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Cumulants of partitions

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Abstract

We utilize the formal equivalence between the number-partitioning problem and a harmonically trapped ideal Bose gas within the microcanonical ensemble for characterizing the probability distribution which governs the number of addends occurring in an unrestricted partition of a natural number n. By deriving accurate asymptotic formulae for its coefficients of skewness and excess, it is shown that this distribution remains non-Gaussian even when n is made arbitrarily large. Both skewness and excess vary substantially before settling to their constant-limiting values for $n > 10^{10}$.

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1. Introduction

Let $\Phi(n, M)$ denote the number of possibilities to partition the natural number n into M integer, positive addends. For instance, for $n = 5$ we have

$$\begin{aligned} 5 &= 1+1+1+1+1 \\ &= 2+1+1+1 \\ &= 2+2+1 \\ &= 3+1+1 \\ &= 3+2 \\ &= 4+1 \\ &= 5 \end{aligned} \tag{1}$$

so that $\Phi(5, 5) = 1$, $\Phi(5, 4) = 1$, $\Phi(5, 3) = 2$, $\Phi(5, 2) = 2$ and $\Phi(5, 1) = 1$; the total number $\Omega(n)$ of partitions of $n = 5$ adds up to $\Omega(5) = 7$.

The number-partitioning problem, i.e., the problem of finding and enumerating all such partitions of a given natural number n, has a long history in mathematics [1–4], and close connections to topical questions in physics [5–8]. Having been treated already by Euler [1], it leads directly to Bose–Einstein condensation: consider an ideal Bose gas of N particles, isolated from its surrounding and confined by a one-dimensional harmonic oscillator potential with angular frequency ω_0, and assume that the total excitation energy E of this gas amounts to n oscillator quanta, $E = n\hbar\omega_0$. Then, as long as $n \leqslant N$, the individual partitions of n correspond precisely to the possible microstates of the physical system: in the above example (1) with five oscillator quanta, there exists one microstate where five different Bose particles each carry one quantum, another microstate where one Boson carries two quanta and three other Bosons each carry one quantum, still another microstate where two particles each carry two quanta and another particle carries the remaining quantum, and so on. Thus, for a given partition each addend of magnitude $m > 0$ corresponds to a particle carrying m quanta of excitation energy, and the total number of addends belonging to that partition corresponds to the total number of excited particles for that particular microstate. The fact that the numbers commute, so that, for instance, $3 + 1 + 1 = 1 + 1 + 3$, reflects the fundamental indistinguishability of the quantum-mechanical particles: the question 'which particle' carries one or three quanta is meaningless. Finally, the logarithm of the total number of microstates compatible with the energy $E = n\hbar\omega_0$ gives the Boltzmann entropy: $S(n) = k_B \ln(\Omega(n))$, with k_B denoting Boltzmann's constant [9]. After the experimental realization of Bose–Einstein condensates of dilute atomic gases, the (non-)equivalence of the statistical ensembles has become a point of concern even for the ideal gas [10–12]. The results obtained in this paper amount to a detailed comparison of canonical and microcanonical statistics for an ideal gas in a one-dimensional harmonic oscillator trap, while the underlying method can be applied to arbitrary trapping potentials.

For moderately large n, it is easy to compute $\Phi(n, M)$ and $\Omega(n) = \sum_{M=1}^{n} \Phi(n, M)$ exactly by means of a recursion relation: if n quanta are to be distributed over $M \leqslant n$ particles, we first take M of the quanta and assign them to M different particles, thus fixing the required number of addends. The remaining $n - M$ quanta can then be distributed in an arbitrary manner over these M excited particles; the maximum number of particles that will finally be equipped with two or more quanta obviously cannot exceed the smaller of the numbers $n - M$ and M:

$$\Phi(n, M) = \sum_{k=1}^{\min\{n-M,M\}} \Phi(n - M, k). \tag{2}$$

Simple as this relation (2) may look, it does require quite substantial resources of computer memory when n is of the order of ten thousand, say, and is impractical to evaluate numerically when n is of the order of a million. One can then resort to approximate asymptotic formulae, such as the Hardy–Ramanujan formula for $\Omega(n)$ [13]:

$$\Omega(n) = \frac{1}{4\sqrt{3}n} \exp\left(\pi\sqrt{\frac{2n}{3}}\right) [1 + \mathcal{O}(n^{-1/2})]. \tag{3}$$

We remark that the first application of this formula in physics appears to be an estimate of the density of energy levels in a heavy nucleus due to Bohr and Kalckar [14].

In this paper, we will focus on the probability distribution $p_{mc}(n, M)$ for finding, in a given partition of n, precisely M nonzero addends (or, coming back to the physical realization, for finding M excited particles in a one-dimensional, harmonically trapped isolated ideal Bose gas with n quanta of excitation energy), and derive asymptotic formulae for the cumulants of this distribution. The first cumulant $\kappa_{mc}^{(1)}(n)$ gives the expectation value of the number of addends (of the number of excited particles); the second cumulant $\kappa_{mc}^{(2)}(n)$ gives the mean-square fluctuation of this quantity. If the distribution $p_{mc}(n, M)$ were Gaussian, the higher cumulants $\kappa_{\mathrm{mc}}^{(k)}(n)$ with $k \geqslant 3$ would be identically zero; thus, their actual magnitude quantifies to what extent this 'number-of-pieces' distribution deviates from a Gaussian. In particular, we will evaluate the coefficient of skewness,

$$\gamma_1(n) = \frac{\kappa_{\mathrm{mc}}^{(3)}(n)}{\left(\kappa_{\mathrm{mc}}^{(2)}(n)\right)^{3/2}} \tag{4}$$

describing the asymmetry of $p_{\mathrm{mc}}(n, M)$, and the coefficient of excess (or kurtosis),

$$\gamma_2(n) = \frac{\kappa_{\mathrm{mc}}^{(4)}(n)}{\left(\kappa_{\mathrm{mc}}^{(2)}(n)\right)^{2}} \tag{5}$$

describing its flatness [15]. As we will show, both skewness and excess approach *constant*, nonzero values in the limit $n \to \infty$, which means that the distribution remains non-Gaussian even in this limit. Interestingly, the convergence turns out to be rather slow; in both cases the respective limiting values are well approached only for $n > 10^{10}$.

While there exist already several attempts in the literature to compute the leading-order terms of the moments (rather than cumulants) of the distribution $p_{\mathrm{mc}}(n, M)$ [16–19], our goal here is somewhat more ambitious, insofar as we aim at a level of precision such that even the *absolute*, rather than merely relative, error of the resulting formulae goes to zero for $n \to \infty$.

As indicated by the subscript 'mc', the above programme is essentially microcanonical in nature: finding all partitions and characterizing $p_{\mathrm{mc}}(n, M)$ means determining the entropy of a harmonically trapped Bose gas that is thermally isolated, so that the amount of energy to be partitioned among the particles is conserved. Nonetheless, we will exploit the physical intuition that follows from the Bose gas analogy, and will first treat the gas within the simpler *canonical* ensemble. In that case, the system has a predetermined temperature T, and exchanges energy with its environment. Most importantly, the ensuing canonical cumulants $\kappa_{\mathrm{cn}}^{(k)}(\beta)$ (where $\beta = 1/(k_{\mathrm{B}}T)$ denotes the inverse temperature) can be expressed through a convenient integral formula that is derived in section 2. Obviously, one then does *not* obtain the desired microcanonical cumulants from their canonical counterparts by simply inverting the energy–temperature relation, that is, by expressing β as a function of n, and inserting $\beta(n)$ into the canonical expressions: for instance, thermal contact and the accompanying energy fluctuation implies that also the number of excited Bose particles fluctuates stronger in a canonical set-up than it does in a microcanonical one [20]. However, we will work out in detail in section 3 how the difference between the canonical and the microcanonical cumulants can systematically be expressed in terms of the known canonical cumulants, and therefore be evaluated in a transparent manner. Via this detour, that is, by assigning 'temperature' to the numbers n on the basis of their entropy $S(n)$, then calculating the canonical cumulants and finally returning to the microcanonical ensemble, we will determine skewness (4) and excess (5) for the number-partitioning problem. Section 4 contains a comparison of exact, numerically computed data with our asymptotic results; some mathematical details have been collected in the appendix.

2. The canonical cumulant formula

In this section we will not restrict ourselves to one-dimensional harmonic oscillator potentials, but consider N non-interacting Bosons in a set-up where they can occupy arbitrary, discrete single-particle levels ε_ν, $\nu \geqslant 0$, and stipulate that the ground state $\nu = 0$ be non-degenerate. Denoting the occupation number of the νth level as n_ν ($n_\nu = 0, 1, 2, \ldots$), the total energy of a particular microstate of this ideal Bose gas is written as

$$\sum_{\nu=0}^{\infty} n_\nu \varepsilon_\nu = \sum_{\nu=1}^{\infty} n_\nu(\varepsilon_\nu - \varepsilon_0) + N\varepsilon_0 \equiv E + N\varepsilon_0 \tag{6}$$

where we have separated the total excitation energy E from the trivial N-particle ground-state energy $N\varepsilon_0$. (Note that the sums in equation (6) actually terminate at some finite ν, since $\sum_\nu n_\nu = N$.) This excitation energy E is the quantity to be partitioned, i.e., shared among the Bosons.

We then denote the total number of microstates compatible with the excitation energy E—the total number of possibilities for distributing the energy E in an arbitrary manner among the N Bosons—as $\omega(E, N)$. Moreover, for $M = 0, 1, 2, \ldots, N$ we introduce

$$\Phi(E, M) = \omega(E, M) - \omega(E, M - 1). \tag{7}$$

These differences count the partitions of E into *exactly* M pieces, corresponding to the microstates with exactly M out of N particles in an excited state, so that the remaining $N - M$ particles occupy the ground state. With $\omega(E, -1) = 0$, equation (7) obviously implies

$$\sum_{M=0}^{N} \Phi(E, M) = \omega(E, N). \tag{8}$$

When E exceeds $N(\varepsilon_1 - \varepsilon_0)$, all particles can be excited. Therefore, for energies higher than this value the circumstance that the number of particles is finite explicitly restricts the possible partitions to partitions with at most N pieces. This restriction is removed when the number of particles is formally taken to be infinite, so that E can be partitioned into an arbitrary number of parts: for each fixed value of E, the number of microstates $\omega(E, N)$ becomes independent of N when N is sufficiently large. We write

$$\Omega(E) = \lim_{N\to\infty} \omega(E, N) \tag{9}$$

for the number of unrestricted partitions of E, and immediately obtain

$$\sum_{M=0}^{\infty} \Phi(E, M) = \Omega(E) \tag{10}$$

keeping in mind that $\Phi(E, M) = 0$ for large M.

The object of interest now is the normalized distribution

$$p_{\mathrm{mc}}(E, M) \equiv \frac{\Phi(E, M)}{\Omega(E)} \qquad M \geqslant 0 \tag{11}$$

which describes the microcanonical probability for finding M excited particles in the thermally isolated Bose gas when the total excitation energy is E, under the further assumption that there is an infinite supply of additional particles still residing in the ground state, i.e., a Bose–Einstein condensate.

As pointed out in the introduction, it will be convenient to consider first the canonical counterpart of the microcanonical distribution (11), given by

$$p_{\mathrm{cn}}(\beta, M) \equiv \frac{\sum_E \mathrm{e}^{-\beta E}\Phi(E, M)}{\sum_E \mathrm{e}^{-\beta E}\Omega(E)} \tag{12}$$

where the sums run over all possible values of E, and $\beta = 1/(k_{\mathrm{B}}T)$. This canonical distribution (12) gives the probability for finding M excited particles when the system is kept at constant temperature T by contact with some thermal reservoir, again assuming the presence of an infinite background of Bose–Einstein-condensed ground-state particles which render the consideration of restricted partitions unnecessary.

Within the canonical ensemble, the M-particle partition function $Z_M(\beta)$ now generates the microcanonical weights $\omega(E, M)$ according to

$$Z_M(\beta) = \sum_E \omega(E, M) \exp(-\beta M \varepsilon_0 - \beta E): \tag{13}$$

these canonical partition functions (13), in their turn, are generated by the grand-canonical partition function

$$\begin{aligned}\Xi(\beta, z) &\equiv \sum_{M=0}^{\infty} (z\,\mathrm{e}^{\beta\varepsilon_0})^M Z_M(\beta) \\ &= \prod_{\nu=0}^{\infty} \frac{1}{1 - z\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]}\end{aligned} \tag{14}$$

where z is a fugacity-type variable [21]. From the definition (13) it follows that $\Xi(\beta, z)$ also has the alternative sum representation

$$\Xi(\beta, z) = \sum_{M=0}^{\infty} z^M \sum_E \omega(E, M) \exp(-\beta E) \tag{15}$$

which enables us to construct a generating function for the microcanonical differences $\Phi(E, M)$: multiplying equation (15) by $(1 - z)$ and appropriately shifting the summation index M, we have

$$\begin{aligned}(1 - z)\Xi(\beta, z) &= \sum_{M=0}^{\infty} (z^M - z^{M+1}) \sum_E \omega(E, M) \exp(-\beta E) \\ &= \sum_{M=0}^{\infty} z^M \sum_E [\omega(E, M) - \omega(E, M-1)] \exp(-\beta E) \\ &= \sum_{M=0}^{\infty} z^M \sum_E \Phi(E, M) \exp(-\beta E).\end{aligned} \tag{16}$$

On the other hand, the product representation (14) yields for this generating function (16) the equivalent expression

$$\begin{aligned}(1 - z)\Xi(\beta, z) &= \prod_{\nu=1}^{\infty} \frac{1}{1 - z\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]} \\ &\equiv \Xi_{\mathrm{ex}}(\beta, z).\end{aligned} \tag{17}$$

This identity has an interesting interpretation: multiplying $\Xi(\beta, z)$ by $(1 - z)$ means discarding the ground-state factor $\nu = 0$ from the product (14) and retaining its 'excited' part $\Xi_{\mathrm{ex}}(\beta, z)$, so that the generating function (16) for the differences $\Phi(E, M)$ corresponds to the grand partition function of an ideal Bose gas from which the single-particle ground state has been removed.

Combining equations (16) and (17), we now find

$$\left. \left(z \frac{\partial}{\partial z} \right)^k \Xi_{\mathrm{ex}}(\beta, z) \right|_{z=1} = \sum_E \exp(-\beta E) \sum_{M=0}^{\infty} M^k \Phi(E, M) \tag{18}$$

which means that the ground-state amputated function $\Xi_{\mathrm{ex}}(\beta, z)$ furnishes, by repeated application of the operator $z\frac{\partial}{\partial z}$, the moments of the non-normalized distribution

$\left\{\sum_E \exp(-\beta E)\Phi(E, M);\, M \geqslant 0\right\}$. According to standard probability theory, this implies that the logarithm of $\Xi_{\rm ex}(\beta, z)$ generates precisely the cumulants of the canonical number-of-pieces distribution (12):

$$\kappa_{\rm cn}^{(k)}(\beta) = \left(z\frac{\partial}{\partial z}\right)^k \ln \Xi_{\rm ex}(\beta, z)\bigg|_{z=1} \tag{19}$$

hence

$$\ln \Xi_{\rm ex}(\beta, z) = \sum_{\nu=0}^{\infty} \frac{\kappa_{\rm cn}^{(\nu)}(\beta)}{\nu!} (\ln z)^{\nu}\,. \tag{20}$$

In general, the cumulants of a probability distribution $\{p(M);\, M \geqslant 0\}$ belonging to an integer-valued stochastic variable are closely related to the central moments $\mu^{(k)} = \sum_{M=0}^{\infty} (M - \bar{m})^k p(M)$, where $\bar{m} = \sum_{M=0}^{\infty} M p(M)$ is the mean value; in particular, one has [15]

$$\kappa^{(1)} = \bar{m} \qquad \kappa^{(2)} = \mu^{(2)} \qquad \kappa^{(3)} = \mu^{(3)} \qquad \kappa^{(4)} = \mu^{(4)} - 3(\mu^{(2)})^2. \tag{21}$$

The merit of cumulants, as opposed to the moments, lies in the fact that when $\widehat{Y}$ is a sum of independent stochastic variables $\widehat{X}_\nu$, then the kth order cumulant of $\widehat{Y}$ equals the sum of the kth order cumulants of its components:

$$\kappa^{(k)}[\widehat{Y}] = \sum_{\nu} \kappa^{(k)}[\widehat{X}_\nu]. \tag{22}$$

In our context, since $\ln \Xi_{\rm ex}(\beta, z)$ is expressed as a sum over contributions from the excited states $\nu \geqslant 1$, all total cumulants $\kappa_{\rm cn}^{(k)}(\beta)$ are given by sums over cumulants pertaining to the individual excited states. For instance, the first cumulant $\kappa_{\rm cn}^{(1)}(\beta)$, which is the canonical expectation value of the number of excited particles, simply equals the sum of the expectation values of the excited-states occupation numbers. While this is obvious, a more interesting statement is obtained for $k = 2$: the canonical mean-square fluctuation $\kappa_{\rm cn}^{(2)}(\beta)$ of the number of excited particles equals, within the 'infinite-condensate assumption', the sum of the mean-square fluctuations of the individual occupation numbers, so that these canonical occupation numbers are uncorrelated stochastic variables.

In order to derive an expression for the canonical cumulants $\kappa_{\rm cn}^{(k)}(\beta)$ that lends itself to a systematic asymptotic expansion, we start from equation (17) and write $\ln \Xi_{\rm ex}(\beta, z)$ in the form

$$\begin{aligned}\ln \Xi_{\rm ex}(\beta, z) &= -\sum_{\nu=1}^{\infty} \ln(1 - z\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]) \\ &= \sum_{\nu=1}^{\infty}\sum_{n=1}^{\infty} \frac{z^n \exp[-\beta(\varepsilon_\nu - \varepsilon_0)n]}{n}.\end{aligned} \tag{23}$$

Recalling now that e^{-a} is the Mellin transform of $\Gamma(t)$, namely

$$\mathrm{e}^{-a} = \frac{1}{2\pi \mathrm{i}} \int_{\tau - \mathrm{i}\infty}^{\tau + \mathrm{i}\infty} \mathrm{d}t\, a^{-t}\Gamma(t) \tag{24}$$

for $\mathrm{Re}\, a > 0$ and $\tau > 0$, one arrives at

$$\begin{aligned}\ln \Xi_{\rm ex}(\beta, z) &= \sum_{\nu=1}^{\infty}\sum_{n=1}^{\infty} \frac{1}{2\pi \mathrm{i}} \int_{\tau - \mathrm{i}\infty}^{\tau + \mathrm{i}\infty} \mathrm{d}t\, \Gamma(t) \frac{z^n}{n} \frac{1}{(\beta[\varepsilon_\nu - \varepsilon_0]n)^t} \\ &= \frac{1}{2\pi \mathrm{i}} \int_{\tau - \mathrm{i}\infty}^{\tau + \mathrm{i}\infty} \mathrm{d}t\, \Gamma(t) \sum_{\nu=1}^{\infty} \frac{1}{(\beta[\varepsilon_\nu - \varepsilon_0])^t} \sum_{n=1}^{\infty} \frac{z^n}{n^{t+1}}.\end{aligned} \tag{25}$$

The interchange of summation and integration performed here is permissible when the resulting series under the integral are absolutely convergent [3]; this requires that the real number τ be chosen such that the path of integration parallel to the imaginary axis lies to the right of the poles of these analytically continued series. We then employ the familiar notation [21]

$$g_\alpha(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\alpha} \tag{26}$$

for the Bose function $g_\alpha(z)$, and introduce the Dirichlet series

$$Z(\beta, t) \equiv \sum_{\nu=1}^{\infty} \frac{1}{(\beta[\varepsilon_\nu - \varepsilon_0])^t} \tag{27}$$

so that

$$\ln \Xi_{\mathrm{ex}}(\beta, z) = \frac{1}{2\pi \mathrm{i}} \int_{\tau-\mathrm{i}\infty}^{\tau+\mathrm{i}\infty} \mathrm{d}t\, \Gamma(t) Z(\beta, t) g_{t+1}(z). \tag{28}$$

Finally, inserting this expression into equation (19), utilizing

$$z\frac{\mathrm{d}}{\mathrm{d}z} g_\alpha(z) = g_{\alpha-1}(z) \tag{29}$$

and

$$g_\alpha(1) = \zeta(\alpha) \tag{30}$$

where $\zeta(\alpha) = \sum_{n=1}^{\infty} n^{-\alpha}$ is the Riemann zeta function, we arrive at the representation

$$\kappa_{\mathrm{cn}}^{(k)}(\beta) = \frac{1}{2\pi \mathrm{i}} \int_{\tau-\mathrm{i}\infty}^{\tau+\mathrm{i}\infty} \mathrm{d}t\, \Gamma(t) Z(\beta, t) \zeta(t + 1 - k). \tag{31}$$

So far, our deliberations refer to an arbitrary single-particle spectrum, and can be applied to quite different types of partitions when this spectrum is adjusted accordingly. For application to the standard number-partitioning problem, we now return to the one-dimensional harmonic oscillator spectrum, so that

$$\varepsilon_\nu = \hbar\omega_0(\nu + 1/2) \tag{32}$$

with integer quantum number $\nu = 0, 1, 2, \ldots,$ and

$$Z(\beta, t) = b^{-t} \zeta(t) \tag{33}$$

with scaled (dimensionless) inverse temperature

$$b \equiv \beta\hbar\omega_0. \tag{34}$$

Hence, simply writing $\kappa_{\mathrm{cn}}^{(k)}(b)$ instead of $\kappa_{\mathrm{cn}}^{(k)}\left(\frac{b}{\hbar\omega_0}\right)$, in this special case the canonical cumulants adopt the form

$$\kappa_{\mathrm{cn}}^{(k)}(b) = \frac{1}{2\pi \mathrm{i}} \int_{\tau-\mathrm{i}\infty}^{\tau+\mathrm{i}\infty} \mathrm{d}t\, b^{-t} \Gamma(t) \zeta(t) \zeta(t + 1 - k). \tag{35}$$

Since we are primarily interested in partitioning large numbers, corresponding to energies that are large compared to the oscillator quantum $\hbar\omega_0$, we need the asymptotic expansion of these cumulants (35) in the regime $b \ll 1$. By means of the residue theorem, this expansion is obtained through collecting, from right to left, the residues of the integrand in equation (35). In this way, we obtain the cumulants of the canonical distribution (12) for harmonically trapped, ideal Bosons in one dimension:

$$\kappa_{\rm cn}^{(0)}(b) = \frac{\pi^2}{6b} + \frac{1}{2}\ln\frac{b}{2\pi} - \frac{b}{24} + \mathcal{O}(b^{15.5}) \tag{36}$$

$$\kappa_{\rm cn}^{(1)}(b) = \frac{1}{b}\left(\ln\frac{1}{b} + \gamma\right) + \frac{1}{4} - \frac{b}{144} + \mathcal{O}(b^{2.5}) \tag{37}$$

$$\kappa_{\rm cn}^{(2)}(b) = \frac{\pi^2}{6b^2} - \frac{1}{2b} + \frac{1}{24} + \mathcal{O}(b^{14.5}) \tag{38}$$

$$\kappa_{\rm cn}^{(3)}(b) = \frac{2\zeta(3)}{b^3} - \frac{1}{12b} + \frac{b}{1440} + \mathcal{O}(b^{2.5}) \tag{39}$$

$$\kappa_{\rm cn}^{(4)}(b) = \frac{\pi^4}{15b^4} - \frac{1}{240} + \mathcal{O}(b^{11.5}) \tag{40}$$

where $\gamma \approx 0.57722$ is Euler's constant. The error terms, as well as the mathematical justification for these approximations, are discussed in detail in the appendix.

3. The microcanonical cumulants

The task now is to abandon the notion of temperature, and to return to the microcanonical distribution (11) for the number-partitioning problem. To this end, we specialize equation (16) to the spectrum of the one-dimensional harmonic oscillator. Thus, we write

$$\begin{aligned}\Xi_{\rm ex}(b, z) &= \sum_{\nu=0}^{\infty} {\rm e}^{-b\nu} \sum_{M=0}^{\infty} z^M \Phi(\nu, M) \\ &\equiv \sum_{\nu=0}^{\infty} {\rm e}^{-b\nu} Y(\nu, z)\end{aligned} \tag{41}$$

where

$$Y(\nu, z) = \sum_{M=0}^{\infty} z^M \Phi(\nu, M) \tag{42}$$

generates the microcanonical moments

$$\left(z\frac{\partial}{\partial z}\right)^k Y(\nu, z)\bigg|_{z=1} = \sum_{M=0}^{\infty} M^k \Phi(\nu, M). \tag{43}$$

Hence, $\ln Y(\nu, z)$ generates the desired microcanonical cumulants, so that this function is of central importance for the partitioning problem. Setting ${\rm e}^{-b} \equiv x$, and using the notation $\Xi_{\rm ex}(-\ln x, z) \equiv \widetilde{\Xi}_{\rm ex}(x, z)$, we have

$$\widetilde{\Xi}_{\rm ex}(x, z) = \sum_{\nu=0}^{\infty} x^\nu Y(\nu, z) \tag{44}$$

and extract the nth coefficient $Y(n, z)$ from this power series by means of a complex contour integral:

$$Y(n, z) = \frac{1}{2\pi {\rm i}} \oint {\rm d}x\, \frac{\widetilde{\Xi}_{\rm ex}(x, z)}{x^{n+1}} \tag{45}$$

where the path of integration encircles the origin of the complex x-plane counter-clockwise. This contour integral (45) will now be evaluated with the help of the saddle-point approximation. Following the standard procedure [22], we define the function $F_n(x,z)$ as the negative logarithm of the integrand,

$$\frac{\widetilde{\Xi}_{\rm ex}(x,z)}{x^{n+1}} \equiv \exp(-F_n(x,z)) \tag{46}$$

so that

$$F_n(x,z) = (n+1)\ln x - \ln\widetilde{\Xi}_{\rm ex}(x,z). \tag{47}$$

The saddle point $x_0(z)$, that is, the location where the optimal path of integration crosses the real axis, is found by setting the first derivative

$$\frac{\partial F_n(x,z)}{\partial x} = \frac{n+1}{x} - \frac{\partial}{\partial x}\ln\widetilde{\Xi}_{\rm ex}(x,z) \tag{48}$$

equal to zero, giving the 'energy–temperature' relation

$$\begin{aligned} n+1 &= x\frac{\partial}{\partial x}\ln\widetilde{\Xi}_{\rm ex}(x,z)\bigg|_{x_0(z)} \\ &= -\frac{\partial}{\partial b}\ln\Xi_{\rm ex}(b,z)\bigg|_{b_0(z)} \end{aligned} \tag{49}$$

with $b_0(z) = -\ln x_0(z)$. Moreover, the required second derivative of $F_n(x,z)$ at the saddle point is determined as

$$\begin{aligned} \frac{\partial^2 F_n(x,z)}{\partial x^2}\bigg|_{x_0(z)} &= -\frac{1}{x_0^2}\left(x\frac{\partial}{\partial x}\right)^2\ln\widetilde{\Xi}_{\rm ex}(x,z)\bigg|_{x_0(z)} \\ &= -{\rm e}^{2b_0}\left(-\frac{\partial}{\partial b}\right)^2\ln\Xi_{\rm ex}(b,z)\bigg|_{b_0(z)} \end{aligned} \tag{50}$$

where equation (49) has been used. Thus, within the usual Gaussian approximation the saddle-point formula [22]

$$Y(n,z) = \frac{\exp(-F_n(x_0(z),z))}{\sqrt{-2\pi\,\partial_x^2 F_n(x_0(z),z)}} \tag{51}$$

yields in the present case

$$\ln Y(n,z) = \ln\Xi_{\rm ex}(b_0(z),z) + nb_0(z) - \frac{1}{2}\ln 2\pi - \frac{1}{2}\ln\left(-\frac{\partial}{\partial b}\right)^2\ln\Xi_{\rm ex}(b_0(z),z) \tag{52}$$

from which the sought-for cumulants are obtained by further differentiation

$$\kappa_{\rm mc}^{(k)}(n) = \left(z\frac{\rm d}{{\rm d}z}\right)^k \ln Y(n,z)\bigg|_{z=1} \tag{53}$$

where the symbol for the total derivative is meant to indicate that also the implicit z-dependence of the saddle point needs to be taken into account.

Let us work out the first cumulant

$$\kappa_{\rm mc}^{(1)}(n) = z\frac{\rm d}{{\rm d}z}\ln Y(n,z)\bigg|_{z=1} \tag{54}$$

in explicit detail: we have

$$\kappa_{\rm mc}^{(1)}(n) = \left[\left(z\frac{\partial}{\partial z}\ln Y(n,z)\right)_{b_0} + z\frac{{\rm d}b_0}{{\rm d}z}\left(\frac{\partial}{\partial b_0}\ln Y(n,z)\right)_z\right]_{z=1} \tag{55}$$

where the subscripts at the round brackets are to indicate which quantity is to be held constant. For the first of these brackets, equation (52) then gives, in a shorthand notation,

$$\left(z\frac{\partial}{\partial z}\ln Y(n,z)\right)_{b_0} = z\frac{\partial}{\partial z}\ln \Xi_{\rm ex}(b_0,z) - \frac{1}{2}z\frac{\partial}{\partial z}\ln\left(-\frac{\partial}{\partial b_0}\right)^2 \ln \Xi_{\rm ex}(b_0,z) \tag{56}$$

while the second leads to

$$\left(\frac{\partial}{\partial b_0}\ln Y(n,z)\right)_{z} = -1 - \frac{1}{2}\frac{\partial}{\partial b_0}\ln\left(-\frac{\partial}{\partial b_0}\right)^2 \ln \Xi_{\rm ex}(b_0,z) \tag{57}$$

where, again, equation (49) defining the saddle point has been used.

To proceed with the evaluation of equation (55), we still need to know $\mathrm{d}b_0/\mathrm{d}z$, i.e., the z-dependence of the saddle point. This is found by taking the derivative of equation (49):

$$z\frac{\partial}{\partial b_0}\frac{\partial}{\partial z}\ln \Xi_{\rm ex}(b_0,z) + z\frac{\mathrm{d}b_0}{\mathrm{d}z}\frac{\partial^2}{\partial b_0^2}\ln \Xi_{\rm ex}(b_0,z) = 0 \tag{58}$$

which, when taken at $z = 1$ and keeping in mind that $\ln \Xi_{\rm ex}$ generates the canonical cumulants, reduces to

$$\left.\frac{\mathrm{d}b_0}{\mathrm{d}z}\right|_{z=1} = -\frac{D\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} \tag{59}$$

where D indicates differentiation with respect to b_0, and $b_1 = b_0(1)$. Expressing, in the same spirit, also the ingredients from equations (56) and (57) in terms of derivatives of canonical cumulants, equation (55) finally takes the form

$$\kappa_{\rm mc}^{(1)}(n) = \kappa_{\rm cn}^{(1)}(b_1) - \frac{1}{2}\frac{D^2\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} + \frac{D\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\left[1 + \frac{1}{2}\frac{D^3\kappa_{\rm cn}^{(0)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\right]. \tag{60}$$

Of course, the inverse temperature has to be expressed in terms of the energy, $b_1 = b_1(n)$. Recalling $\ln \Xi_{\rm ex}(b,1) = \kappa_{\rm cn}^{(0)}(b)$, equations (49) and (36) yield the relation

$$n + 1 = \frac{\pi^2}{6b_1^2} - \frac{1}{2b_1} + \frac{1}{24} \tag{61}$$

which, upon inversion, gives

$$\frac{1}{b_1} = \frac{\sqrt{6n}}{\pi} + \frac{3}{2\pi^2} + \mathcal{O}(n^{-1/2}). \tag{62}$$

Inserting this expression into the canonical first cumulant (37), one is led to [16]

$$\kappa_{\rm cn}^{(1)}(b_1(n)) = \frac{\sqrt{6n}}{\pi}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] + \frac{3}{2\pi^2}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma + 1 + \frac{\pi^2}{6}\right] + \mathcal{O}(n^{-1/2}). \tag{63}$$

To arrive at the proper microcanonical first cumulant, one still has to evaluate the rest of equation (60). Employing the expressions (36) and (37), doing the derivatives, and inserting equation (62), we obtain the difference between the microcanonical and the canonical first cumulant in the form

$$\kappa_{\rm mc}^{(1)}(n) - \kappa_{\rm cn}^{(1)}(b_1(n)) = \frac{3}{2\pi^2}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] + \mathcal{O}(n^{-1/2}). \tag{64}$$

Therefore, the expectation value of the number of addends in a partition of the natural number n finally becomes

$$\kappa_{\rm mc}^{(1)}(n) = \frac{\sqrt{6n}}{\pi}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma\right] + \frac{3}{2\pi^2}\left[2\ln\left(\frac{\sqrt{6n}}{\pi}\right) + 2\gamma + 1 + \frac{\pi^2}{6}\right] + \mathcal{O}(n^{-1/2}). \tag{65}$$

This example shows how to proceed in the general case: starting from the microcanonical generating function $\ln Y(n, z)$, given, within the usual saddle-point approximation, by equation (52), the microcanonical cumulants are determined by equation (53). Although the practical evaluation of this equation is somewhat tedious, due to the implicit dependence of the saddle point b_0 on z, there are no principal technical difficulties, so that the kth microcanonical cumulant can eventually be expressed in terms of the ℓth canonical cumulants, $\ell = 0, \ldots, k$, and their derivatives with respect to the scaled temperature b. Computing the second cumulant in the same manner, we obtain the rms fluctuation of the number of addends in a partition of n

$$\begin{aligned} \sigma(n) &= \left(\kappa_{\mathrm{mc}}^{(2)}(n)\right)^{1/2} \\ &= \sqrt{n} - \frac{3\sqrt{6}}{2\pi^3}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma + 1\right]^2 + \mathcal{O}(n^{-1/2}) \end{aligned} \tag{66}$$

or, in a numerically convenient form,

$$\sigma(n) = \sqrt{n} - 0.118\,50[\ln(\sqrt{n})]^2 - 0.314\,80\ln(\sqrt{n}) - 0.209\,08 + \mathcal{O}(n^{-1/2}). \tag{67}$$

Proceeding further, the above strategy produces the third cumulant

$$\begin{aligned} \kappa_{\mathrm{mc}}^{(3)}(n) &= \frac{12\sqrt{6}\zeta(3)}{\pi^3}n^{3/2} - \frac{18}{\pi^2}n\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma + 1\right] + \mathcal{O}(n^{1/2}) \\ &= 1.1395n^{3/2} - 1.8238n[\ln(\sqrt{n}) + 1.3283] + \mathcal{O}(n^{1/2}) \end{aligned} \tag{68}$$

while the fourth cumulant reads

$$\begin{aligned} \kappa_{\mathrm{mc}}^{(4)}(n) &= \frac{12}{5}n^2 - n^{3/2}\left(\frac{42\sqrt{6}}{5\pi} + \frac{432\sqrt{6}\zeta(3)}{\pi^5}\left[\ln\left(\frac{\sqrt{6n}}{\pi}\right) + \gamma + 1\right]\right) + \mathcal{O}(n) \\ &= 2.4n^2 - n^{3/2}[4.1566\ln(\sqrt{n}) + 12.071] + \mathcal{O}(n). \end{aligned} \tag{69}$$

The derivation of higher-order terms for these expansions is straightforward. In particular, we state the coefficients of skewness (4) and excess (5) for the number-of-pieces distribution (11) with an absolute error of the order of only $\mathcal{O}(n^{-3/2})$: the skewness becomes

$$\begin{aligned} \gamma_1(n) = 1.1395 &+ \frac{1}{\sqrt{n}}[0.101\,28[\ln(n)]^2 - 0.373\,76\ln(n) - 1.7078] \\ &+ \frac{1}{n}[0.007\,5008[\ln(n)]^4 + 0.025\,681[\ln(n)]^3 + 0.020\,024[\ln(n)]^2 \\ &- 0.230\,28\ln(n) - 0.569\,84] + \mathcal{O}(n^{-3/2}) \end{aligned} \tag{70}$$

and the flatness takes the form

$$\begin{aligned} \gamma_2(n) = 2.4 &+ \frac{1}{\sqrt{n}}[0.284\,40[\ln(n)]^2 - 0.567\,14\ln(n) - 10.064] \\ &+ \frac{1}{n}[0.025\,276[\ln(n)]^4 + 0.022\,329[\ln(n)]^3 - 0.338\,09[\ln(n)]^2 \\ &+ 0.735\,38\ln(n) + 3.7863] + \mathcal{O}(n^{-3/2}). \end{aligned} \tag{71}$$

4. Discussion

We now check the accuracy of the preceding results by comparing the predictions of the asymptotic formulae with exact numerical data, computed with the help of the recursion formula (2). Figure 1 shows exact values of the expectation value $\kappa_{\mathrm{mc}}^{(1)}(n)$ (full line),

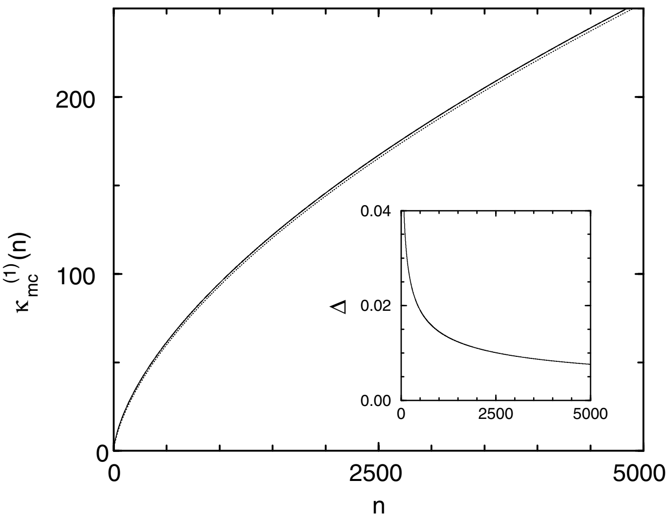

Figure 1. Numerically computed, exact values (full line) of the expectation value $\kappa_{\mathrm{mc}}^{(1)}(n)$ of the number of addends in a partition of n, compared to the leading-order term (dotted line) of the asymptotic formula (65), excluding terms of the order $\mathcal{O}(1)$. When these terms are included, the resulting graph is, on the scale of this plot, indistinguishable from that of the exact data. The inset quantifies the absolute value of the error term of order $\mathcal{O}(n^{-1/2})$ in equation (65).

in comparison to the leading-order term (excluding terms of order $\mathcal{O}(1)$, dotted line) of equation (65). When the next-to-leading term of order $\mathcal{O}(1)$ is included, the plot of the approximate data coincides, on the scale of the figure, with that of the exact ones. The inset quantifies the absolute value Δ of the error term in equation (65), as resulting from the exact numerical calculation, and confirms that this absolute error vanishes with increasing n. The accuracy reached by equation (65) indeed is remarkable: for $n = 5000$, say, the number of partitions is $\Omega(5000) \approx 1.6982 \times 10^{74}$, the exact value of the expected number of addends is $\kappa_{\mathrm{mc}}^{(1)}(5000) \approx 254.70$, and equation (65) is off by less than 0.01.

Figure 2 depicts the corresponding comparison for the rms fluctuation $\sigma(n)$ of the number of addends: the full line visualizes the exact data, the dotted line stems from the leading term of equation (66), $\sigma(n) \sim \sqrt{n}$, while the long-dashed line (coinciding almost with the full line) is obtained when the terms of order $\mathcal{O}(1)$ are included, so that the remaining absolute error Δ again decreases with increasing n (see the inset).

As already indicated, the non-vanishing skewness (4) of the number-of-pieces distribution (11) indicates the non-Gaussian nature of the number-partitioning problem. It is easily seen that this non-Gaussian nature persists in the limit $n \to \infty$,

$$\lim_{n\to\infty} \gamma_1(n) = \frac{12\sqrt{6}\zeta(3)}{\pi^3} \approx 1.1395 \tag{72}$$

and thus is not a finite-size effect. Moreover, it is interesting to observe that this limiting value (72) is reached only for fairly large numbers n, due to the logarithmic corrections found in equation (70): as illustrated by figure 3, $\gamma_1(n)$ significantly overshoots the limit when n is 'merely' of the order of 10^4, and well approaches that limit only for $n > 10^{10}$. The same type of 'creeping convergence' is also observed for the excess (5), as witnessed by figure 4: here, the logarithmic corrections collected in equation (71) prevent $\gamma_2(n)$ from approaching its limit

$$\lim_{n\to\infty} \gamma_2(n) = \tfrac{12}{5} \tag{73}$$

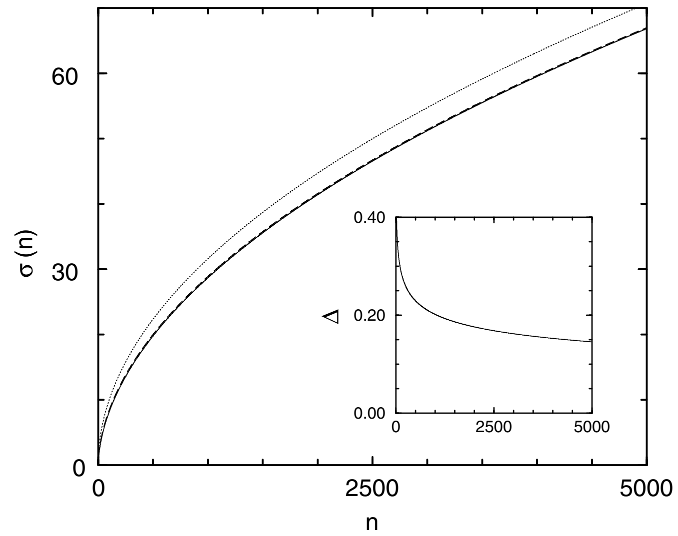

Figure 2. Exact values (full line) of the rms fluctuation $\sigma(n)$ of the number of addends in a partition of n, compared to the leading-order term $\sqrt{n}$ (dotted line), and to the prediction of the asymptotic formula (66), including terms of the order $\mathcal{O}(1)$ (dashed line, almost coinciding with the full line). The inset quantifies the absolute value of the error term of order $\mathcal{O}(n^{-1/2})$.

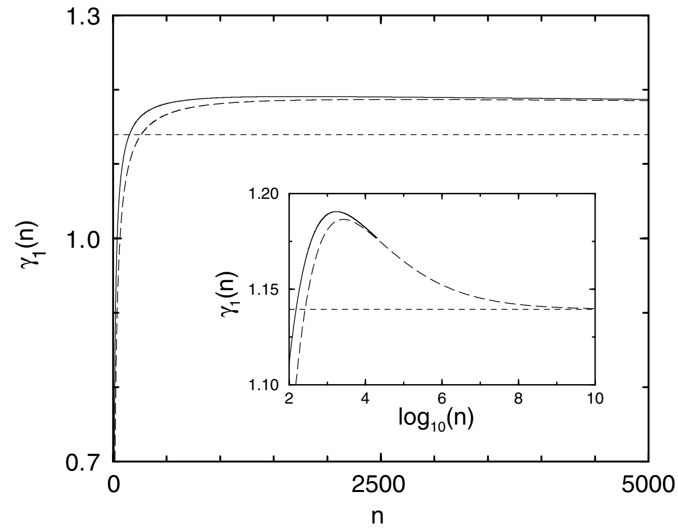

Figure 3. Exact values (full lines) of the coefficient of skewness (4) of the 'number-of-pieces' distribution (11), compared to the prediction of the asymptotic formula (70) (long-dashed lines), and the limiting value (72) (short-dashed lines). The inset, with its logarithmic n-scale, emphasizes the slow convergence.

as long as n stays below 10^{10}. Finally, it should be noted that the microcanonical limiting values (72) and (73) agree to the corresponding values for the canonical ensemble, as follows immediately from equations (38)–(40).

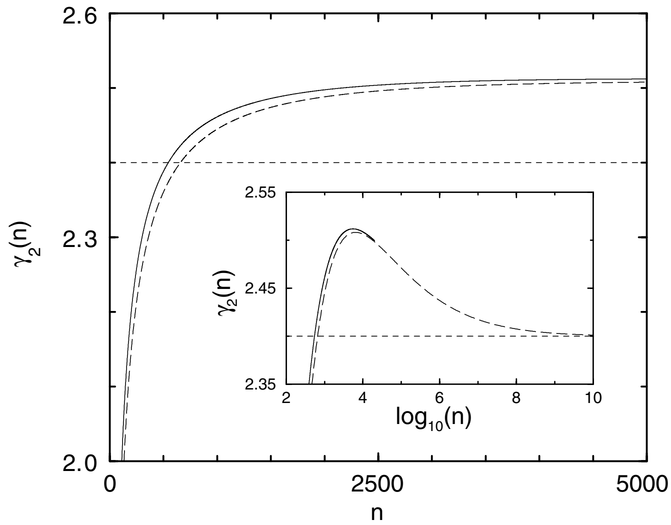

Figure 4. Exact values (full lines) of the coefficient of excess (5) of the 'number-of-pieces' distribution (11), compared to the prediction of the asymptotic formula (71) (long-dashed lines), and the limiting value (73) (short-dashed lines). Again, the inset reveals the 'creeping convergence'.

To summarize, we have exploited the formal equivalence of the number-partitioning problem and a thermally isolated ideal gas of infinitely many Bose particles stored in a one-dimensional harmonic oscillator potential for studying the distribution (11) which governs the number of addends in a partition of a natural number n. This distribution turns out to be essentially non-Gaussian even for $n \to \infty$. However, the standard quantities that measure the deviations from a Gaussian, the coefficients of skewness (4) and excess (5), still vary substantially for $n < 10^{10}$, before approaching the constant limiting values (72) and (73), respectively. In this particular sense, only numbers exceeding 10^{10} can be considered 'large'. We point out that when calculating the moments

$$t_k(n) = \sum_{M=1}^{n} M^k \Phi(n, M) \tag{74}$$

from our cumulants $\kappa_{\mathrm{mc}}^{(k)}(n)$, one does not recover the results obtained in [18]; the asymptotic formula for the moments of partitions derived there is erroneous.

Our approach treats the 'microcanonical' partition problem via a detour to the canonical ensemble, where the degree of excitation of the Bose gas is not quantified by its total energy, but rather in terms of a temperature. In this respect, it constitutes a physical interpretation of the strategy already implicit in the work of Meinardus [3, 17]. In contrast to that work, in our case the return from the canonical to the microcanonical ensemble hinges on the use of the generating function $Y(\nu, z)$ defined in equation (42). Obviously, this generating function can be interpreted as the partition function for a statistical ensemble which uses the 'energy' ν and the fugacity z as its basic variables; this ensemble is precisely the 'Maxwell's Demon ensemble' recently introduced in [20].

The close connection between asymptotic number theory and statistical mechanics can also be exploited for studying other kinds of partition problems, if the single-particle spectrum of the ideal Bose gas is chosen appropriately. For instance, a Bose gas in a d-dimensional oscillator trap images certain d-dimensional partitions, while partitions into sums of d squares correspond to an ideal gas in a d-dimensional box with hard walls. Asymptotic formulae pertaining to these and further partitions can be obtained by exactly retracing the steps made in this paper, the only modification consisting in the replacement of the Riemann zeta function $b^{-t}\zeta(t)$ in the canonical cumulant formula (35) by the appropriate generalized zeta function (27). For example, in the case of a three-dimensional isotropic harmonic trapping potential with oscillator frequency ω_0 one has

$$Z(\beta,t) = (\beta\hbar\omega_0)^{-t}\left[\tfrac{1}{2}\zeta(t-2) + \tfrac{3}{2}\zeta(t-1) + \zeta(t)\right]. \tag{75}$$

The recurrence relation required for generating the exact numerical data for this case and others can be found, e.g., in [23].

Appendix. The canonical cumulants

In this appendix, we provide some technical background concerning the derivation of the canonical cumulants, equations (36)–(40).

We have to evaluate the integral (35),

$$\kappa_{\mathrm{cn}}^{(k)}(b) = \frac{1}{2\pi\mathrm{i}}\int_{\tau-\mathrm{i}\infty}^{\tau+\mathrm{i}\infty}\mathrm{d}t\, b^{-t} f_k(t) \tag{A1}$$

where

$$f_k(t) \equiv \Gamma(t)\zeta(t)\zeta(t+1-k) \tag{A2}$$

and $\tau > 0$ is a real number such that all poles of $f_k(t)$ in the complex t-plane have real parts less than τ. Since $\Gamma(t)$ has poles at $t = 0, -1, -2, -3, \ldots, \zeta(t)$ has a pole at $t = 1$, and $\zeta(t+1-k)$ has a pole at $t = k$, this requirement means $\tau > 1$ for $k = 0$ and $k = 1$, or $\tau > k$ for $k \geqslant 2$.

As a first step, we show that the integral

$$I(x_1, x_2; y) \equiv \frac{1}{2\pi\mathrm{i}}\int_{x_1}^{x_2}\mathrm{d}x\, b^{-x-\mathrm{i}y} f_k(x+\mathrm{i}y) \tag{A3}$$

taken along the finite path parallel to the x-axis from $x_1+\mathrm{i}y$ to $x_2+\mathrm{i}y$, vanishes when $|y| \to \infty$. To this end, we start with the estimate

$$|I(x_1, x_2; y)| \leqslant \frac{1}{2\pi}\int_{x_1}^{x_2}\mathrm{d}x\, b^{-x}|\Gamma(x+\mathrm{i}y)\zeta(x+\mathrm{i}y)||\zeta(x+\mathrm{i}y+1-k)|. \tag{A4}$$

Now the gamma function $\Gamma(x+\mathrm{i}y)$ becomes exponentially small in $|y|$ for large $|y|$ (see equation (6.1.45) in [15]):

$$|\Gamma(x+\mathrm{i}y)| \sim \sqrt{2\pi}|y|^{x-1/2}\,\mathrm{e}^{-\pi|y|/2}. \tag{A5}$$

On the other hand, for $x \geqslant \frac{1}{2}$ Cheng [24] has established the following explicit upper bound on the absolute magnitude of the Riemann zeta function $\zeta(x+\mathrm{i}y)$ for $|y| \geqslant 2$ (see also [25] and references therein):

$$|\zeta(x+\mathrm{i}y)| \leqslant \begin{cases} 175|y|^{46(1-x)^{3/2}}\ln^{2/3}|y| & \text{for} \quad \frac{1}{2} \leqslant x \leqslant 1 \\ 175\ln^{2/3}|y| & \text{for} \quad x \geqslant 1 \end{cases}. \tag{A6}$$

In order to control the zeta function also for $x < \frac{1}{2}$, we employ the reflection formula [15]

$$\zeta(t) = 2^t\pi^{t-1}\sin\left(\frac{\pi}{2}t\right)\Gamma(1-t)\zeta(1-t) \tag{A7}$$

which gives

$$|\zeta(x+\mathrm{i}y)| = 2^x\pi^{x-1}\left|\sin\left(\frac{\pi}{2}(x+\mathrm{i}y)\right)\right||\Gamma(1-x-\mathrm{i}y)\zeta(1-x-\mathrm{i}y)|. \tag{A8}$$

Using the simple inequality

$$\left|\sin\left(\frac{\pi}{2}(x+\mathrm{i}y)\right)\right| \leqslant \exp\left(\frac{\pi}{2}|y|\right) \tag{A9}$$

together with the asymptotic expression (A5), equation (A8) leads, for large $|y|$, to

$$|\zeta(x+\mathrm{i}y)| \lesssim 2\left(\frac{2\pi}{|y|}\right)^{x-\frac{1}{2}} |\zeta(1-x-\mathrm{i}y)| \qquad \text{for} \quad x < \frac{1}{2}. \tag{A10}$$

Since with $x < \frac{1}{2}$ an upper bound on $|\zeta(1-x-\mathrm{i}y)|$ is provided again by equation (A6), equations (A6) and (A10) state that for fixed x the magnitude $|\zeta(x+\mathrm{i}y)|$ of the Riemann zeta function does not increase exponentially with $|y|$. Because of equation (A5), we then have the desired limit

$$\lim_{|y|\to\infty} I(x_1, x_2; y) = 0. \tag{A11}$$

In a second step, this result (A11) now allows us to shift the path of integration in equation (A1) from $x = \tau$ parallel to the imaginary axis to $x = -m - \frac{1}{2}$, where $m > 0$ is an integer, and to employ the residue theorem

$$\kappa_{\mathrm{cn}}^{(k)}(b) = \sum_{\text{residues}} + b^{m+\frac{1}{2}} r_{k,m}(b) \tag{A12}$$

where the sum symbolically collects all the residues of $b^{-t} f_k(t)$ in the stripe between $x = -m - \frac{1}{2}$ and $x = \tau$, and

$$r_{k,m}(b) \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}y\, b^{-\mathrm{i}y} f_k(-m-1/2+\mathrm{i}y) \tag{A13}$$

is the remainder.

We now distinguish two cases: since $\zeta(t) = 0$ when t is a negative, even integer, it follows that $f_k(t)$ possesses only a *finite* number of poles when k is even: for $k = 0$, there are poles at $t = 1, 0, -1$; for $k = 2$, at $t = 2, 1, 0$; and for $k = 4$, at $t = 4, 0$. Choosing some *arbitrary* $m > 0$, and calculating the respective residues, then gives equations (36), (38) and (40), but still leaves the error terms stated therein to be explained. In contrast, for odd k there are *infinitely* many poles: for $k = 1$, at $t = 1, 0$ and all odd negative integers; for $k = 3$, at $t = 3, 1$ and all odd negative integers. Choosing $m = 2$ for both $k = 1$ and $k = 3$, and collecting the residues, produces equations (37) and (39). However, this naive application of the residue theorem only makes sense if the magnitude of the remainder,

$$|r_{k,m}(b)| \leqslant \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}y |f_k(-m-1/2+\mathrm{i}y)| \tag{A14}$$

actually is small, which is what we will show next.

For even k, the reflection formula (A7) leads to

$$|f_k(t)| = |2^{2t+1-k}\pi^{2t-1-k}| \left|\sin\left(\frac{\pi}{2}t\right)\cos\left(\frac{\pi}{2}t\right)\right| |\Gamma(t)\Gamma(1-t)\Gamma(k-t)\zeta(1-t)\zeta(k-t)| \tag{A15}$$

for odd k, the factor $\left|\sin\left(\frac{\pi}{2}t\right)\cos\left(\frac{\pi}{2}t\right)\right|$ has to be replaced by $\sin^2\left(\frac{\pi}{2}t\right)$. However, for $t = -m - \frac{1}{2} + \mathrm{i}y$ and integer m one has $\left|\sin\left(\frac{\pi}{2}t\right)\right| = \left|\cos\left(\frac{\pi}{2}t\right)\right|$, so that it actually suffices to consider equation (A15) for all integer k.

Using $2\sin(\alpha)\cos(\alpha) = \sin(2\alpha)$ and the reflection formula for the gamma function [15],

$$\Gamma(t)\Gamma(1-t) = \frac{\pi}{\sin(\pi t)} \tag{A16}$$

one finds

$$|f_k(t)| = |2^{2t+1-k}\pi^{2t-1-k}|\frac{\pi}{2}|\Gamma(k-t)\zeta(1-t)\zeta(k-t)|. \tag{A17}$$

Thus,

$$\begin{aligned}|f_k(-m-1/2+\mathrm{i}y)| &= (2\pi)^{-2m-1-k}|\Gamma(k+m+1/2-\mathrm{i}y)| \\ &\quad\times |\zeta(m+3/2-\mathrm{i}y)\,\zeta(k+m+1/2-\mathrm{i}y)|.\end{aligned} \tag{A18}$$

Using the inequality

$$|\zeta(x+\mathrm{i}y)| = \left|\sum_{n=1}^{\infty}\frac{1}{n^{x+\mathrm{i}y}}\right| \leqslant \sum_{n=1}^{\infty}\left|\frac{1}{n^{x+\mathrm{i}y}}\right| = \zeta(x) \tag{A19}$$

which is valid for $x > 1$, together with

$$|\Gamma(k+m+1/2-\mathrm{i}y)| \leqslant |(k+m-1/2-\mathrm{i}y)^{k+m}\Gamma(1/2-\mathrm{i}y)| \tag{A20}$$

and [15]

$$|\Gamma(1/2-\mathrm{i}y)| = \sqrt{\frac{\pi}{\cosh(\pi y)}} \leqslant \frac{\sqrt{2\pi}}{\exp(\pi|y|/2)} \tag{A21}$$

equation (A18) finally leads to an inequality that lends itself to numerical evaluation,

$$\begin{aligned}|f_k(-m-1/2+\mathrm{i}y)| &\leqslant (2\pi)^{-2m-\frac{1}{2}-k}\zeta(m+3/2)\,\zeta(k+m+1/2) \\ &\quad\times [(k+m-1/2)^2+y^2]^{(k+m)/2}\exp(-\pi|y|/2).\end{aligned} \tag{A22}$$

With the help of this inequality, one can now compute upper bounds on the remainder in equation (A12). With $m=2$ for both $k=1$ and $k=3$, we find

$$|r_{k,2}(b)| \leqslant \begin{cases} 2.1\times 10^{-4} & \text{for}\quad k=1 \\ 5\times 10^{-4} & \text{for}\quad k=3 \end{cases} \tag{A23}$$

which specifies the error terms (i.e., the coefficients of $b^{2.5}$) in equations (37) and (39). On the other hand, for $k=0$, $k=2$, or $k=4$, we are free to choose $m>0$ such that the remainder in equation (A12) is minimized: for $b<1$, we then find

$$\min_{m>0}\left|b^{m+\frac{1}{2}}r_{k,m}(b)\right| \leqslant \begin{cases} 2.5\times 10^{-8}b^{15.5} & \text{for}\quad k=0 \\ 1\times 10^{-6}b^{14.5} & \text{for}\quad k=2 \\ 4\times 10^{-5}b^{11.5} & \text{for}\quad k=4. \end{cases} \tag{A24}$$

This estimate underlies the error terms stated in equations (36), (38) and (40), respectively. For $b \leqslant \frac{1}{2}$, the estimate is even better:

$$\min_{m>0}\left|b^{m+\frac{1}{2}}r_{k,m}(b)\right| \leqslant \begin{cases} 8.6\times 10^{-15}(2b)^{29.5} & \text{for}\quad k=0 \\ 1.4\times 10^{-12}(2b)^{27.5} & \text{for}\quad k=2 \\ 2.2\times 10^{-10}(2b)^{25.5} & \text{for}\quad k=4. \end{cases} \tag{A25}$$

References

[1] Euler L 1911 De partitione numerorum 1753 *Leonardi Euleri opera omnia* (Leipzig: Teubner)
[2] Rademacher H 1973 *Topics in Analytic Number Theory* (Berlin: Springer)
[3] Andrews G E 1976 *The Theory of Partitions (Encyclopedia of Mathematics and its Applications vol 2)* (Reading, MA: Addison-Wesley) ch 6
[4] Ahlgren S and Ono K 2001 *Notices AMS* **48** 978
[5] Wu F Y, Rollet G, Huang H Y, Maillard J M, Hu Chin-Kun and Chen Chi-Ning 1996 *Phys. Rev. Lett.* **76** 173
[6] Schönhammer K and Meden V 1996 *Am. J. Phys.* **64** 1168

[7] Bhatia D P, Prasad M A and Arora D 1997 *J. Phys. A: Math. Gen.* **30** 2281
[8] Mertens S 1998 *Phys. Rev. Lett.* **81** 4281
[9] Auluck F C and Kothari D S 1946 *Proc. Cambridge Phil. Soc.* **42** 272
[10] Scully M O 1999 *Phys. Rev. Lett.* **82** 3927
[11] Kocharovsky V V, Kocharovsky Vl V and Scully M O 2000 *Phys. Rev.* A **61** 053606
[12] Tran M N and Bhaduri R K 2002 *Preprint* cond-mat/0210624, and references cited therein
[13] Hardy G H and Ramanujan S 1918 *Proc. Lond. Math. Soc.* **17** 75
[14] Bohr N and Kalckar F 1937 *Kgl. Danske Vid. Selskab. Math. Phys. Medd.* **14** 10
[15] Abramowitz M and Stegun I A (ed) 1972 *Handbook of Mathematical Functions* (New York: Dover)
[16] Nanda V S 1953 *Proc. Nat. Inst. Sci. (India)* **19** 681
[17] Meinardus G 1954 *Math. Z.* **59** 388
[18] Richmond B 1975 *Acta Arith.* **26** 411
[19] Holthaus M, Kalinowski E and Kirsten K 1998 *Ann. Phys., NY* **270** 198
[20] Navez P, Bitouk D, Gajda M, Idziaszek Z and Rzążewski K 1997 *Phys. Rev. Lett.* **79** 1789
[21] Pathria R K 1996 *Statistical Mechanics* (Oxford: Butterworth-Heinemann)
[22] Dingle R B 1973 *Asymptotic Expansions: Their Derivation and Interpretation* (New York: Academic)
[23] Weiss C and Wilkens M 1997 *Opt. Express* **1** 272
[24] Cheng Y 1999 *Rocky Mtn. J. Math.* **29** 115
[25] Ford K 2002 *Proc. Lond. Math. Soc.* **85** 565