Topics in Statistical Mechanics and Quantum Optics

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Outline

- Problems in Statistical Mechanics: Condensate statistics of ideal Bose gases
  - Introduction to Bose-Einstein Condensation (BEC)
  - Master equation approach
  - Study through independent oscillator picture
  - Microcanonical ensemble investigations
- Problems in Quantum Optics: Atomic coherence effects and their applications
  - Spontaneous emission quenching
  - Possible violation of the Third Law of Thermodynamics
  - Lasing without inversion in a transient regime

Bosons and Fermions

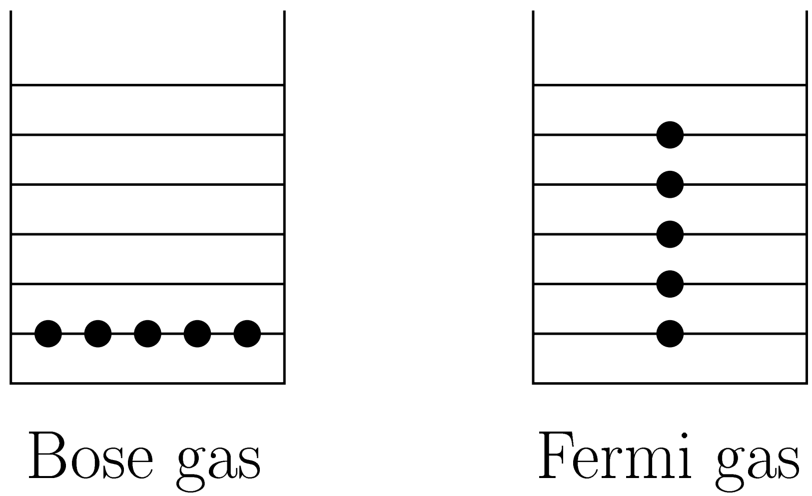
Fermions

- Half-integral spin
- Antisymmetric wavefunction
- No two of them can have the same quantum numbers

Bosons

- Integral spin
- Symmetric wavefunction
- A large number of them can have the same quantum numbers

Difference between the fermionic and bosonic systems as $T \to 0$.



Introduction to BEC

Signatures

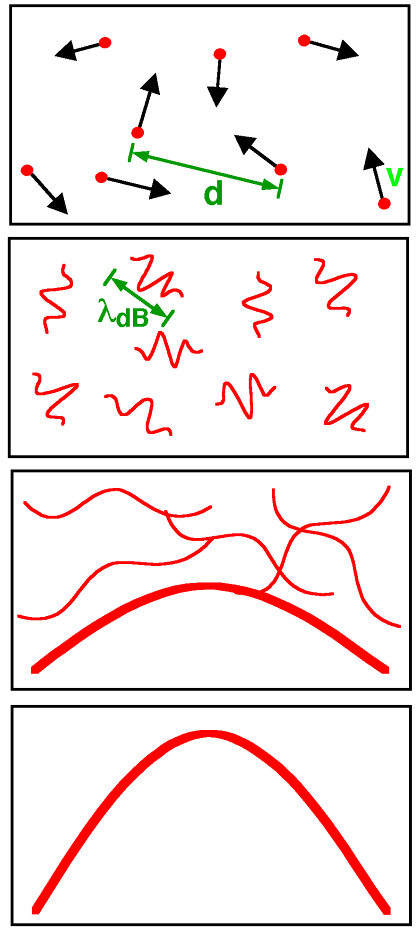
- Macroscopic occupation of the ground state below some critical temperature T_c.
- Chemical potential, $\mu \to 0$ as $T \to T_c^+$ and it remains locked to 0 below T_c.
- Spatial confinement in trapping potentials.
- Appearance of macroscopic phase

Competing Processes

- Liquefaction and solidification
- Dissociation of the fermion pairs
- Disorder and localization

Physically more transparent picture of BEC

What is Bose-Einstein condensation (BEC)?



High Temperature T:

thermal velocity v

density d^{-3}

"Billiard balls"

Low Temperature T:

De Broglie wavelength

$\lambda_{dB} = h/mv \propto T^{-1/2}$

"Wave packets"

$T = T_{crit}$: Bose-Einstein Condensation

$\lambda_{dB} \approx d$

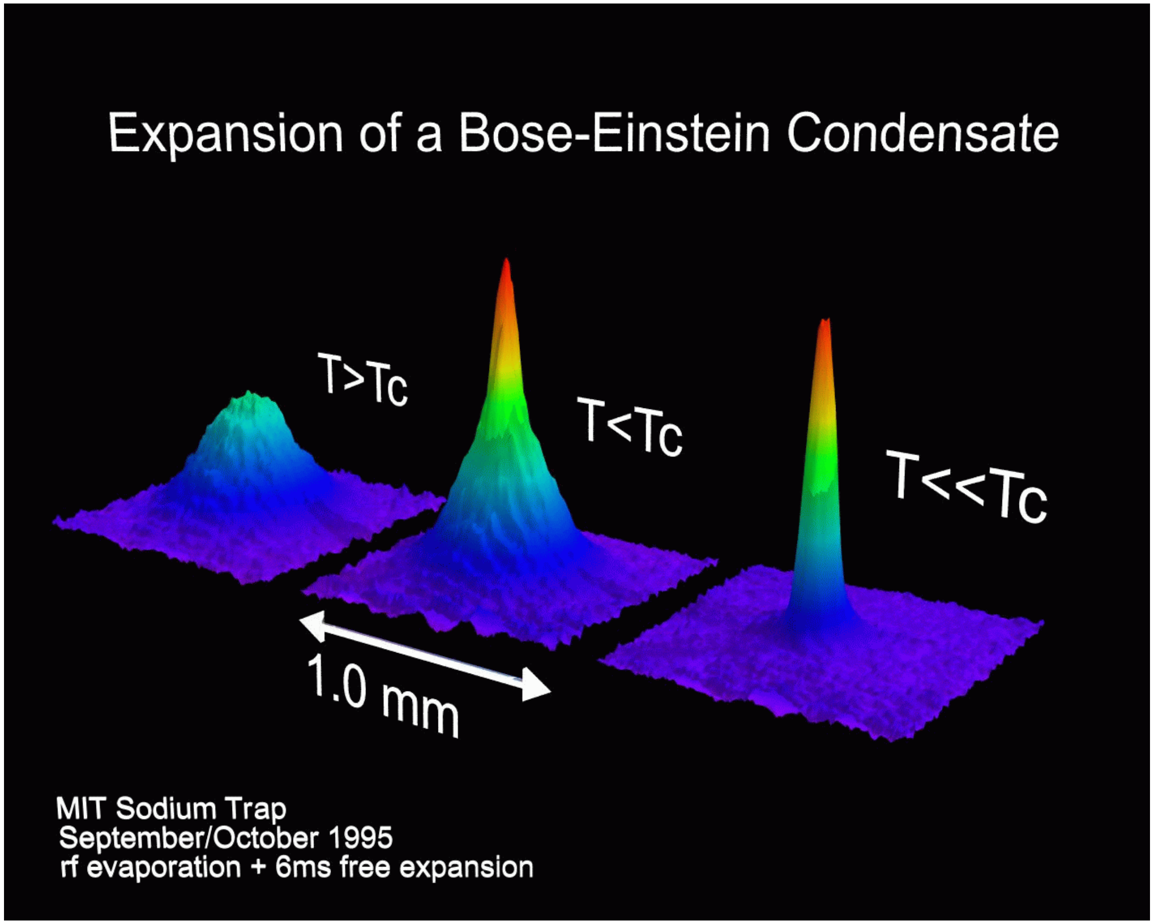
"Matter wave overlap"

T=0: Pure Bose condensate

"Giant matter wave"

One of Prof W. Ketterle's viewgraphs

Physically more transparent picture of BEC



Another one of Prof W. Ketterle's viewgraphs

Grand Canonical Picture of BEC

- Energy as well as matter is exchanged by the system with its surrounding.
- Very easy to evaluate the partition function
- Fluctuations in the condensate occupation

$$\Delta n_0^2 = N(N+1) \qquad \text{as} \quad T \rightarrow 0.$$

Current experiments certainly do not observe this.

- Microcanonical treatment is more relevant to the recent experiments.
- Considering the difficulty involved in evaluating the microcanonical partition function, canonical ensemble constitutes an easier and natural intermediate step.

BEC through canonical ensemble

Canonical Ensemble

- The system exchanges energy with the surrounding but not the matter.
- Thus in a BEC system one has to conserve the number of particles, N, inside the trap.
- This constraint becomes the main hurdle to study BEC within the canonical ensemble.

Various methods employed

- Non-equilibrium Master Equation.
- Canonical ensemble quasiparticles.
- Conventional statistical mechanics with a twist.

Exact Numerical Method for an Ideal Bose Gas

- **Recursion Relation for N Particle Canonical Partition Function** [a]

$$Z_N(T) = \frac{1}{N}\sum_{k=1}^{N} Z_1(T/k) Z_{N-k}(T)$$

- **Ground State Probability Distribution**

$$p_{n_0} = \exp(-n_0\beta\varepsilon_0)\frac{Z_{N-n_0}}{Z_N} - \exp(-(n_0+1)\beta\varepsilon_0)\frac{Z_{N-n_0-1}}{Z_N}$$

The above recursion relation can be evaluated very easily numerically, and hence the ground state probability distribution, thus giving the complete statistics of an ideal Bose gas.

[a] M. Wilkens and C. Weiss, J. Mod. Optics **44**, 1801 (1997);C. Weiss and M. Wilkens, Optics Express **1**, 272 (1997);S. Grossmann and M. Holthaus, Phys. Rev. Lett.**79**, 3557 (1997); henceforth referred to as WWGH

Alternative approaches to the canonical ensemble study of BEC

Canonical ensemble quasiparticles

- Allows one to satisfy the particle number conservation condition through the novel particle number conserving quasiparticles [a].
- Generates cumulants/moments to an arbitrary order very precisely within the condensate regime.
- Very straightforward calculational technique but answers have to be evaluated numerically.

Conventional statistical mechanical approach with a twist.

- Physically equivalent to the quasiparticle approach. [b]
- The form of cumulants obtained this way suggest a nice regularization technique for converting the sums to the integrals.
- The integral representation allow one to obtain analytic expressions for all cumulants very easily.

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[a] V. V. Kocharovsky, Vl. V. Kocharovsky, and M. O. Scully Phys. Rev. A **61**, 053606 (2000).

[b] M. Holthaus, K.T. kapale, V.V. Kocharovsky, and M.O. Scully, "Master equation vs. partition function: Canonical statistics of ideal Bose–Einstein condensates", Physica A **300**,433-467 (2001)

We start from the familiar representation[a]

$$Z_N(\beta) = \sum_{\{n_\nu\}}{}' \exp\left(-\beta \sum_\nu n_\nu \varepsilon_\nu\right) \tag{1}$$

of the canonical N-particle partition function, where the prime indicates that the summation runs only over those sets of occupation numbers $\{n_\nu\}$ that comply with the constraint $\sum_\nu n_\nu = N$. Singling out the ground-state energy $N\varepsilon_0$, we write the total energy of each such configuration as

$$\begin{aligned} \sum_\nu n_\nu \varepsilon_\nu &= \sum_\nu n_\nu \left(\varepsilon_\nu - \varepsilon_0\right) + N\varepsilon_0 \\ &\equiv E + N\varepsilon_0 \ , \end{aligned} \tag{2}$$

so that E denotes the true excitation energy of the respective config-

[a]C. Kittel, *Elementary Statistical Physics* (John Wiley, New York, 1958); K. Huang, *Statistical Mechanics* (John Wiley, New York, 1963); R. K. Pathria, *Statistical Mechanics* (Pergamon Press, Oxford, 1985)

uration. Grouping together configurations with identical excitation energies, we have

$$Z_N(\beta) = \sum_E \Omega(E,N) \exp(-\beta E - N\beta\varepsilon_0) \ , \qquad (3)$$

with $\Omega(E,N)$ denoting the number of microstates accessible to an N-particle system with excitation energy E, that is, the number of microstates where E is distributed over N *or less* particles: $\Omega(E,N)$ counts all the configurations where E is concentrated on one particle only, or shared among two particles, or three, or any other number M up to N.

Detailed understanding of canonical (or microcanonical) statistics, however, requires knowledge of the number of microstates with *exactly* M excited particles, for all M up to N; these numbers are provided by the differences

$$\Phi(E,M) \equiv \Omega(E,M) - \Omega(E,M-1) \ ; \qquad M = 0,1,2,\ldots,N \ . \qquad (4)$$

By definition, $\Omega(E,-1) = 0$. Given $\Phi(E,M)$, the canonical probability distribution for finding M excited particles (and, hence, $N-M$ particles still residing in the ground state) at inverse temperature β is determined by

$$p_N^{(\mathrm{ex})}(M;\beta) \equiv \frac{\sum_E \mathrm{e}^{-\beta E}\Phi(E,M)}{\sum_E \mathrm{e}^{-\beta E}\Omega(E,N)} \; ; \qquad M = 0,1,2,\ldots,N \; . \tag{5}$$

This distribution is merely the mirror image of the condensate distribution p_{n_0} considered in the previous section, *i.e.*, we have $p_N^{(\mathrm{ex})}(M;\beta) = p_{N-M}$. Since the definition (4) obviously implies

$$\sum_{M=0}^{N} \Phi(E,M) = \Omega(E,N) \; , \tag{6}$$

it is properly normalized,

$$\sum_{M=0}^{N} p_N^{(\mathrm{ex})}(M;\beta) = 1 \; . \tag{7}$$

In the following we will derive a general formula which gives all cumulants of the canonical distribution (5), provided the temperature is so low that a significant fraction of the particles occupies the ground state — that is, provided there is a condensate.

To this end, we recall that the set of canonical M-particle partition functions $Z_M(\beta)$ is generated by the grand canonical partition function, which has a simple product form:

$$\sum_{M=0}^{\infty} z^M Z_M(\beta) = \prod_{\nu=0}^{\infty} \frac{1}{1 - z\exp(-\beta\varepsilon_\nu)} \; ; \tag{8}$$

here, z is a complex variable. However, every single M-particle partition function enters into this expression with its own, M-particle ground-state energy $M\varepsilon_0$. In order to remove these unwanted contributions, we define a slightly different function $\Xi(\beta, z)$ by multiplying each $Z_M(\beta)$ by $(z\mathrm{e}^{\beta\varepsilon_0})^M$, instead of z^M, and then summing over M, obtaining

$$\Xi(\beta, z) \equiv \sum_{M=0}^{\infty} (z\mathrm{e}^{\beta\varepsilon_0})^M Z_M(\beta) = \prod_{\nu=0}^{\infty} \frac{1}{1 - z\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]} \; . \tag{9}$$

On the other hand, in view of Eq. (3) this function also has the representation

$$\Xi(\beta, z) = \sum_{M=0}^{\infty} z^M \sum_E \Omega(E, M) \exp(-\beta E) \; . \tag{10}$$

Therefore, multiplying $\Xi(\beta, z)$ by $1-z$ and suitably shifting the summation index M, we arrive at a generating function for the desired differences $\Phi(E, M)$:

$$
\begin{aligned}
(1-z)\,\Xi(\beta, z) &= \sum_{M=0}^{\infty} (z^M - z^{M+1}) \sum_E \Omega(E, M) \exp(-\beta E) \\
&= \sum_{M=0}^{\infty} z^M \sum_E \left[\Omega(E, M) - \Omega(E, M-1)\right] \exp(-\beta E) \\
&= \sum_{M=0}^{\infty} z^M \sum_E \Phi(E, M) \exp(-\beta E) \; . \qquad (11)
\end{aligned}
$$

Going back to the representation (9) now reveals that multiplying $\Xi(\beta, z)$ by $1 - z$ means amputating the ground-state factor $\nu = 0$ from this product and retaining only its "excited" part; we therefore denote the result as $\Xi_{\rm ex}(\beta, z)$:

$$
\begin{aligned}
(1-z)\,\Xi(\beta, z) &= \prod_{\nu=1}^{\infty} \frac{1}{1 - z \exp[-\beta(\varepsilon_\nu - \varepsilon_0)]} \\
&\equiv \Xi_{\rm ex}(\beta, z) \; . \qquad (12)
\end{aligned}
$$

Moreover, from Eq. (11) it is obvious that the canonical moments of the unrestricted set $\Phi(E,M)$ (that is, the moments pertaining to *all* $\Phi(E,M)$ with $M \geq 0$) are obtained by repeatedly differentiating $\Xi_{\rm ex}(\beta,z)$ with respect to z, and then setting $z=1$:

$$\left(z \frac{\partial}{\partial z} \right)^k \Xi_{\rm ex}(\beta,z) \bigg|_{z=1} = \sum_E \exp(-\beta E) \sum_{M=0}^{\infty} M^k \Phi(E,M) \; . \qquad (13)$$

So far, all rearrangements have been exact.

For making contact with the actual N-particle system under consideration, we now have to restrict the summation index M: If the sum over M did not range over all particle numbers from zero to infinity, but rather were restricted to integers not exceeding the actual particle number N, then the equation (13), together with the representation (12), would yield precisely the non-normalized k-th moments of the canonical distribution (5). As it stands, however, exact equality is spoiled by the unrestricted summation. At this point, there is one crucial observation to be made: In the condensate regime the difference between the exact k-th moment, given by a restricted sum, and the right hand side of Eq. (13) must be exceedingly small [?]. Namely, if there is a condensate, then $\Phi(E,N)/\Omega(E,N)$ is negligible, since the statistical weight of those microstates with the energy E spread over all N particles must be insignificant — if it were not, so that there were a substantial probability for all N particles being excited, there would be no condensate! Consequently, we have $\Phi(E,M)/\Omega(E,N) \approx 0$ also for all M larger than N: In the condensate regime it does not matter whether the upper limit of the sum over M in Eq. (13) is the actual particle number N, or infinity;

$$\sum_{M=0}^{\infty} M^k \Phi(E,M) \approx \sum_{M=0}^{N} M^k \Phi(E,M) \quad \text{in the condensate regime} . \tag{14}$$

Within this approximation — which will remain the only approximation in the entire argument! — the amputated function $\Xi_{\rm ex}(\beta,z)$

provides, by means of Eq. (13), the moments of the excited-states distribution (5), as long as one stays in the condensate regime.

The rationale behind this reasoning can be interpreted in a twofold manner. Intuitively, one may divide a partially condensed Bose gas into the excited-states subsystem, and a supply of condensate particles. The approximation (14) then means replacing the actual condensate, consisting of a finite number of particles, by an infinite particle reservoir [**?**]; this point of view goes back to Fierz [**?**]. Of course, the added condensate particles do not take part in the dynamics, so that the statistical properties of the excited subsystem remain unchanged. For our purposes, another interpretation is more telling: For $k = 0$, and utilizing the representation (12) of the moment-generating function $\Xi_{\rm ex}(\beta, z)$, the approximation (14) brings Eq. (12) into the form

$$\prod_{\nu=1}^{\infty} \frac{1}{1-\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]} = \sum_E \exp(-\beta E) \sum_{M=0}^{N} \Phi(E,M) = \sum_E \exp(-\beta E)\, \Omega(E,N) \qquad (15)$$

— stating that in the condensate regime, where (14) holds, the canonical partition function of the Bose gas on the right hand side equals that of a system of harmonic oscillators, with frequencies $\varepsilon_\nu - \varepsilon_0$ ($\nu \geq 1$), on the left hand side of Eq. (15). While the original particles are indistinguishable, and subject to Bose statistics, the substituting oscillators obey Boltzmann statistics; the partition function of the oscillator system being the simple product of the geometric series representing the partition functions of the individual oscillators. It should be noted that this (almost-) isomorphism of a partially condensed, ideal Bose gas and a Boltzmannian harmonic oscillator system holds for any form of the single-particle spectrum, *not* only for harmonic traps.

Since, according to Eq. (13), the function $\Xi_{\rm ex}(\beta, z)$ generates the moments of the canonical distribution (5) in the condensate regime, its logarithm generates the cumulants $\kappa_k(\beta)$:

$$\kappa_k(\beta) = \left(z \frac{\partial}{\partial z} \right)^k \ln \Xi_{\rm ex}(\beta, z) \Big|_{z=1} \quad . \tag{16}$$

As is well known from elementary statistics, the k-th order cumulant of the sum of independent stochastic variables is the sum of their individual k-th order cumulants; moreover, all cumulants higher than the second vanish exactly for a Gaussian stochastic variable [**?**]. In the present case, taking the required derivatives of $\ln \Xi_{\rm ex}(\beta, z)$ and using the expression (**??**) for the canonical occupation numbers $\langle n_\nu \rangle$ in the condensate regime, we find for $k = 1, \ldots, 4$:

Calculation of the cumulants

- Grand canonical partition function for the independent oscillators

$$\Xi_{\rm ex}(\beta, z) \equiv (1-z)\,\Xi(\beta, z) = \prod_{\nu=1}^{\infty} \frac{1}{1 - z\exp[-\beta(\varepsilon_\nu - \varepsilon_0)]}$$

- Logarithm of the grand canonical partition function:

$$\ln \Xi_{\rm ex}(\beta, z) = \sum_{\nu=1}^{\infty}\sum_{n=1}^{\infty} \frac{z^n \exp[-\beta(\varepsilon_\nu - \varepsilon_0)n]}{n} \ ,$$

- The cumulant formula [a] :

$$\kappa_k(\beta) = \left(z\frac{\partial}{\partial z}\right)^k \Xi_{\rm ex}(\beta, z)\bigg|_{z=1} = \frac{1}{2\pi i}\int_{\tau-i\infty}^{\tau+i\infty} {\rm d}t\, \Gamma(t)\, Z(\beta, t)\, \zeta(t+1-k)$$

[a] Where we have used the following definitions of the spectral Zeta function and the Riemann Zeta functions and the Mellin Barnes Integral representation:

$$Z(\beta, t) \equiv \sum_{\nu=1}^{\infty} \frac{1}{(\beta[\varepsilon_\nu - \varepsilon_0])^t}\ ;\ \zeta(\alpha) = \sum_{n=1}^{\infty}\frac{1}{n^\alpha}\ ;\ {\rm e}^{-a} = \frac{1}{2\pi i}\int_{\tau-i\infty}^{\tau+i\infty} {\rm d}t\ a^{-t}\,\Gamma(t)\ [[\tau > 0, {\rm Re}(a) > 0]]$$

Relation between cumulants and centered moments

- Cumulants in terms of the excited state subsystem occupancies:

$$\begin{aligned}
\kappa_1(\beta) &= \sum_{\nu\geq 1}\langle n_\nu\rangle \;, \\
\kappa_2(\beta) &= \sum_{\nu\geq 1}\langle n_\nu\rangle\left(\langle n_\nu\rangle + 1\right) \;, \\
\kappa_3(\beta) &= \sum_{\nu\geq 1}\left(\langle n_\nu\rangle + 3\langle n_\nu\rangle^2 + 2\langle n_\nu\rangle^3\right) \;, \\
\kappa_4(\beta) &= \sum_{\nu\geq 1}\left(\langle n_\nu\rangle + 7\langle n_\nu\rangle^2 + 12\langle n_\nu\rangle^3 + 6\langle n_\nu\rangle^4\right) \;.
\end{aligned}$$

- Cumulants in terms of the condensate population

$$\begin{aligned}
\kappa_1(\beta) &= N - \langle n_0\rangle \;, \\
\kappa_2(\beta) &= \left\langle (n_0 - \langle n_0\rangle)^2 \right\rangle \;, \\
\kappa_3(\beta) &= -\left\langle (n_0 - \langle n_0\rangle)^3 \right\rangle \;, \\
\kappa_4(\beta) &= \left\langle (n_0 - \langle n_0\rangle)^4 \right\rangle - 3\left\langle (n_0 - \langle n_0\rangle)^2 \right\rangle^2 \;.
\end{aligned}$$

Pole structure of Riemann Zeta, Gamma and Spectral Zeta Functions

- $\zeta(z)$ possesses only one simple pole, located at $z = 1$ with residue $+1$, i.e.,

  $$\zeta(z) \approx \frac{1}{z-1} + \gamma \qquad \text{for } z \approx 1 \ ,$$

  where $\gamma \approx 0.57722$ is Euler's constant.

- $\Gamma(t)$ has poles at $t = 0, -1, -2, \ldots$

- $Z(\beta, t)$ pole structure depends on the energy levels of the trap, and hence on the details of the trapping potential.

Poles and residues of generalized Zeta functions

If $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \ldots$ is a sequence of real numbers with $\lambda_\nu \to \infty$, such that the partition function

$$\Theta(\beta) = \sum_{\nu=1}^{\infty} \exp(-\beta\lambda_\nu) \tag{17}$$

converges for $\mathrm{Re}(\beta) > 0$, and possesses for $\beta \to 0$ (*i.e.*, for high temperatures) the asymptotic expansion

$$\Theta(\beta) \sim \sum_{n=0}^{\infty} c_{i_n} \beta^{i_n} \tag{18}$$

with a strictly increasing sequence of real exponents i_n starting with a negative number $i_0 < 0$, then $\Theta(\beta)$ admits, for $\mathrm{Re}(t) > -i_0$, a Mellin transform $\mathcal{M}\Theta(t)$, defined by

$$\mathcal{M}\Theta(t) = \int_0^\infty \mathrm{d}\beta\, \beta^{t-1}\Theta(\beta)\ ; \tag{19}$$

this Mellin transform exhibits simple poles at $t = -i_n$ with residues c_{i_n}. The associated Zeta function, that is, the analytic continuation of

$$Z(t) = \sum_{\nu=1}^{\infty} \frac{1}{\lambda_\nu^t} \; , \tag{20}$$

is then given by

$$Z(t) = \frac{1}{\Gamma(t)} \mathcal{M}\Theta(t) \; . \tag{21}$$

Therefore, there are potential poles of $Z(t)$ at

$$t = -i_n \quad \text{with residue } c_{i_n}/\Gamma(-i_n) \; ; \tag{22}$$

keeping in mind that the singularities of the Gamma function will eliminate those poles of $\mathcal{M}\Theta(t)$ that are located at zero or negative integer numbers.

This connection provides the strategy we have to follow: Given some Zeta function of the form (20), defined for such t which render the sum absolutely convergent, we focus on the corresponding partition function (17) and find its asymptotic (high-temperature) expansion (18). The exponents and coefficients emerging in this expansion then provide, by means of Eq. (22), the positions and residues of the poles of the analytically continued Zeta function.

To see how this works in practice, let us first study the Zeta function

$$E_1(t) = \sum_{n=1}^{\infty} (n^2)^{-t} \; . \tag{23}$$

To find the expansion (18), we recall the Poisson resummation formula

$$\sum_{n=-\infty}^{+\infty} \exp(-\beta n^2) = \left(\frac{\pi}{\beta}\right)^{1/2} \sum_{n=-\infty}^{+\infty} \exp(-\pi^2 n^2/\beta) \; , \tag{24}$$

and rearrange it to read

$$\sum_{n=1}^{\infty} \exp(-\beta n^2) = \frac{1}{2}\left[\left(\frac{\pi}{\beta}\right)^{1/2} - 1 + 2\left(\frac{\pi}{\beta}\right)^{1/2} \sum_{n=1}^{\infty} \exp(-\pi^2 n^2/\beta)\right] . \tag{25}$$

Seen from the viewpoint of statistical mechanics, this identity links the low–temperature behavior ($\beta \to \infty$ on the left hand side) of the partition function of a system with quadratic spectrum to its high-temperature counterpart ($1/\beta \to \infty$ on the right hand side). Leaving out those terms in Eq. (25) that are exponentially damped for $\beta \to 0$, we arrive at the required asymptotic expansion,

$$\sum_{n=1}^{\infty} \exp(-\beta n^2) \sim \frac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2} - \frac{1}{2} . \tag{26}$$

Thus, we have $i_0 = -1/2$, $c_{i_0} = \sqrt{\pi}/2$, and $i_1 = 0$, $c_{i_1} = -1/2$; all other coefficients c_{i_n} vanish. Since the Gamma function is singular at $t = 0$, the analytic continuation of $E_1(t)$ has merely a single pole, located at

$$t = -i_0 = 1/2 \quad \text{with residue } \frac{c_{-1/2}}{\Gamma(1/2)} = \frac{1}{2} \,. \tag{27}$$

Of course, since $E_1(t) = \zeta(2t)$, we could also have inferred this result from Eq. (**??**). But now we got our machinery running: Multiplying the expansion (26) with itself, we find

$$\sum_{n_1,n_2=1}^{\infty} \exp\bigl(-\beta(n_1^2+n_2^2)\bigr) \sim \frac{\pi}{4\beta} - \frac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2} + \frac{1}{4} \,, \tag{28}$$

implying that the Epstein function $E_2(t)$ defined in Eq. (**??**) has poles at

$$t = 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{1}{2} \,. \tag{29}$$

Multiplying then Eq. (26) by Eq. (28), we arrive at

$$\sum_{n_1,n_2,n_3=1}^{\infty} \exp\bigl(-\beta(n_1^2+n_2^2+n_3^2)\bigr)$$

$$\sim \frac{1}{8}\left(\frac{\pi}{\beta}\right)^{3/2} - \frac{3\pi}{8\beta} + \frac{3}{8}\left(\frac{\pi}{\beta}\right)^{1/2} - \frac{1}{8}\ , \qquad (30)$$

stating that $E_3(t)$ has poles at

$$t = 3/2, 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{3\pi}{8}, \frac{3}{8}\ . \qquad (31)$$

Next, we turn to the inhomogeneous Epstein functions introduced in equation (**??**). The partition function associated with $\widetilde{E}_1(t)$, namely

$$\Theta(\beta) = \exp(\beta)\sum_{n=2}^{\infty}\exp(-\beta n^2)\ , \qquad (32)$$

forces us to rewrite the identity (24) as

$$\sum_{n=2}^{\infty}\exp(-\beta n^2)$$

$$= \frac{1}{2}\left[\left(\frac{\pi}{\beta}\right)^{1/2} - 1 - 2\exp(-\beta) + 2\left(\frac{\pi}{\beta}\right)^{1/2}\sum_{n=1}^{\infty}\exp(-\pi^2 n^2/\beta)\right] \quad (33)$$

Again discarding terms that are exponentially damped for $\beta \to 0$, multiplying by $\exp(\beta)$, and expanding this latter exponential, we find

$$\sum_{n=2}^{\infty}\exp\big(-\beta(n^2-1)\big) \sim \frac{1}{2}\left(\frac{\pi}{\beta}\right)^{1/2} - \frac{3}{2} + \frac{(\pi\beta)^{1/2}}{2} - \frac{\beta}{2} + \ldots \, . \quad (34)$$

In contrast to its counterpart (26), this expansion in powers of $\beta^{1/2}$ does not terminate, so that $\widetilde{E}_1(t)$ possesses infinitely many poles. For our purposes, it will be sufficient to account for only the leading of these poles, located at

$$t = 1/2 \quad \text{with residue } \frac{1}{2} \, . \quad (35)$$

Multiplying Eq. (34) by itself, we obtain

$$\sum_{n_1,n_2=2}^{\infty} \exp\bigl(-\beta(n_1^2+n_2^2-2)\bigr)$$

$$\sim \frac{\pi}{4\beta} - \frac{3}{2}\left(\frac{\pi}{\beta}\right)^{1/2} + \frac{2\pi+9}{4} - 2(\pi\beta)^{1/2} + \dots\,, \tag{36}$$

so that the leading poles of $\widetilde{E}_2(t)$ are found at

$$t = 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{3}{2}\,. \tag{37}$$

Finally, multiplying Eq. (34) by Eq. (36) results in

$$\sum_{n_1,n_2,n_3=2}^{\infty} \exp\bigl(-\beta(n_1^2+n_2^2+n_3^2-3)\bigr)$$

$$\sim \frac{1}{8}\left(\frac{\pi}{\beta}\right)^{3/2} - \frac{9\pi}{8\beta} + \frac{27+3\pi}{8}\left(\frac{\pi}{\beta}\right)^{1/2} + \dots\,, \tag{38}$$

from which we deduce in the usual manner that the leading poles of $\widetilde{E}_3(t)$ lie at

$$t = 3/2, 1, 1/2 \quad \text{with residues } \frac{\pi}{4}, -\frac{9\pi}{8}, \frac{27+3\pi}{8} \ . \tag{39}$$

Comparing the poles and residues of the inhomogeneous Zeta functions $\widetilde{E}_d(t)$ to those of their homogeneous counterparts $E_d(t)$, we see that neither the positions nor the residues of the leading poles at $t = d/2$ are affected by the inhomogeneity, whereas the next-to-leading poles of $\widetilde{E}_d(t)$, which are found at the same positions as those of $E_d(t)$ for $d \geq 2$, already exhibit a different residue.

3D-Harmonic trap

- Single-particle energy spectrum for the case of an isotropic, three-dimensional harmonic oscillator potential with oscillator frequency ω:

$$\varepsilon_\nu = \hbar\omega(\nu + 1/2) \quad , \quad \nu = 0, 1, 2, \dots \ .$$

- Each level has the degree of degeneracy

$$g_\nu = \frac{1}{2}\nu^2 + \frac{3}{2}\nu + 1 \ .$$

- Therefore, the generalized Zeta function reduces to a sum of Riemann Zeta functions:

$$\begin{aligned} Z(\beta, t) &= \sum_{\nu=1}^{\infty} \frac{g_\nu}{(\beta\hbar\omega\nu)^t} \\ &= (\beta\hbar\omega)^{-t}\left[\frac{1}{2}\zeta(t-2) + \frac{3}{2}\zeta(t-1) + \zeta(t)\right] \ . \end{aligned}$$

- For $\beta\hbar\omega \ll 1$, dependence of the k-th cumulant $\kappa_k(\beta)$ is governed by the factor $(\beta\hbar\omega)^{-p}$, where p is the position of the rightmost pole appearing in the integrand.

Cumulants: BEC in a 3D-Harmonic trap

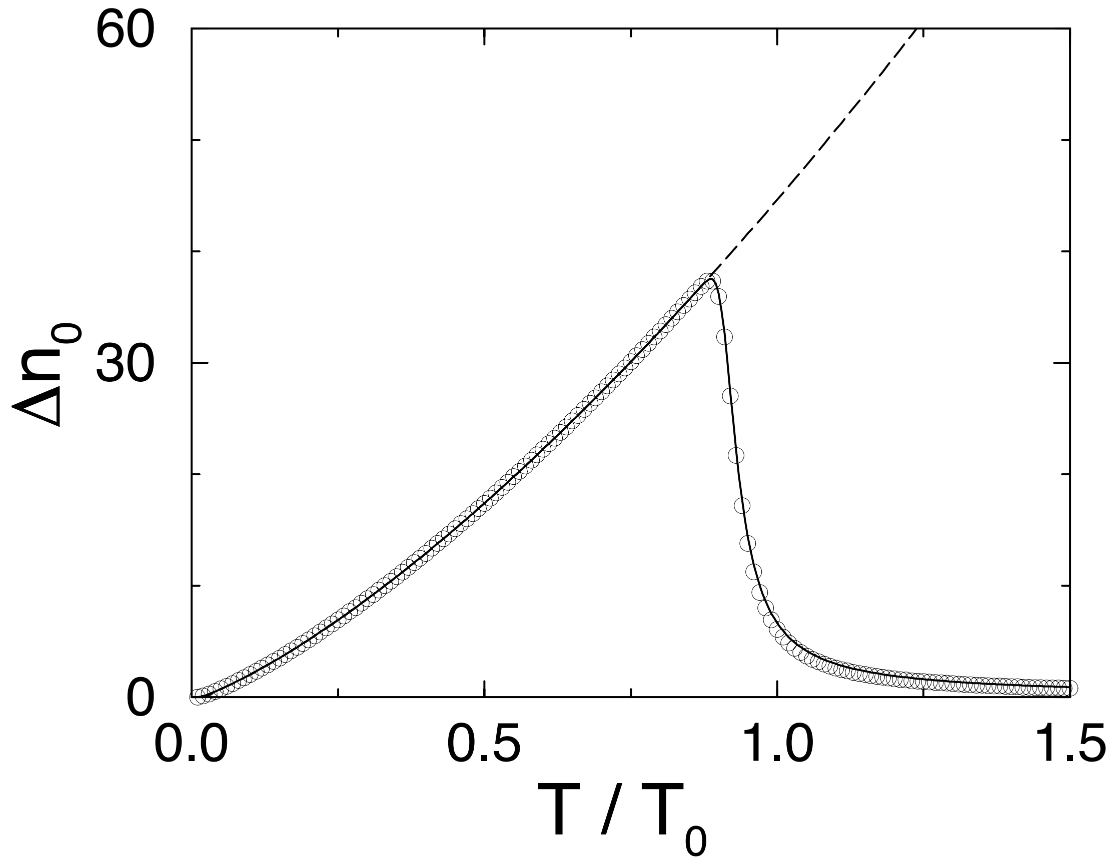
$$\langle n_0 \rangle \sim N - \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) - \frac{3}{2}\zeta(2)\left(\frac{k_B T}{\hbar\omega}\right)^2 - \frac{k_B T}{\hbar\omega}\left[\ln\left(\frac{k_B T}{\hbar\omega}\right) + \gamma - \frac{19}{24}\right],$$

$$\kappa_2(\beta) \sim \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(2) + \left(\frac{k_B T}{\hbar\omega}\right)^2 \left[\frac{3}{2}\ln\left(\frac{k_B T}{\hbar\omega}\right) + \frac{3}{2}\gamma + \frac{5}{4} + \zeta(2)\right] - \frac{1}{2}\frac{k_B T}{\hbar\omega},$$

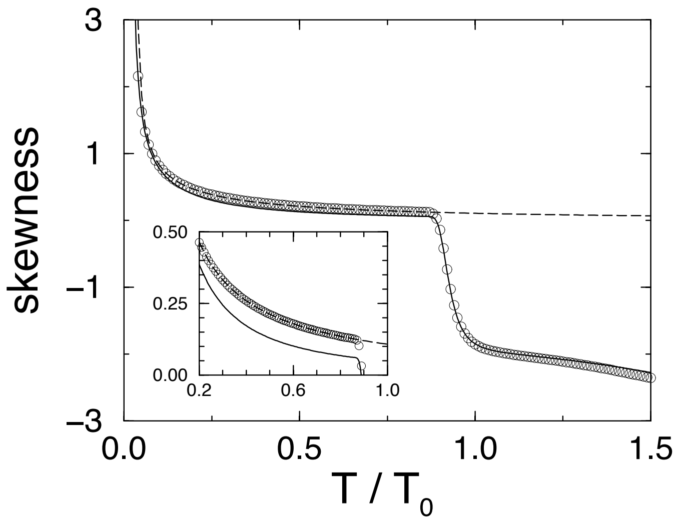
$$-\kappa_3(\beta) \sim -\left(\frac{k_B T}{\hbar\omega}\right)^3 \left[\ln\left(\frac{k_B T}{\hbar\omega}\right) + \gamma + \frac{3}{2} + 3\zeta(2) + 2\zeta(3)\right] + \frac{3}{4}\left(\frac{k_B T}{\hbar\omega}\right)^2 + \frac{1}{12}\frac{k_B T}{\hbar\omega},$$

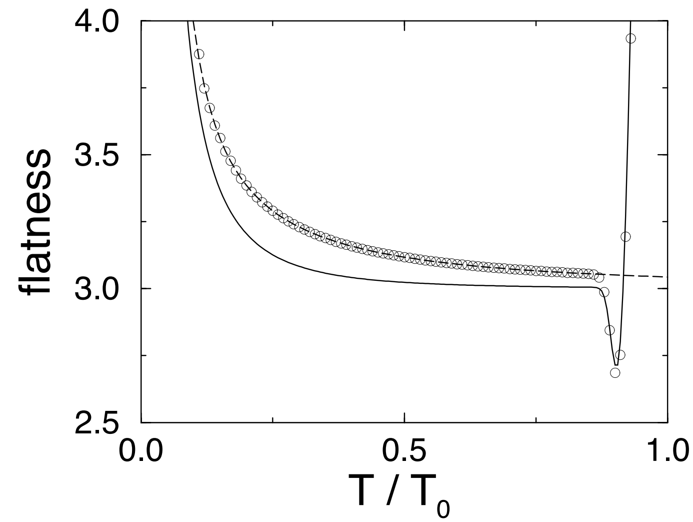
$$\kappa_4(\beta) \sim \left(\frac{k_B T}{\hbar\omega}\right)^4 \left[3\zeta(2) + 9\zeta(3) + 6\zeta(4)\right] - \frac{1}{2}\left(\frac{k_B T}{\hbar\omega}\right)^3 - \frac{1}{8}\left(\frac{k_B T}{\hbar\omega}\right)^2.$$

BEC in 3D-harmonic trap: Root-mean-square fluctuations



BEC in 3D-harmonic trap : skewness and flatness (non-Gaussian Character)





3D-Box

(Periodic Boundary Conditions)

- **Single-particle energy spectrum**

$$\varepsilon_{n_1,n_2,n_3} = \frac{\hbar^2(2\pi)^2}{2mL^2}\left(n_1^2+n_2^2+n_3^2\right) \equiv \hbar\Omega\left(n_1^2+n_2^2+n_3^2\right)$$

$$\text{with } n_\nu = 0, \pm 1, \pm 2 \pm \ldots \; .$$

- **Spectral Zeta function**

$$\begin{aligned} Z(\beta,t) &= (\beta\hbar\Omega)^{-t} \sum_{n_1,n_2,n_3=-\infty}^{+\infty}{}' \frac{1}{\left(n_1^2+n_2^2+n_3^2\right)^t} \\ &\equiv (\beta\hbar\Omega)^{-t} S(t) \; . \end{aligned}$$

- **Pole structure**

  $S(t)$ has one simple pole at $t = 3/2$ with residue 2π.

3D-Box

(Dirichlet Boundary Conditions)

- **Single-particle energy spectrum** [a]

$$\varepsilon_{n_1,n_2,n_3} = \frac{1}{4}\hbar\Omega\left(n_1^2 + n_2^2 + n_3^2\right) \quad \text{with } n_\nu = 1, 2, 3, \ldots\ ,$$

- **Spectral Zeta function**

$$\begin{aligned} Z(\beta, t) &= \left(\frac{1}{4}\beta\hbar\Omega\right)^{-t} \sum_{n_1,n_2,n_3=1}^{\infty}{}' \frac{1}{\left(n_1^2 + n_2^2 + n_3^2 - 3\right)^t} \\ &\equiv \left(\frac{1}{4}\beta\hbar\Omega\right)^{-t} \widetilde{S}(t)\ , \end{aligned}$$

- **Pole structure**
  the leading three poles of $\widetilde{S}(t)$ reside at $t = 3/2, 1, 1/2$ with residues $\frac{\pi}{4}$, $-\frac{3\pi}{8}$ and $\frac{3+3\pi}{8}$ respectively.

---

[a] Energy level spacings are reduced compared to PBC, but owing to $n_\nu > 0$, the leading term in the density of states remain the same.

Cumulants: BEC in a 3D Box

- Periodic boundary conditions:

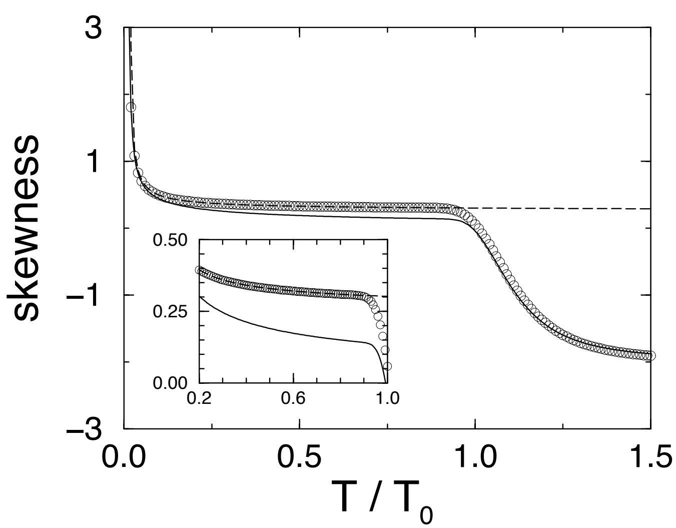
$$\begin{aligned}\langle n_0\rangle &\sim N-\pi^{3/2}\zeta(3/2)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}-S(1)\,\frac{k_BT}{\hbar\Omega}\\ \kappa_k(\beta) &\sim (k-1)!\,S(k)\left(\frac{k_BT}{\hbar\Omega}\right)^{k}+\pi^{3/2}\zeta(5/2-k)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}.\end{aligned}$$

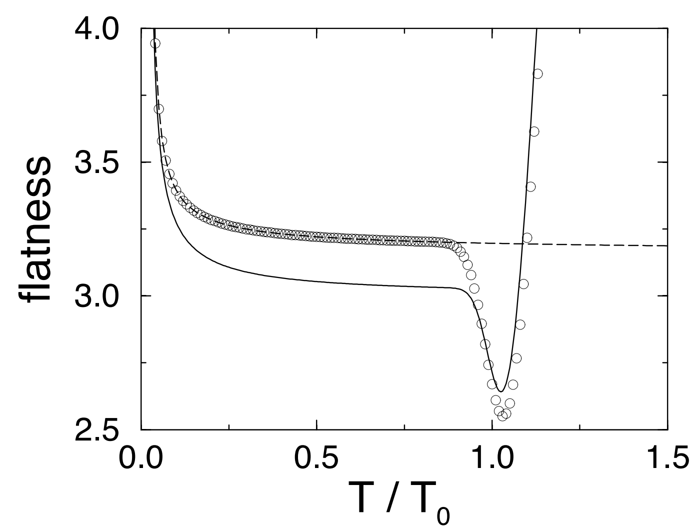
- Dirichlet boundary conditions (hard walls) [a]:

$$\begin{aligned}\langle n_0\rangle &\sim N-\pi^{3/2}\zeta(3/2)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}+\left[\frac{3\pi}{2}\ln\left(\frac{4k_BT}{\hbar\Omega}\right)-4\delta\right]\frac{k_BT}{\hbar\omega}\\ &\quad -\frac{3}{4}(1+\pi)\sqrt{\pi}\,\zeta(1/2)\left(\frac{k_BT}{\hbar\Omega}\right)^{1/2},\\ \kappa_k(\beta) &\sim 4^k(k-1)!\,\widetilde{S}(k)\left(\frac{k_BT}{\hbar\Omega}\right)^{k}+\pi^{3/2}\zeta(5/2-k)\left(\frac{k_BT}{\hbar\Omega}\right)^{3/2}\\ &\quad -\frac{3\pi}{2}\zeta(2-k)\,\frac{k_BT}{\hbar\Omega}+\frac{3}{4}(1+\pi)\sqrt{\pi}\,\zeta(3/2-k)\left(\frac{k_BT}{\hbar\Omega}\right)^{1/2}.\end{aligned}$$

[a] Higher moments differ in the both cases even with thermodynamic limit.

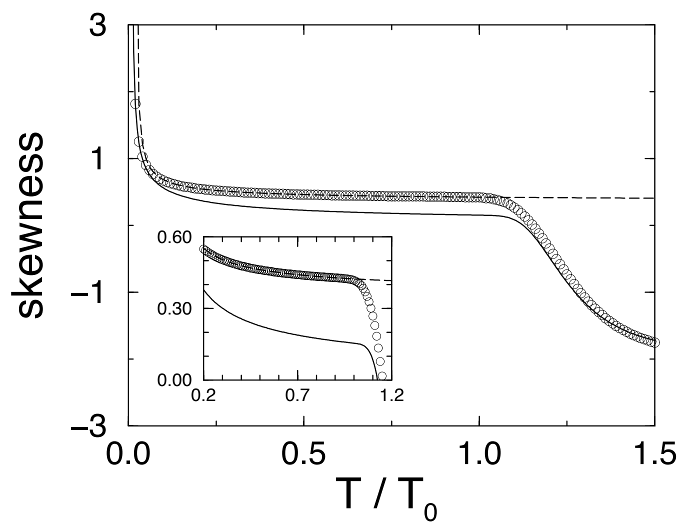
BEC in 3D-Box with Periodic Boundary Conditions: skewness and flatness[a]

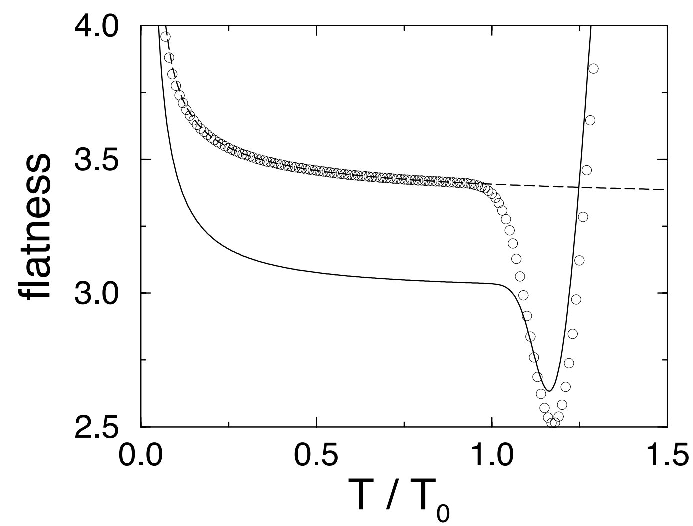




[a] Skewness: $\kappa_3(\beta)/\kappa_2(\beta)^{3/2}$ and flatness:$\kappa_4(\beta)/\kappa_2(\beta)^2 + 3$

BEC in 3D-Box with Dirichlet Boundary Conditions:skewness and flatness





Thermodynamic Limit

- Using

$$\Omega = \frac{\hbar(2\pi)^2}{2mL^2}, \; V = L^3 \text{ and } \lambda_T = \frac{2\pi\hbar}{\sqrt{2\pi m k_B T}}$$

  we can show

$$\langle n_0 \rangle \sim N - \zeta(3/2)\,\frac{V}{\lambda_T^3} - S(1)\,\frac{V^{2/3}}{\pi\lambda_T^2}\ .$$

- In the **thermodynamic limit**[a] the last term on the right hand side may be neglected, giving familiar textbook expression for the number of condensate particles, usually derived within the grand canonical ensemble, valid as long as $\langle n_0 \rangle > 0$.
- The equation $\langle n_0 \rangle = 0$ defines the condensation temperature T_0: In the thermodynamic limit, one has

$$T_0 = \frac{\hbar\Omega}{\pi k_B}\left(\frac{N}{\zeta(3/2)}\right)^{2/3}.$$

- For finite systems, where the additional term effectively increases the ground state occupation number[b], the *transition temperature is minutely shifted upward.*
- The situation is different for the higher cumulants as the dominant pole is of that of the Riemann Zeta function $\zeta(t+1-k)$ in this case.

[a] (i.e., for $N \to \infty$ and $V \to \infty$, such that the density N/V remains constant)
[b] since $S(1) \approx -8.9136$ is *negative*

Comments on the Boundary Condition Dependence

- The usual substitution:

$$\sum_{\nu\geq 1} \frac{1}{\exp[\beta(\varepsilon_\nu - \varepsilon_0)] - 1} \approx \int_0^\infty \frac{\rho(\varepsilon)\,\mathrm{d}\varepsilon}{\exp(\beta\varepsilon) - 1}.$$

- In the thermodynamic limit the boundary-condition independence of the leading term of $\rho(\varepsilon)$ implies the boundary-condition independence of $\kappa_1(\beta)$ and T_0.

- However, for higher cumulants, the emerging integrals are formally divergent, and the above continuous approximation does not work.

- Thus, **in the thermodynamic limit** only quantities that can be evaluated with the help of the density of states do not depend on the respective boundary conditions.

Comments on Boundary Condition Dependence (contd...)

- Compared to the case of periodic box, the density of states for Dirichlet boundary conditions is slightly reduced.
- Thus, the leading volume term in the density of states remains the same and only a surface correction arises in the next term.
- At low temperatures there are slightly less states accessible in a hard box than there would be in a hypothetical, same-sized box with periodic boundary conditions.
- This lack of states results in an enlarged ground state occupation number, so that Bose-Einstein condensation sets in at a higher temperature in the hard-walled box than it would in the periodic case.

Microcanonical Ensemble Analysis

Motivation

- Canonical ensemble is a helpful intermediate step but not quite relevant to the recent experiments.
- Microcanonical ensemble by itself is very difficult to study and it is very difficult to calculate corresponding partition functions.
- However, there is a well established prescription to convert the canonical ensemble results to the microcanonical ones.

Prescription to obtain the microcanonical partition function from the canonical one

- Definition:

$$Z_N(\beta) = \sum_E e^{-\beta E}\Omega(E, N)$$

- Let $x = e^{-\beta\hbar\omega}$ and $m = E/\hbar\omega$
  where $\hbar\omega$ is the single quantum of energy say corresponding to the trap

- Giving:

$$Z_N(\beta) = \sum_{m=0}^{\infty} x^m \Omega(m, N)$$

- Inverting the above expression one obtains

$$\Omega(m, N) = \frac{1}{2\pi i}\oint \frac{Z_N(\beta)}{x^{m+1}}$$

Condensate Statistics through microcanonical partition function

- Microcanonical probability distribution:

$$P_{mc}(N_0|N) = \frac{\Omega(N - N_0, E) - \Omega(N - N_0 - 1, E)}{\Omega(N, E)}$$

- Average occupation of the condensate:

$$\langle n_0 \rangle_{mc} = \sum_{n_0=0}^{N} n_0 P_{mc}(n_0|N)$$

- Condensate fluctuations:

$$\langle \delta^2 n_0 \rangle_{mc} = \sum_{n_0=0}^{N} (n_0 - \langle n_0 \rangle)^2 P_{mc}(n_0|N).$$

Microcanonical partition function for an ideal gas in an isotropic 3-D harmonic trap

- The canonical partition function[a]

$$Z_N(T) = \left(\frac{T}{T_c}\right)^{3(N+1)} \int_0^\infty dt\, e^{-t\left(\frac{T}{T_c}\right)^3} (t+N)^N = \sum_i \frac{N!}{(N-i)!}\left[N\left(\frac{T}{T_c}\right)^3\right]^{N-i}$$

- The saddle point equation

$$\boxed{m+1 = x\frac{\partial}{\partial x}\ln Z_N(T).}$$

- Taking the contours through the extrema (saddle point) $x = 0$ of $\phi(x) \equiv Z_N(\beta)/x^{m+1}$ we get for $m \to \infty$ the following asymptotic formula:

$$\Omega(N, m) = \frac{1}{[2\pi\phi^{(2)}(x_0)]^{1/2}}\frac{Z_N(x_0)}{x_0^{m+1}}$$

where $\phi^{(2)}(x_0)$ is the second derivative of $\phi(x)$ evaluated at the saddle point.

- Unfortunately, theoretical analysis is impossible as there is no way to invert the saddle point equation. Numerical analysis shows inadequacy of the method.

[a] M. Scully, Phys. Rev. Lett. **82** 3927, (1999).

Exact numerical procedure

- There is a formal equivalence between the microcanonical distribution of the energy among the particles and the integer number partitioning problem.
- Let $\Phi(n, M)$: number of possibilities to partition the integer number n into M integer, nonzero summands.
- If n quanta are to be distributed over $M \leq n$, we first take M of the quanta and assign them to M different particles, thus fixing the required number of parts. 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 can not exceed the smaller of the numbers $n - M$ and M:

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

- Corresponding microcanonical probability distribution:

$$p_{\rm mc} \equiv \frac{\Phi(n, M)}{\Omega(n)}, \quad \text{with } \Omega(n) = \sum_{M=1}^{n} \Phi(n, M)$$

Recall canonical cumulants

Results for 1D harmonic potential

$$
\begin{aligned}
\kappa_{\rm cn}^{(0)}(b) &= \frac{\pi^2}{6b} + \frac{1}{2}\ln\frac{b}{2\pi} - \frac{b}{24} \\
\kappa_{\rm cn}^{(1)}(b) &= \frac{1}{b}\left(\ln\frac{1}{b} + \gamma\right) + \frac{1}{4} - \frac{b}{144} + \mathcal{O}(b^3) \\
\kappa_{\rm cn}^{(2)}(b) &= \frac{\pi^2}{6b^2} - \frac{1}{2b} + \frac{1}{24} \\
\kappa_{\rm cn}^{(3)}(b) &= \frac{2\zeta(3)}{b^3} - \frac{1}{12b} + \frac{b}{1440} + \mathcal{O}(b^3) \\
\kappa_{\rm cn}^{(4)}(b) &= \frac{\pi^4}{15b^4} - \frac{1}{240}\ ,
\end{aligned}
$$

Results for 3D harmonic potential

$$
\begin{aligned}
\kappa_{\rm cn}^{(0)}(b) &= \frac{\zeta(4)}{b^3} + \frac{3\zeta(3)}{2b^2} + \frac{\pi^2}{6b} + \frac{3\ln b}{24} + \frac{1}{2}\ln\frac{b}{2\pi} \\
&\quad + \frac{1}{2}\Big(\zeta'(-2) + 3\zeta'(-1)\Big) \\
\kappa_{\rm cn}^{(1)}(b) &= \frac{\zeta(3)}{b^3} + \frac{3}{2}\frac{\zeta(2)}{b^2} + \frac{1}{b}\left(\ln\frac{1}{b} + \gamma - \frac{19}{24}\right) \\
\kappa_{\rm cn}^{(2)}(b) &= \frac{\zeta(2)}{b^3} + \frac{1}{b^2}\left(\frac{3}{2}\ln\frac{1}{b} + \frac{3}{2}\gamma + \frac{5}{4} + \zeta(2)\right) - \frac{1}{2b} \\
\kappa_{\rm cn}^{(3)}(b) &= \frac{1}{b^3}\left(\ln\frac{1}{b} + \gamma + \frac{3}{2} + 3\zeta(2) + 2\zeta(3)\right) \\
&\quad - \frac{3}{4}\frac{1}{b^2} - \frac{1}{12b} \\
\kappa_{\rm cn}^{(4)}(b) &= \frac{1}{b^4}[3\zeta(2) + 9\zeta(3) + 6\zeta(4)] - \frac{1}{2b^3} - \frac{1}{8b^2}
\end{aligned}
$$

where $b = \beta\hbar\omega$ and $\gamma \approx 0.57722$ is Euler's constant.

Relation between microcanonical and canonical cumulants

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

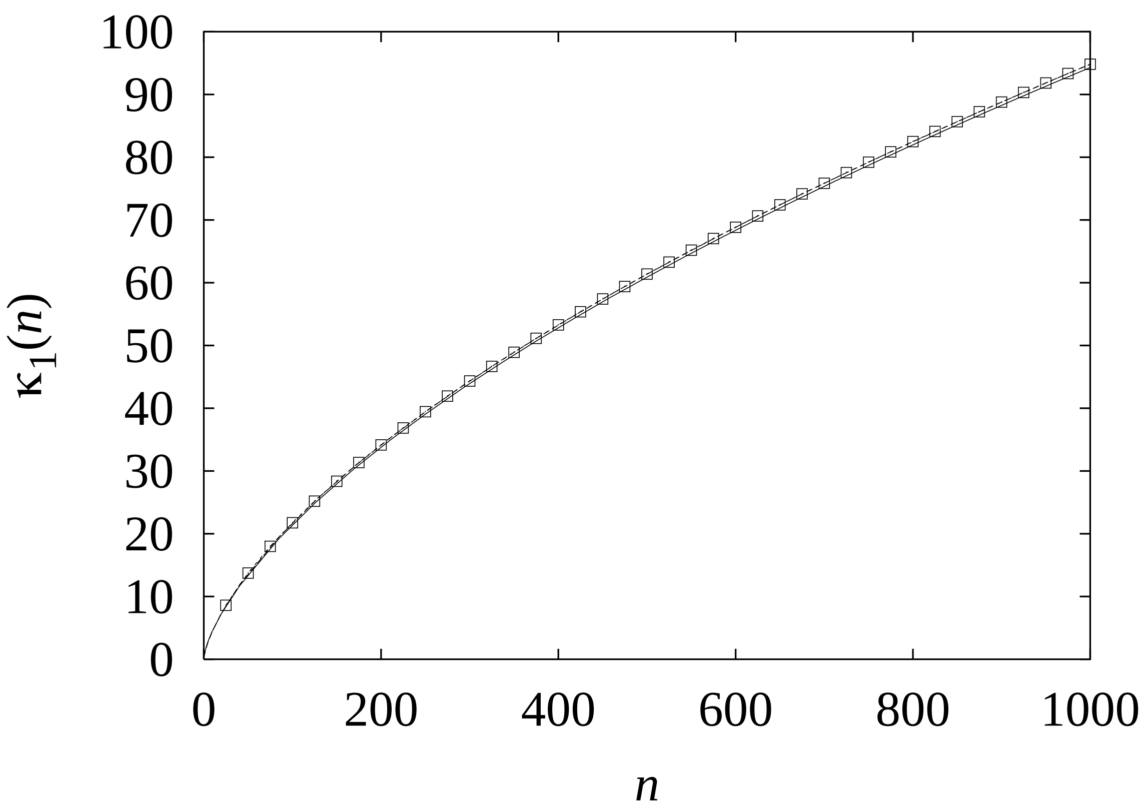
$$\begin{aligned}\kappa_{\rm mc}^{(2)}(n) = \; & \kappa_{\rm cn}^{(2)}(b_1) - \frac{1}{2}\left(\frac{D^2\kappa_{\rm cn}^{(2)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} - \left[\frac{D^2\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\right]^2\right) + \left[\frac{D\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\right] \\ & \left(1 + \frac{1}{2}\frac{D^3\kappa_{\rm cn}^{(0)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\right) + \frac{D\kappa_{\rm cn}^{(2)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} - \frac{D\kappa_{\rm cn}^{(1)}(b_1)D^2\kappa_{\rm cn}^{(1)}(b_1)}{[D^2\kappa_{\rm cn}^{(0)}(b_1)]^2} \\ & + \frac{1}{2}\left\{\frac{D\kappa_{\rm cn}^{(2)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\frac{D^3\kappa_{\rm cn}^{(0)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} + \frac{D\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\left(\frac{D^3\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)} - \frac{D^2\kappa_{\rm cn}^{(1)}(b_1)}{[D^2\kappa_{\rm cn}^{(0)}(b_1)]^2}\right)\right. \\ & \left. -2D\kappa_{\rm cn}^{(1)}(b_1)\frac{D^3\kappa_{\rm cn}^{(0)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\frac{D^2\kappa_{\rm cn}^{(1)}(b_1)}{[D^2\kappa_{\rm cn}^{(0)}(b_1)]^2}\right\} - \frac{D\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\left(\kappa_{\rm cn}^{(1)}(b_1) - \frac{1}{2}\frac{D^2\kappa_{\rm cn}^{(1)}(b_1)}{D^2\kappa_{\rm cn}^{(0)}(b_1)}\right)\end{aligned}$$

Here D denotes the derivative with respect to b, and $b_1 = b_0(z=1)$ is to be taken as a function of n through

$$n + 1 = x\,\frac{\partial}{\partial x}\ln \Xi_{\rm ex}(x,z)\bigg|_{x_0(z)} = -\frac{\partial}{\partial b}\ln \Xi_{\rm ex}(b,z)\bigg|_{b_0(z)} .$$

Numerical Results

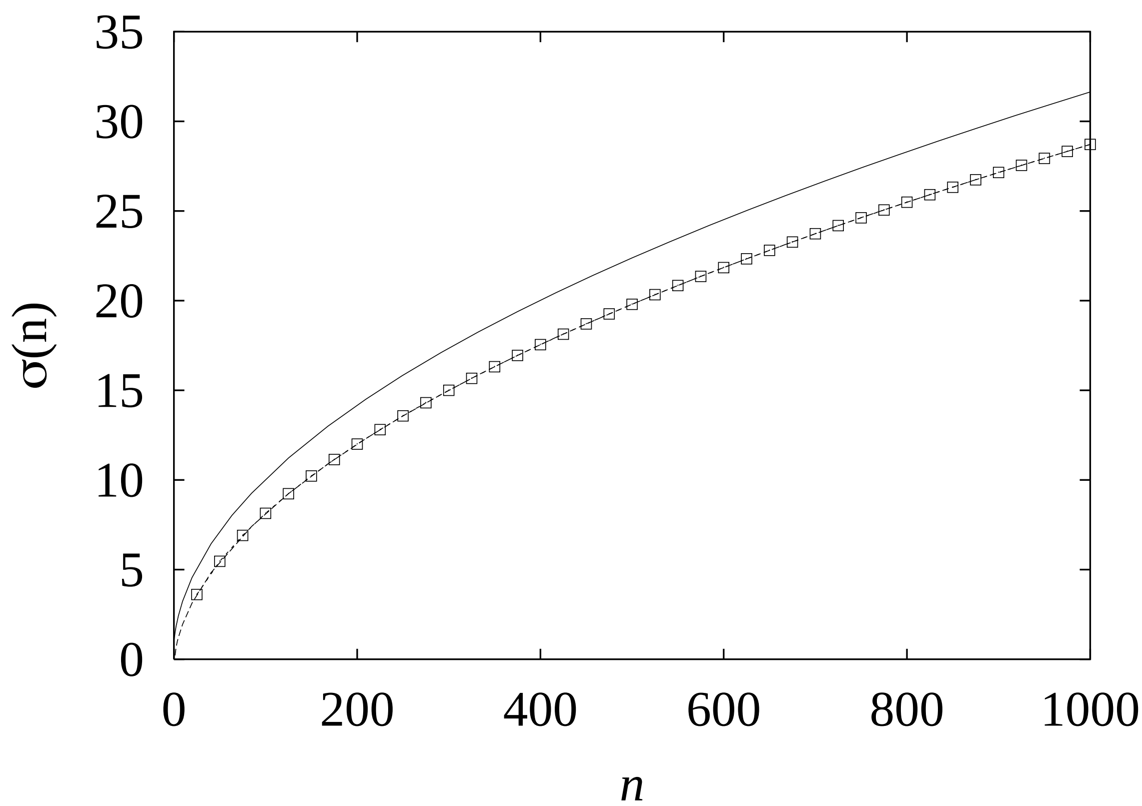
First cumulant 1D harmonic trap



Solid line: Canonical ensemble result, **dashed line:** Microcanonical result, and **squares:** Exact numerical result.

Numerical Results

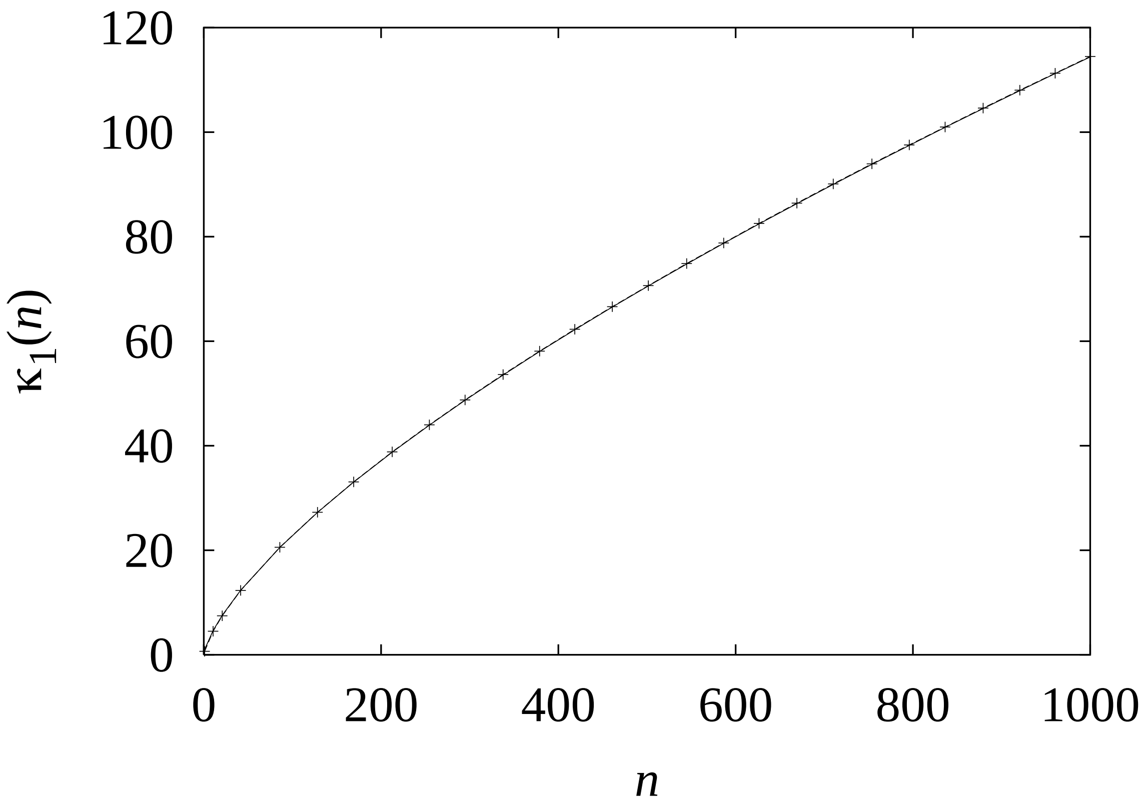
RMS fluctuations 1D harmonic trap



Solid line: Canonical ensemble result, **dashed line:** Microcanonical result, **squares:** Exact numerical result.

Numerical Results

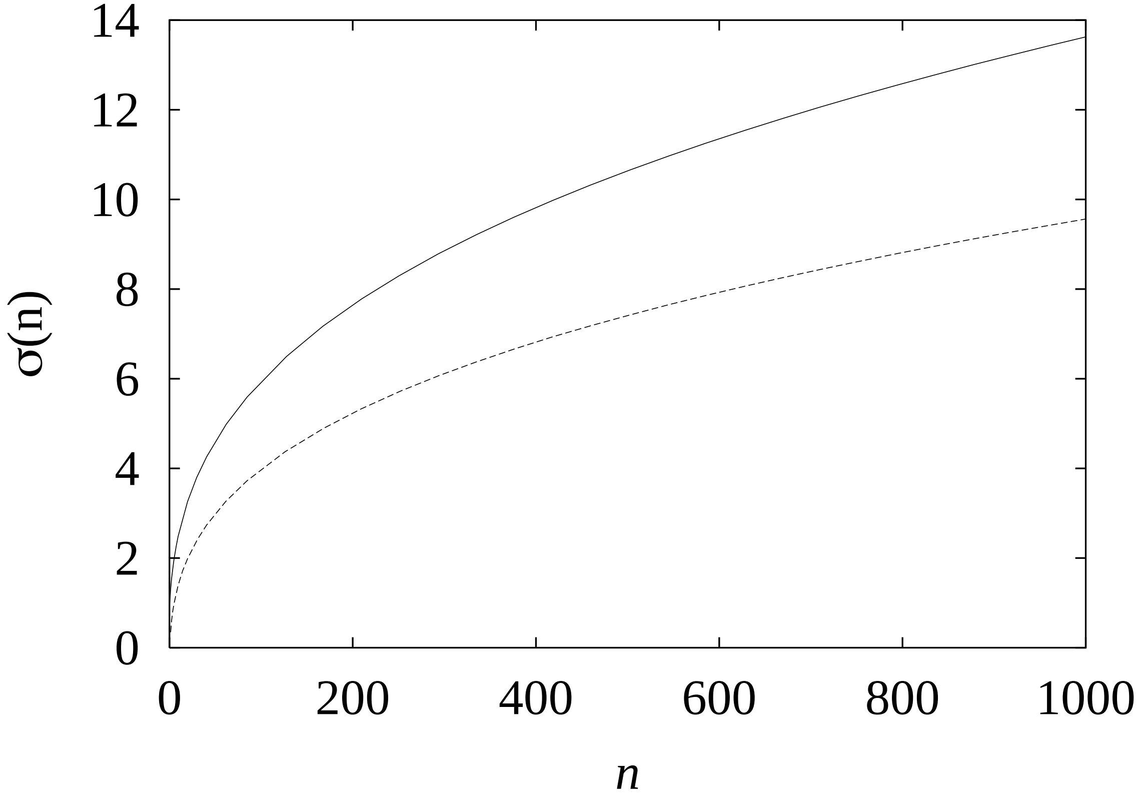
First cumulant 3D harmonic trap



Solid line: Canonical ensemble result, **Dashed line:** Microcanonical result.

Numerical Results

RMS fluctuations 3D harmonic trap



Solid line: Canonical ensemble result, **Dashed line:** Microcanonical result.

Summary

- We have obtained analytical expressions for the cumulants for an ideal Bose trapped in various potentials through the Mellin-Barnes integral representation.
- Illustration of the dependence of higher statistics on the boundary conditions of the problem is given.
- A general strategy for transforming the canonical results into microcanonical ones is discussed.
- Microcanonical cumulants for the 1D and 3D harmonic trap have been calculated.