2} n^{-1/2} + \frac{15^{1/4} (a_1 a_3 \pi^6 - 45 a_2^2 \zeta(3)^2)}{24 a_1^{5/4} \pi^5} n^{-3/4} + O(n^{-1}). \quad (\text{A4})$$

Evaluating the integral about this saddle point, we obtain

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

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