Asymptotics of the number partitioning distribution

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Abstract

The number partitioning problem can be interpreted physically in terms of a thermally isolated non-interacting Bose gas trapped in a one-dimensional harmonic oscillator potential. We exploit this analogy to characterize, by means of a detour to the Bose gas within the canonical ensemble, the probability distribution for finding a specified number of summands in a randomly chosen partition of an integer n. It is shown that this distribution approaches its asymptotics only for $n > 10^{10}$.

Consider the decompositions of a natural number n into natural summands, without regard to order. Let $\Phi(n, M)$ denote the number of such partitions which consist of M parts, and $\Omega(n) = \sum_{M=1}^{n} \Phi(n, M)$ the total number of partitions. For $n = 4$, for instance, we have

$$\begin{aligned} 4 &= 1+1+1+1 \\ &= 2+1+1 \\ &= 2+2 = 3+1 \,, \end{aligned} \tag{1}$$

hence $\Phi(4,4) = 1$, $\Phi(4,3) = 1$, $\Phi(4,2) = 2$, $\Phi(4,1) = 1$, adding up to $\Omega(4) = 5$. It is known that $\Omega(n)$ grows exponentially with $\sqrt{n}$ [1], so that the enumeration of the individual partitions soon becomes impractical when n gets larger. It is then useful to focus on the distribution

$$p_{\mathrm{mc}}(n, M) \equiv \frac{\Phi(n, M)}{\Omega(n)} \qquad (0 \le M \le n) \,, \tag{2}$$

which gives the probability for finding M summands in a randomly chosen partition of n. For moderately large n, this distribution can be computed numerically with the help of the recursion relation

$$\Phi(n, M) = \sum_{k=1}^{\min\{n-M, M\}} \Phi(n - M, k) \; ; \tag{3}$$

fig. 1 depicts the results for $n = 1000$ and $n = 5000$.

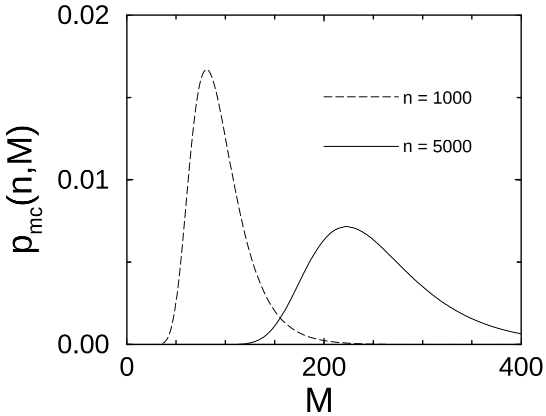

Figure 1: Exact "microcanonical" probability distribution (2) for finding M summands in a randomly chosen partition of n, for $n = 1000$ (dashed) and $n = 5000$ (full line).

The number partitioning problem [2, 3, 4, 5] finds profound applications in various areas of statistical physics, ranging from lattice animals [6, 7] over combinatorial optimization [8] to Fermion-Boson transmutation [9]. Therefore, it is of substantial interest to characterize the distribution (2) for asymptotically large n: Does it, for instance, become Gaussian?

In this Letter we tackle this number-theoretical question within a physical framework. There is a one-to-one correspondence between the individual partitions of an integer and the individual microstates of a gas of ideal Bose particles stored in a one-dimensional harmonic oscillator potential with frequency ω_0. If the total excitation energy E of the gas amounts to n oscillator quanta, $E = n\hbar\omega_0$, then each partition of n labels one possibility for distributing E among the particles. For $n = 4$, the first line in eq. (1) indicates a microstate with four quanta $\hbar\omega_0$ bestowed on four different particles, the second line indicates another microstate where one particle carries two quanta while two other particles account for the remaining ones, and so forth. For any value of E, we assume that the number of particles be at least as large as the number of quanta, so that no restriction (with respect to the number of summands) on the partitions occurs. Hence, each excited Bose particle gives a nonzero summand in a partition of $E/(\hbar\omega_0) = n$, while the remaining ground-state particles correspond to additional zeroes.

Thus, the partitioning problem is mapped to *microcanonical* statistics: Given the total energy (the number to be partitioned) of the thermally isolated gas, the task is to count all accessible microstates. The physical model now suggests to consider first the simpler *canonical* version of this problem, *i.e.*, a gas of infinitely many, harmonically trapped ideal Bosons in thermal contact with a reservoir of temperature T [10]. Then the microcanonical distribution (2) is replaced by its canonical counterpart

$$p_{\rm cn}(b, M) \equiv \frac{\sum_n \mathrm{e}^{-bn}\,\Phi(n, M)}{\sum_n \mathrm{e}^{-bn}\,\Omega(n)} \;, \tag{4}$$

where $b \equiv \hbar\omega_0/(k_{\rm B}T)$ quantifies the inverse temperature, made dimensionless with the quantum $\hbar\omega_0$ and Boltzmann's constant $k_{\rm B}$. Within the canonical ensemble, the analysis starts from the M-particle partition functions

$$Z_M(b) = \sum_{n=0}^{\infty} \omega(n, M)\; \exp(-Mb/2 - bn) \;\;, \tag{5}$$

where the weight $\omega(n, M)$ is the number of possibilities for distributing n quanta over *up to* M Bosons. Since $\Phi(n, M)$ counts the number of possibilities for distributing the n quanta over *exactly* M particles, we have

$$\omega(n, M) - \omega(n, M-1) = \Phi(n, M) . \tag{6}$$

Following textbook practice [11], we proceed from the canonical to the grand canonical ensemble by introducing the fugacity z, and defining the grand partition function

$$\begin{aligned} \Xi(b, z) &\equiv \sum_{M=0}^{\infty} (z e^{b/2})^M Z_M(b) \\ &= \sum_{M=0}^{\infty} z^M \sum_{n=0}^{\infty} \omega(n, M) \exp(-bn) \\ &= \prod_{\nu=0}^{\infty} \frac{1}{1 - z \exp(-b\nu)} . \end{aligned} \tag{7}$$

If we now multiply this function (7) by $(1 - z)$, so that the ground-state factor $(\nu = 0)$ is removed, eq. (6) provides the necessary link to the desired quantities $\Phi(n, M)$:

$$\begin{aligned} \Xi_{\rm ex}(b, z) &\equiv (1 - z)\, \Xi(\beta, z) \\ &= \sum_{M=0}^{\infty} z^M \sum_{n=0}^{\infty} \Phi(n, M) \exp(-bn) \\ &= \prod_{\nu=1}^{\infty} \frac{1}{1 - z \exp(-b\nu)} . \end{aligned} \tag{8}$$

Thus, the grand partition function $\Xi_{\rm ex}(b, z)$ of an ideal Bose gas with amputated ground state generates the microcanonical weights $\Phi(n, M)$. According to probability theory [12], the logarithm of $\Xi_{\rm ex}(b, z)$ then generates the cumulants $\kappa_{\rm cn}^{(k)}(b)$ of the canonical distribution (4):

$$\ln \Xi_{\rm ex}(b, z) = \sum_{\nu=0}^{\infty} \frac{\kappa_{\rm cn}^{(\nu)}(b)}{\nu!} (\ln z)^\nu . \tag{9}$$

The first cumulant $\kappa_{\rm cn}^{(1)}(b)$ is the expectation value of the number of excited particles at the given temperature, the second cumulant $\kappa_{\rm cn}^{(2)}(b)$ its mean-square fluctuation; in general, $\kappa_{\rm cn}^{(k)}$ is related to the k-th central moment of the underlying probability distribution [12]. In particular, $\kappa_{\rm cn}^{(k)} = 0$ for $k \geq 3$ if that distribution is Gaussian.

It is crucial that these *canonical* cumulants can easily be calculated in the relevant temperature regime $k_{\rm B}T \gg \hbar\omega_0$, that is, for $b \ll 1$: Starting from the product representation (8), one derives [13] the *exact* formula

$$\kappa_{\rm cn}^{(k)}(b) = \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} {\rm d}t\, b^{-t}\, \Gamma(t)\, \zeta(t)\, \zeta(t + 1 - k) , \tag{10}$$

where $\Gamma(t)$ denotes the Gamma function, and $\zeta(t)$ is Riemann's Zeta function. This formula (10) allows one to determine the asymptotic expansion of the cumulants from the residues of the integrand. Doing the math yields

$$\kappa_{\rm cn}^{(0)}(b) \sim \frac{\pi^2}{6b} + \frac{1}{2} \ln \frac{b}{2\pi} - \frac{b}{24} \tag{11}$$

$$\kappa_{\rm cn}^{(1)}(b) \sim \frac{1}{b}\left(\ln \frac{1}{b} + \gamma\right) + \frac{1}{4} - \frac{b}{144} + \mathcal{O}(b^3) \tag{12}$$

$$\kappa_{\rm cn}^{(2)}(b) \sim \frac{\pi^2}{6b^2} - \frac{1}{2b} + \frac{1}{24} \tag{13}$$

$$\kappa_{\rm cn}^{(3)}(b) \sim \frac{2\zeta(3)}{b^3} - \frac{1}{12b} + \frac{b}{1440} + \mathcal{O}(b^3) \tag{14}$$

$$\kappa_{\rm cn}^{(4)}(b) \sim \frac{\pi^4}{15b^4} - \frac{1}{240}\ , \tag{15}$$

where $\gamma \approx 0.57722$ is Euler's constant; all higher cumulants are obtained in the same manner.

For applications to the partitioning problem, however, we have to abandon the notion of an externally imposed temperature, and to return to a thermally isolated gas. To this end, we write the generating function (8) as

$$\Xi_{\rm ex}(b,z) = \sum_{\nu=0}^{\infty} {\rm e}^{-b\nu}\, Y(\nu,z)\ , \tag{16}$$

where the series

$$Y(\nu,z) = \sum_{M=0}^{\infty} z^M\, \Phi(\nu,M) \tag{17}$$

is of central importance, since the microcanonical weights $\Phi(\nu,M)$ directly figure as coefficients. Hence, its logarithm generates the cumulants $\kappa_{\rm mc}^{(k)}(n)$ of the microcanonical distribution (2). This function $Y(n,z)$ describes an ideal Bose gas which exchanges particles, but no energy with a reservoir, and thus coincides with the partition function for the recently introduced Maxwell's Demon ensemble [14]. Writing ${\rm e}^{-b} \equiv x$, we extract $Y(n,z)$ from the series (16) by means of a complex contour integral,

$$Y(n,z) = \frac{1}{2\pi i}\oint {\rm d}x\, \frac{\Xi_{\rm ex}(b(x),z)}{x^{n+1}}\ , \tag{18}$$

where the path of integration encircles the origin of the complex x-plane counter-clockwise, and evaluate this integral within the usual saddle-point approximation [15]. The saddle point $b_0(z)$ is determined by setting the logarithmic derivative of the integrand to zero, resulting in the equation which links energy with temperature,

$$n + 1 = -\frac{\partial}{\partial b} \ln \Xi_{\rm ex}(b,z)\Big|_{b_0(z)}\ . \tag{19}$$

Within the Gaussian approximation, one is then led to

$$\ln Y(n,z) = \ln \Xi_{\rm ex}(b_0(z),z) + n b_0(z) - \frac{1}{2}\ln 2\pi - \frac{1}{2}\ln\left(-\frac{\partial}{\partial b}\right)^2 \ln \Xi_{\rm ex}(b,z)\Big|_{b_0(z)}\ , \tag{20}$$

from which the desired microcanonical cumulants are obtained by further differentiation,

$$\kappa_{\rm mc}^{(k)}(n) = \left(z\frac{\rm d}{{\rm d}z}\right)^k \ln Y(n,z)\Big|_{z=1}\ . \tag{21}$$

The calculations now are straightforward, but tedious, because of the z-dependence of the saddle point. We omit the technical details [16] and state the result for $k = 1$: When the thermally isolated gas carries the excitation energy $E = n\hbar\omega_0$, with $n \gg 1$, the expectation value of the number of excited Bose particles takes the form

$$\kappa_{\rm mc}^{(1)}(n) = \kappa_{\rm cn}^{(1)}(b_1) - \frac{1}{2}\frac{D^2\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} + \frac{D\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\left[1 + \frac{1}{2}\frac{D^3\kappa_{\rm cn}^{(0)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\right]\ , \tag{22}$$

where $\kappa_{\rm cn}^{(0)}(b) = \ln \Xi_{\rm ex}(b,1)$, D denotes the derivative with respect to b, and $b_1 \equiv b_0(1)$ has to be taken as function of n. This latter task is achieved by inverting the saddle-point equation (19) for $z = 1$, yielding

$$\frac{1}{b_1} = \frac{\sqrt{6n}}{\pi} + \frac{3}{2\pi^2} + \mathcal{O}(n^{-1/2}) \; . \tag{23}$$

Hence, the canonical expectation value (12), expressed in terms of the scaled energy n, reads

$$\kappa_{\rm cn}^{(1)}(b_1(n)) = \frac{\sqrt{6n}}{\pi}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] + \frac{3}{2\pi^2}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma + 1 + \frac{\pi^2}{6}\right] + \mathcal{O}(n^{-1/2}) \; . \tag{24}$$

The difference between the canonical and the microcanonical expectation value then follows from eq. (22), utilizing the explicit expressions (11) and (12) of the canonical cumulants $\kappa_{\rm cn}^{(0)}$ and $\kappa_{\rm cn}^{(1)}$:

$$\kappa_{\rm mc}^{(1)}(n) \quad - \quad \kappa_{\rm cn}^{(1)}(b_1(n)) = \frac{3}{2\pi^2}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] + \mathcal{O}(n^{-1/2}) \; . \tag{25}$$

Thus, we finally obtain the desired asymptotic formula for the expectation value of the number of summands in a randomly chosen partition of a large integer n:

$$\kappa_{\rm mc}^{(1)}(n) = \frac{\sqrt{6n}}{\pi}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] + \frac{3}{2\pi^2}\left[2\ln\left(\frac{\sqrt{6n}}{\pi}\right) + 2\gamma + 1 + \frac{\pi^2}{6}\right] + \mathcal{O}(n^{-1/2}) \; . \tag{26}$$

For example, for $n = 1000$ this expression (26) yields $\kappa_{\rm mc}^{(1)}(1000) = 94.8073...$, while the exact value is 94.82177..., so that the error is only about 0.015%.

The above calculation of the expectation value $\kappa_{\rm mc}^{(1)}(n)$ illustrates the general strategy for computing an arbitrary *microcanonical* cumulant from eq. (21): Starting from the saddle-point approximation (20) to the generating function $\ln Y(n,z)$, the k-th cumulant $\kappa_{\rm mc}^{(k)}(n)$ is expressed in terms of derivatives of *canonical* cumulants $\kappa_{\rm cn}^{(\ell)}(b)$, with $0 \le \ell \le k$, which, in their turn, are obtained explicitly from the integral fromula (10). In the same manner, the r.m.s.-fluctuation of the number of summands is determined as

$$\sigma(n) = \left(\kappa_{\rm mc}^{(2)}(n)\right)^{1/2} = \sqrt{n} - \frac{3\sqrt{6}}{2\pi^3}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma + 1\right]^2 + \mathcal{O}(n^{-1/2}) \; . \tag{27}$$

Of particular interest are the coefficient $\gamma_1(n)$ of skewness, and the coefficient $\gamma_2(n)$ of excess (or kurtosis) [12],

$$\gamma_1(n) = \frac{\kappa_{\rm mc}^{(3)}(n)}{\left(\kappa_{\rm mc}^{(2)}(n)\right)^{3/2}} \quad \text{and} \quad \gamma_2(n) = \frac{\kappa_{\rm mc}^{(4)}(n)}{\left(\kappa_{\rm mc}^{(2)}(n)\right)^{2}} \; ,$$

which quantify the deviation of the number partitioning distribution (2) from a Gaussian; in the Gaussian case, both γ_1 and γ_2 are equal to zero. Determining the third and fourth cumulant as outlined above, we find

$$\begin{aligned} \gamma_1(n) \;\; = \;\; & 1.1395 + \frac{1}{\sqrt{n}}\Big[0.10128\,[\ln(n)]^2 - 0.37376\;\ln(n) - 1.7078\Big] \\ + \;\; & \frac{1}{n}\Big[0.0075008\,[\ln(n)]^4 + 0.025681\,[\ln(n)]^3 \\ & +0.020024\,[\ln(n)]^2 - 0.23028\;\ln(n) - 0.56984\Big] + \mathcal{O}(n^{-3/2}) \end{aligned} \tag{28}$$

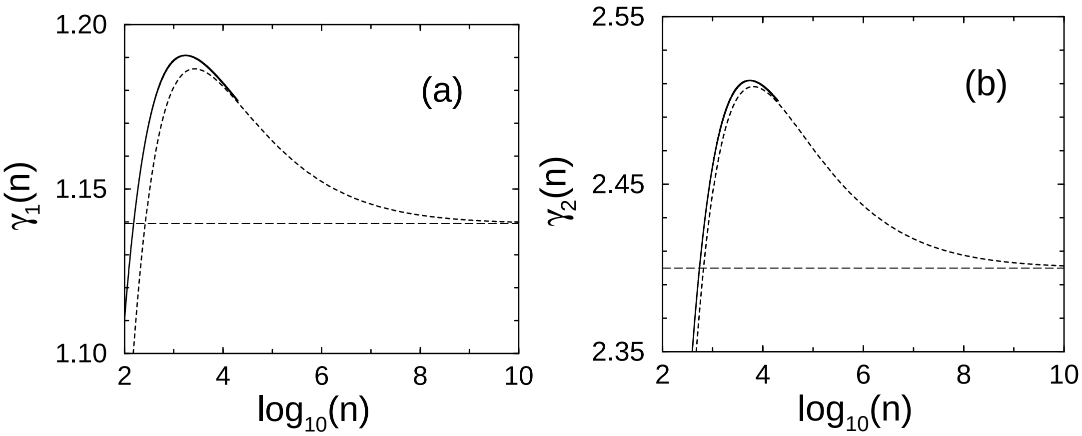

Figure 2: (a) Skewness $\gamma_1(n)$ and (b) excess $\gamma_2(n)$ of the number partitioning distribution (2). The solid lines indicate numerically computed, exact data; the short-dashed lines are the predictions of the asymptotic formulae (28) and (29), respectively. The horizontal lines mark the limiting values.

and, again including terms of order $\mathcal{O}(n^{-1})$,

$$\begin{aligned}\gamma_2(n) &= 2.4 + \frac{1}{\sqrt{n}}\left[0.28440\,[\ln(n)]^2 - 0.56714\,\ln(n) - 10.064\right] \\ &+ \frac{1}{n}\Big[0.025276\,[\ln(n)]^4 + 0.022329\,[\ln(n)]^3 \\ &\quad -0.33809\,[\ln(n)]^2 + 0.73538\,\ln(n) + 3.7863\Big] + \mathcal{O}(n^{-3/2})\;. \end{aligned} \tag{29}$$

Thus, $\gamma_1(n)$ and $\gamma_2(n)$ approach nonzero constants, so that the distribution (2) remains non-Gaussian:

$$\lim_{n\to\infty}\gamma_1(n) = \frac{12\sqrt{6}\,\zeta(3)}{\pi^3} \approx 1.1395\;, \quad \lim_{n\to\infty}\gamma_2(n) = \frac{12}{5}\;.$$

However, due to the vexating logarithmic corrections in eqs. (28) and (29), this asymptotic behaviour is still masked for merely moderately large n: Figure 2 (a) depicts exact values of $\gamma_1(n)$, computed numerically with the help of eq. (3), together with the prediction of the asymptotic formula (28); fig. 2 (b) shows the same comparison for $\gamma_2(n)$. It should be noted that the exact evaluation of the recursion relation (3) requires a substantial amount of computer memory and therefore becomes quite demanding when n is of the order of 10^5, say, while the limiting values of skewness and excess are well approached only for $n > 10^{10}$.

To conclude: While the number partitioning problem is essentially microcanonical in nature, so that one associates "temperature" to natural numbers n on the basis of their entropy $\ln\Omega(n)$, the equivalent problem of harmonically trapped ideal Bosons is approached exactly within the canonical ensemble, when temperature is imposed by an external heat bath. By means of such a detour to the canonical ensemble, we have characterized the number partitioning distribution in terms of its coefficients of skewness and excess. Central to our approach is the fact that statistical mechanics concepts, such as the partition function, have an intrinsic number-theoretical meaning [2]. Even subtle differences between the two ensembles come into play here, such as the usually neglected difference between microcanonical and canonical expectation values; see eqs. (22) and (25). Our results show that the number partitioning distribution adopts its asymptotic shape only for $n > 10^{10}$, so that numerical simulations which inherently rely on partitions might not reach the proper asymptotics. The analytical method we have employed for computing microcanonical cumulants can be generalized to Bosons stored in different types of traps, and thus allows one to study the statistical mechanics of thermally isolated Bose gases.

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