Fluctuations of Trapped Particles

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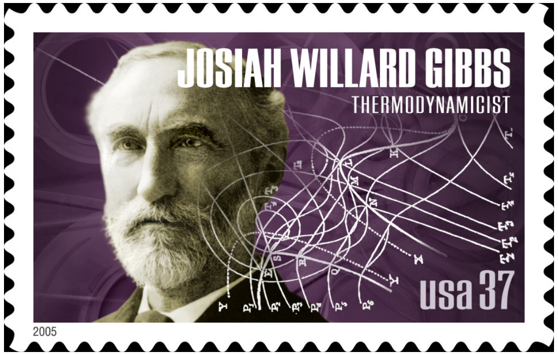
Ground State Fluctuations



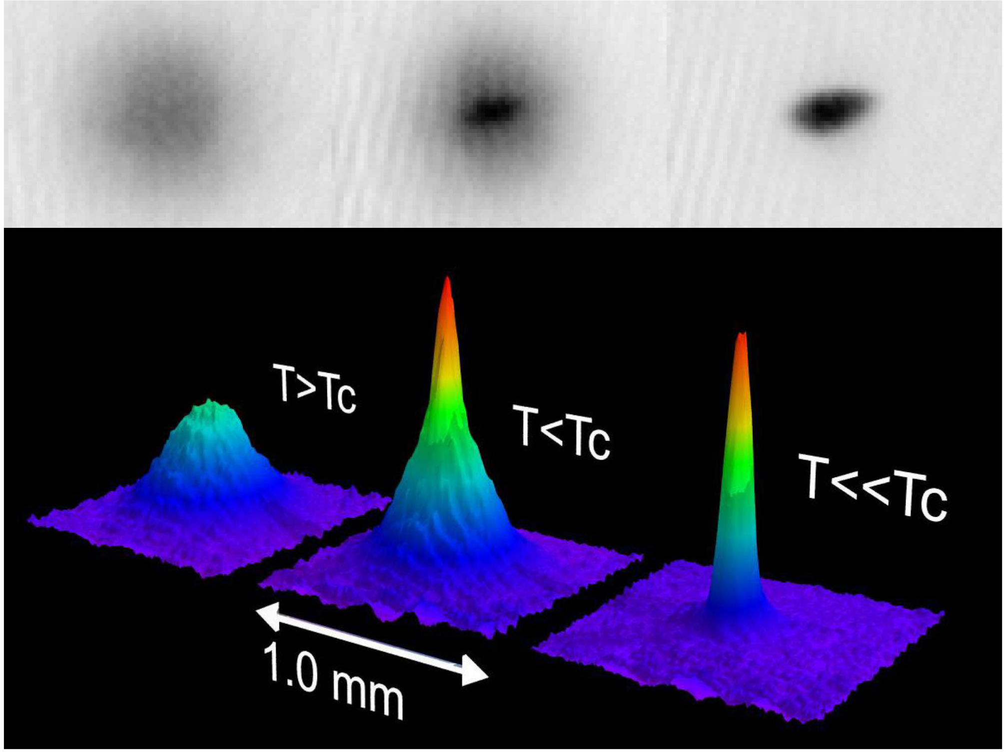
- Ensembles in Statistical Mechanics.
- Ensemble equivalence ? GCE Catastrophe.
- Partitions and micro-canonical ensemble.
- Fluctuations in micro-canonical and canonical ensembles.
- A pathological case.
- Interacting systems - Landau conjecture

Statistical Ensembles

J. Willard Gibbs(1878): Ensemble is an idealisation consisting of a large number of mental copies (infinitely many) of a system, considered all at once, each represents a possible state that the real system.

- *Micro-canonical ensemble – an ensemble of systems, each of which is required to have the same total energy (ie thermally isolated).*
- *Canonical ensemble – an ensemble of systems, each of which can share its energy with a large heat bath (in effect, fixing the temperature).*
- *Grand canonical ensemble – an ensemble of systems, each of which can share both its energy and its particles with a reservoir (ie an open system, at a given temperature).*

BEC-Ensemble equivalence



After the breakthrough in Bose-Einstein Condensation of Rubidium, sodium and lithium, second generation experiments are probing the temperature dependence of condensate fraction, collective excitations of the condensate. A condensate is indeed a mesoscopic matter wave-interference fringes in two freely expanding condensates.

Ensemble equivalence

In the limit of large systems, the macroscopic behaviour of a system does not depend on the particular ensemble used! Choice of the ensemble rests on how best or easily the properties of the macroscopic system may be derived.

- A condensate is neither in thermal contact with a heat bath, nor exchanging particles with a particle reservoir.
- The only ensemble that is appropriate for describing BEC is the microcanonical ensemble.
- However, theoretical description until now relies mainly on the grand canonical ensemble. For example calculation of T_c- see any text on statistical mechanics!
- Equivalence of ensemble is generally assumed- how far is this justified?

Ground state fluctuations - the catastrophe

- Consider a system of bosons: Number fluctuation is

$$\delta N^2 = \langle N^2 \rangle - \langle N \rangle^2 = \sum_{k=1}^{\infty} \langle n_k \rangle (1 + \langle n_k \rangle)$$

That is $\delta N^2 \rightarrow N^2$ as $T \rightarrow 0$.

The ground state fluctuation diverges as the size of the system! A problem referred to as the GCE catastrophe.

- No such problem for a system of Fermions:

$$\delta N^2 = \langle N^2 \rangle - \langle N \rangle^2 = \sum_{k=1}^{\infty} \langle n_k \rangle (1 - \langle n_k \rangle)$$

That is $\delta N^2 \rightarrow 0$ as $T \rightarrow 0$

Moral: start with micro-canonical ensemble-ie., state counting

Micro Canonical Ensemble - Introduction

Consider a system of particles occupying single particle levels: $\epsilon_0, \epsilon_1, \epsilon_2, \cdots$. The partition function of the system is:

$$Z_1(\beta) = \sum_{k=0}^{\infty} e^{-\beta \epsilon_k}, \quad \beta = 1/kT$$

and for N particles

$$Z_N(\beta) = \sum_{k=0}^{\infty} \Omega(E_k, N) e^{-\beta E_k} = e^{-\beta E_0} \sum_{k=0}^{\infty} \Omega(E_k^x, N) e^{-\beta E_k^x}$$

where $\Omega(E_k^x, N)$ is the number of ways of sharing the excitation energy E_k^x among utmost N particles.

This is what we need for state counting.

Fluctuations from counting

The number of ways of distributing excitation energy may be further divided:

$$\Omega(E_k^x, N) = \sum_{N_x=1}^{N} \omega(E_k^x, N_x, N)$$

$\omega(E_k^x, N_x, N)$ is the number of ways of sharing the excitation energy E_k^x among exactly N_x particles.
Now, we can construct a probability distribution:

$$P(E^x, N_x, N) = \frac{\omega(E^x, N_x, N)}{\Omega(E^x, N)}$$

This is the fundamental quantity that one uses in Micro-Canonical calculations.

Moments

Given the fundamental probability distribution,

$$P(E^x, N_x, N) = \frac{\omega(E^x, N_x, N)}{\Omega(E^x, N)}$$

we have

$$\langle N_x \rangle = \sum_{N_x=1}^{N} N_x P(E^x, N_x, N), \quad \langle N_x^2 \rangle = \sum_{N_x=1}^{N} N_x^2 P(E^x, N_x,$$

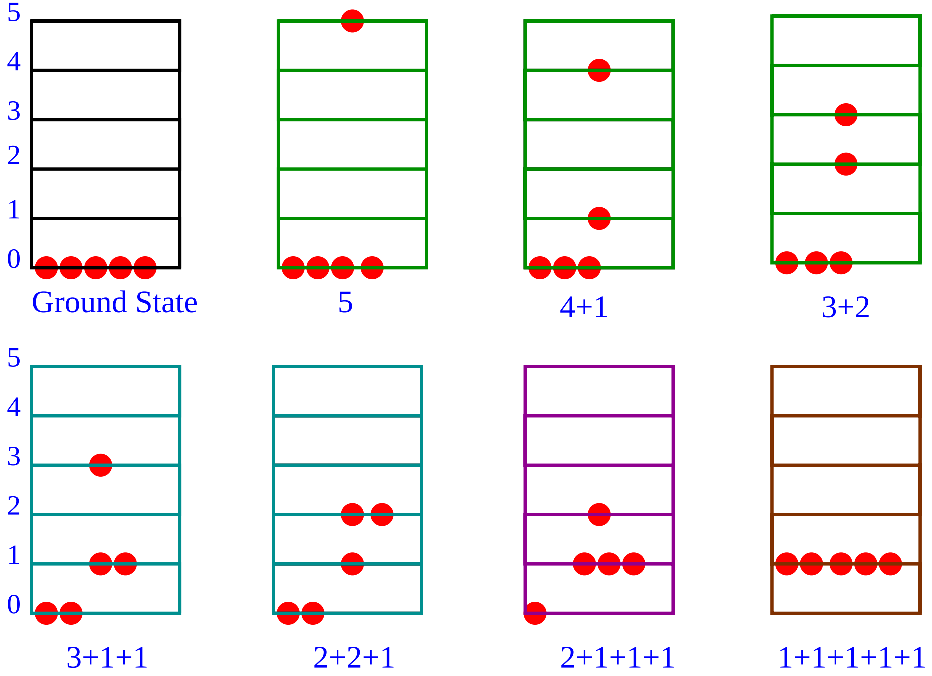
The fluctuation for fixed N

$$\delta N^2 = \langle N_x^2 \rangle - \langle N_x \rangle^2 = \langle N_0^2 \rangle - \langle N_0 \rangle^2; \quad N = N_0 + N_x$$

The fluctuation in the ground state occupancy- Bose, or Fermi.

Example: Bosons in a harmonic trap

Consider distributing the bosons in a harmonic trap with E=5, in energy units.



Bosonic excitations in Harmonic Oscillator System

The problem of state counting with harmonic spectrum is the same as the number partitioning problem- gets complicated with large numbers. (Hardy and Ramanujan, 1918)

$$\omega(5,1,5)=1, \omega(5,2,5)=2, \omega(5,3,5)=2, \omega(5,4,5)=1, \omega(5,$$

$$\Omega(5,5)=7$$

Digression: Euler and Ramanujan

Euler's Recurrence Formula:

$$\prod_{n=1}^{N} \frac{1}{1-x^n} = 1 + x + x^2 + x^3 + \cdots$$

$$\times 1 + x^2 + x^4 + \cdots$$

$$\times 1 + x^3 + x^6 + \cdots$$

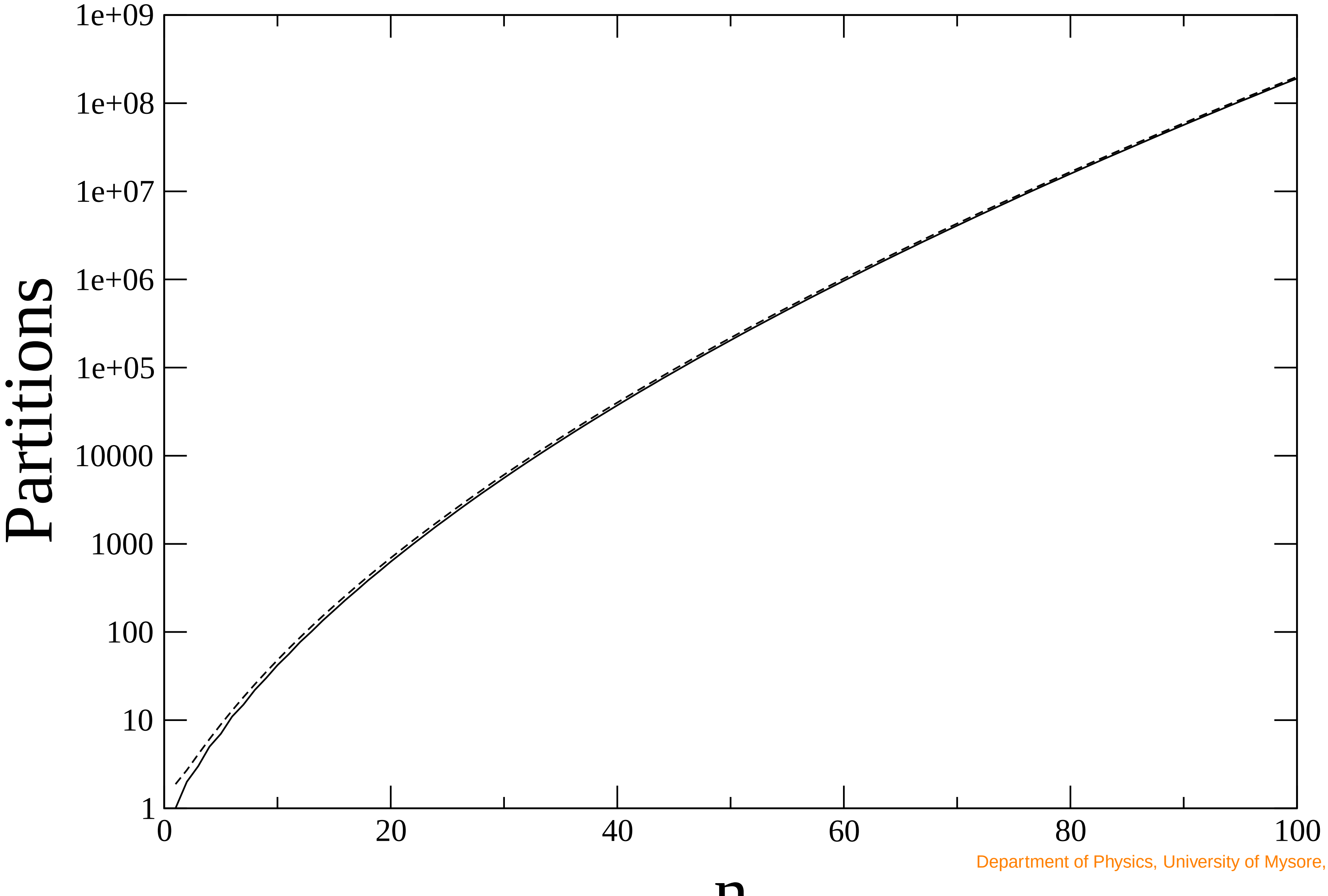
$$\times \cdots\cdots\cdots$$

$$= 1 + x + 2x^2 + 3x^3 + 5x^4 + 7x^5 + \cdots \quad = \sum_{n=0}^{N} \Omega(n, N) x^n$$

Asymptotic formula for $\Omega(n)$: Hardy and Ramanujan

$$\boldsymbol{\Omega(n) \Rightarrow \frac{\exp[\pi\sqrt{\frac{2n}{3}}]}{4\sqrt{3n}}, \quad N \to \infty}$$

Harmonic spectrum: Exact-Asymptotic Ω



Fluctuations from canonical averaging

The microcanonical ensemble is the simplest of the ensembles of statistical mechanics, in which each system of the ensemble is assumed to have the same total energy. Quantum mechanically, this means that every system within the ensemble is known to be in a quantum state of equal energy. The microcanonical partition function is simply the quantum degeneracy of the energy state corresponding to the fixed energy of the ensemble, Ω.

Unlike the micro-canonical ensemble, in the canonical ensemble description of statistical system, we have a large system that is in thermal contact with the environment, which has temperature T*, with both the volume of the system and the number of constituent particles fixed.*

The canonical partition function is

$$Z_N = \sum_j \Omega(E_j, N) e^{-\beta E_j} = \frac{1}{N} \sum_{j=1}^{N} Z_1(j\beta) Z_{N-j}(\beta)$$

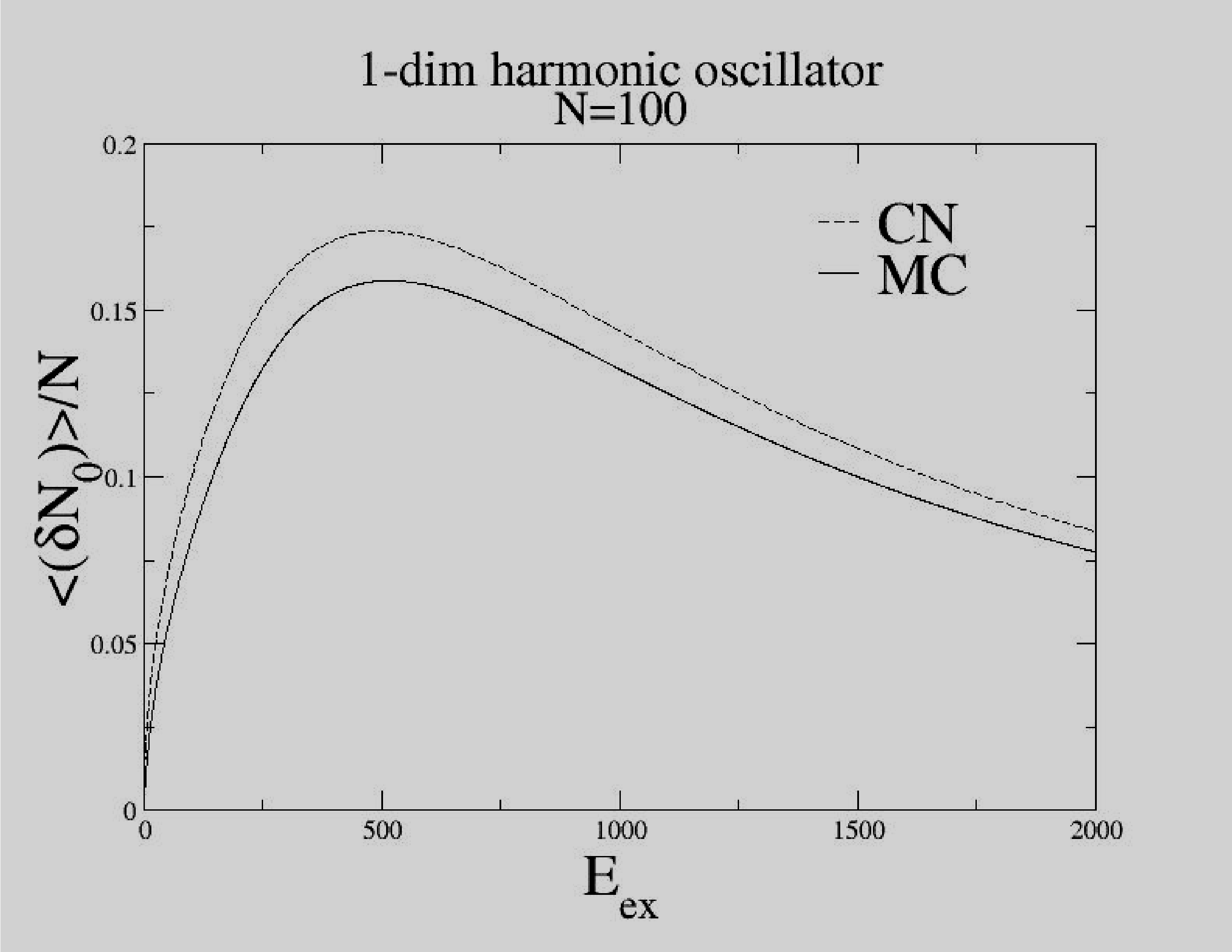
where j labels the micro states with energy E_j. In such a system we have,

$$\begin{aligned} \langle n_k \rangle &= \frac{1}{Z_N} \sum_{j=1}^{N} e^{-j\beta\epsilon_k} Z_{N-j}(\beta) \\ \langle n_k^2 \rangle &= \frac{1}{Z_N} \sum_{j=1}^{N} (2j-1) e^{-j\beta\epsilon_k} Z_{N-j}(\beta) \end{aligned}$$

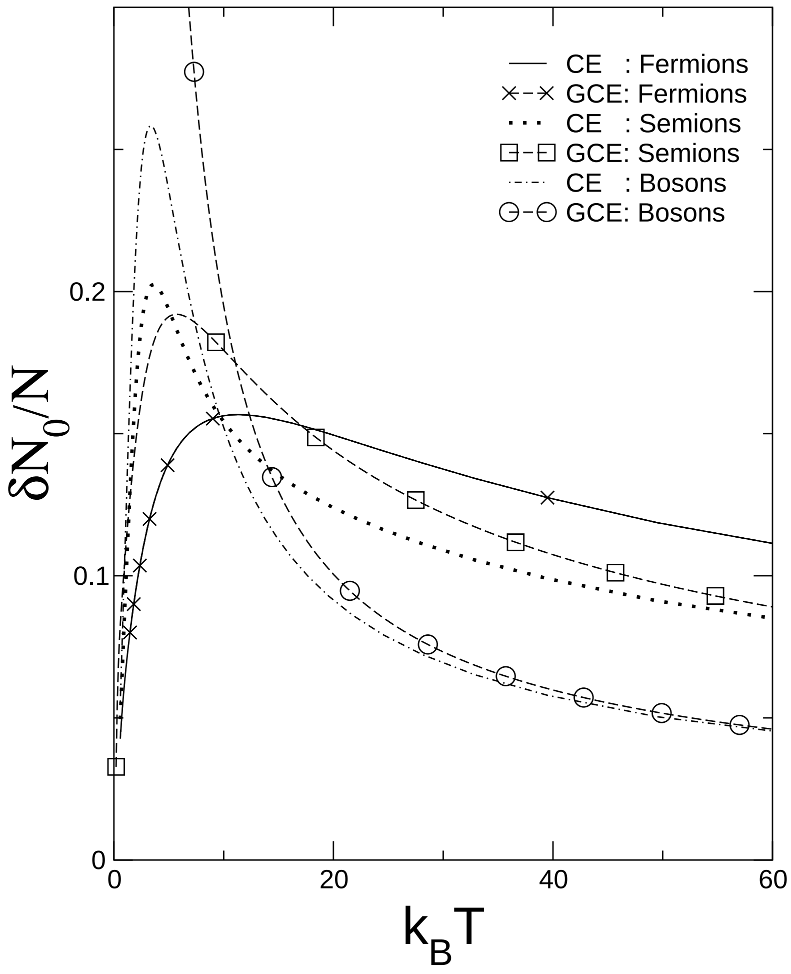
The number fluctuation (no divergence as in GCE) is,

$$\delta N_0^2 = \sum_{gs} [\langle n_k^2 \rangle - \langle n_k \rangle^2]$$

Comparison of MCE and CE



Comparison of CE and GCE



A Pathological case

Consider a single particle spectrum $\epsilon_0 = 0, \epsilon_p = \ln p,\ p = 2, 3, 5, ...$

In how many ways an excited energy E^x *may be shared by* N_x *particles?*

1. $E^x \neq \ln(n)$ (n-integer), then $\omega(E^x, N_x, N) = 0$.

2. $E^x = \ln(n) = n_1 \ln(p_1) + n_2 \ln(p_2) + \cdots + n_r \ln(p_r)$

since $n = p_1^{n_1} p_2^{n_2} \cdots p_r^{n_r}$

This is unique from the Fundamental theorem of Arithmetic- Euclid.

For example, Let

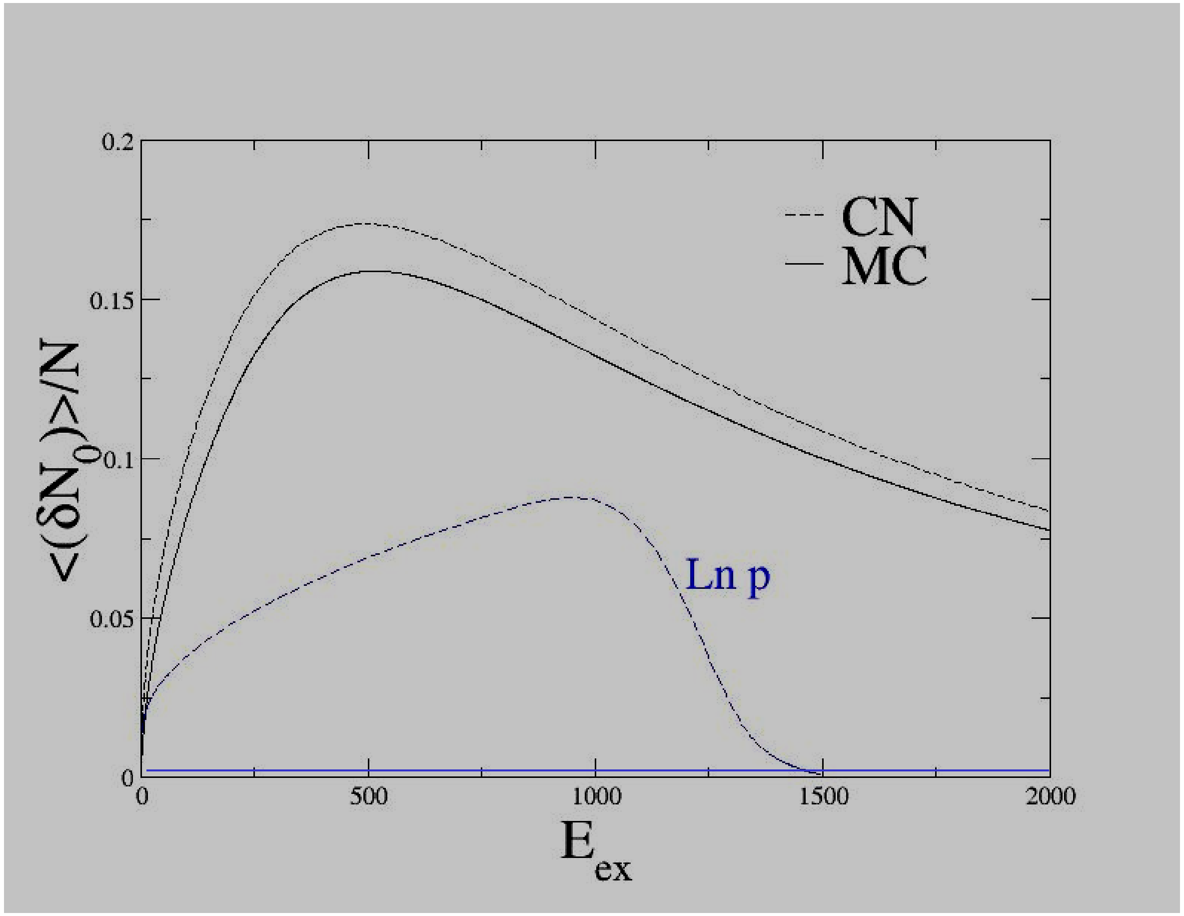
$E^x = \ln(20) = 2\ln(2) + ln(5)$

$\Rightarrow \omega(\ln(20), 3, N) = 1, \quad \omega(\ln(20), N_x \neq 3, N) = 0$

Thus the fluctuation $\delta N_0^2 = 0\ \forall\ \ E^x$ (in MCE)

Tran and Bhaduri, 2003

Microcanonical vs canonical (Ln p and 1- dimensional harmonic oscillator)



Here even CE and MCE equivalence breaks down!

Interacting systems: Landau's conjecture

It is well known that the number fluctuation in the grand canonical ensemble which is directly proportional to the compressibility, diverges for an ideal Bose gas as $T \to 0$*....when interactions, which must exist in any actual gas, are taken into account the resulting fluctuations must be finite.*

We illustrate this using a one-dimensional Model.

Calogero-Sutherland Model in 1-d

An exactly solvable many body Hamiltonian with non-trivial correlations

The Hamiltonian: $\hbar = 1, m = 1, c = 1$

$$\boldsymbol{H = \frac{1}{2}\left[\sum_i p_i^2 + \omega^2 \sum_i x_i^2 + \lambda \sum_{i,j} \frac{1}{(x_i - x_j)^2}\right]}$$

The Spectrum of system of N interacting Bosons:

$$\boldsymbol{E(g) = E(g = 0) + g\omega \frac{N(N-1)}{2}}$$

where $\lambda = g(g-1)$

Thermodynamics of interacting bosons

The distribution function for interacting bosons is given by,

$$\boldsymbol{\langle n_\epsilon \rangle = \frac{1}{w(\epsilon) + g}; \qquad w^g (1 + w)^{1-g} = e^{\beta(\epsilon - \mu)}}$$

Fluctuations: $(\delta n_k)^2 = T \frac{\partial \langle n_k \rangle}{\partial \mu}$. Therefore

$$\begin{aligned}
(\delta N)^2 &= \sum_{k=0}^{\infty} (\delta n_k)^2 = \sum_{k=0}^{\infty} w_k (1 + w_k) \langle n_k \rangle^3 \\
(\delta N)^2 &= \sum_{k=0}^{\infty} \langle n_k \rangle (1 - g \langle n_k \rangle)(1 + (1 - g) \langle n_k \rangle)
\end{aligned}$$

where $\langle n_k \rangle \to 1/g, \;\; T \to 0$

Thus the fluctuation goes to zero as $T \to 0$, no matter how small g is, or how small the interaction is.

Summary

- For Thermodynamic systems ensemble equivalence is taken for granted.
- However this equivalence breaks down in some special cases, especially bosons and fermions in a trap.
- The mean occupation number in the ground state is in general thermodynamically equivalent in all ensembles. An exception to this rule is the system whose single particle spectrum is given by logarithm of the prime number sequence.
- The ground state number fluctuation, however, is very sensitive to the ensemble used as illustrated in some special cases.