Lecture 4 :

Ideal gases of bosons and fermions

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Reminder on equilibrium statistical mechanics : grand canonical ensemble

- non-interacting particles of mass M in a potential $U(\boldsymbol{r})$, characterized by a single-particle states i with energy ε_i.
- contact with a heat bath fixes the mean energy $\overline{E}$.
- contact with a particle reservoir fixes the mean number of particles $\overline{N}$.
- microstate : a configuration $\{N; n_i\}$ of occupation numbers for each energy level, with total energy $E_i = \sum_{n_i} n_i \varepsilon_i$ such that $\sum_i n_i = N$ and $0 \leq N \leq +\infty$.

Grand partition function:
Maximization of entropy under the fixed $\overline{E}$ and $\overline{N}$ constraints implemented by two Lagrange multipliers $\beta = \frac{1}{k_B T}$ and μ (chemical potential). This leads to a statistical density operator $\hat{\rho} = \frac{1}{\Theta} e^{-\beta(\hat{H} - \mu \hat{N})}$ in equilibrium, with the grand partition function

$$\Theta = \mathrm{Tr}\left[e^{-\beta(\hat{H} - \mu \hat{N})}\right]$$

Grand potential :

$$\Omega(T, \mu, \cdots) = -k_B T \ln \Theta = \overline{E} - TS - \mu \overline{N}$$

- For uniform systems (U =cst), equivalence between all statistical ensembles in the *thermodynamic limit*:
  number of particles $N \to \infty$, volume $V \to \infty$, density $\frac{N}{V} \to \mathrm{cst}$
- What about non-uniform systems ?

Grand partition function for ideal gases

Factorization into a product of individual partition functions ζ_i for each energy level,

$$\Theta = \prod_i \zeta_i, \qquad \zeta_i = \sum_{n_i=0}^{\infty} e^{-\beta(\varepsilon_i - \mu)n_i},$$

ε_i: energy of state i, $\mu = \left.\frac{\partial \overline{E}}{\partial N}\right|_T$: chemical potential

Grand potential :

$$\ln\Theta = \sum_i \ln\zeta_i = -\frac{\Omega}{k_B T}$$

Particle number :

$$\overline{N} = \frac{1}{\beta}\left.\frac{\partial \ln\Theta}{\partial \mu}\right|_T = \sum_i \frac{1}{\beta}\left.\frac{\partial \ln\zeta_i}{\partial \mu}\right|_T = \sum_i n(\epsilon_i)$$

$n(\epsilon_i)$: *average* occupation number

Bosons : $0 \leq n_i \leq \infty$

$$\ln\zeta_i = -\ln\left(1 - e^{-\beta(\epsilon_i - \mu)}\right)$$

$$\Longrightarrow \; n_{\mathrm{BE}}(\epsilon_i) = \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1}$$

Fermions: $n_i = 0, 1$

$$\ln\zeta_i = 1 + e^{\beta(\epsilon_i - \mu)}$$

$$\Longrightarrow \; n_{\mathrm{FD}}(\epsilon_i) = \frac{1}{e^{\beta(\epsilon_i - \mu)} + 1}$$

Classical limit : $\frac{\mu}{k_B T} \to -\infty$

$$n_{\mathrm{BE/FD}}(\epsilon_i) \approx z e^{-\beta\epsilon_i} \;\; \text{(Boltzmann)}$$

with $z = e^{\beta\mu}$ the *fugacity*.

Bose-Einstein condensation

Single out the lowest energy state, with energy $\epsilon_{\rm min}$ and population N_0:

$$N = \sum_i n_{BE}(\epsilon_i) = \sum_{\epsilon_i} \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1} = N_0 + N'$$

$$N_0 = \frac{z}{1-z}, \qquad z = e^{\beta(\mu - \epsilon_{\rm min})} \qquad\qquad N' = \sum_{\epsilon_i > \epsilon_{\rm min}} \frac{1}{z^{-1} e^{\beta(\epsilon_i - \epsilon_{\rm min})} - 1}$$

Saturation of excited states when $\mu = \epsilon_{\rm min}$ $(z = 1)$:

$$N' \leq N'_{\rm max}(T) = \sum_{\epsilon_i > \epsilon_{\rm min}} \frac{1}{e^{\beta(\epsilon_i - \epsilon_{\rm min})} - 1}$$

Low temperature : BEC

- $z \approx 1$ $(\mu - \epsilon_{\rm min} \approx -\frac{k_B T}{N_0})$
- $N' = N'_{\rm max}$
- $N_0 = N - N'_{\rm max}$: Macroscopic accumulation of particles in the lowest energy state

Increasing N at fixed T: BEC when $N \geq N_c = N'_{\rm max}$
Decreasing T at fixed N: BEC when $T \leq T_c$ such that $N'_{\rm max}(T_c) = N$

Large box of size L with periodic boundary conditions.

Single particle states: plane waves $\boldsymbol{k}$ with energy $\frac{\hbar^2 \boldsymbol{k}^2}{2M}$ $(\epsilon_{\min} = 0)$.

Excited states population:

$$N' = \sum_{\boldsymbol{k}} n_{\mathrm{BE}} \left(\frac{\hbar^2 \boldsymbol{k}^2}{2M} \right) = \int \frac{d^3 \boldsymbol{k}}{\left(\frac{2\pi}{L}\right)^3} \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2M} - \mu\right)} - 1} = \left(\frac{L}{\lambda_{\mathrm{th}}} \right)^3 g_{3/2}(z)$$

- $z = e^{\beta\mu}$: fugacity
- $g_\alpha(z) = \sum_{l=1}^{+\infty} \frac{z^l}{l^\alpha}$: Bose-Einstein functions
- $\lambda_{\mathrm{th}} = \sqrt{\frac{2\pi\hbar^2}{M k_B T}}$: thermal De Broglie wavelength

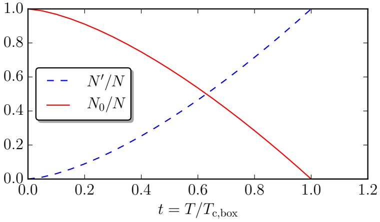
Saturation of excited states:

$$N'_{\max} = \left(\frac{L}{\lambda_{\mathrm{th}}} \right)^3 \underbrace{g_{3/2}(1)}_{\approx 2.612}$$

Fixing $n = N/V$:

$$T_{\mathrm{c,box}} \approx \frac{2\pi\hbar^2}{M} \left(\frac{n}{2.612} \right)^{2/3}$$

NB: $T_{\mathrm{c,box}} = \frac{2\pi\hbar^2}{2ML^2} N^{2/3} \gg \frac{2\pi\hbar^2}{2ML^2}$



Derivation

Excited states population:

$$N' = \int \frac{d^3\boldsymbol{k}}{\left(\frac{2\pi}{L}\right)^3} \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2M} - \mu\right)} - 1}$$

$$= \left(\frac{L}{2\pi}\right)^3 \sum_{p=1}^{+\infty} e^{p\beta\mu} \int d^3\boldsymbol{k} e^{-\frac{p(k\lambda_{\text{th}})^2}{4\pi}}$$

$$= \left(\frac{L}{2\pi}\right)^3 \sum_{p=1}^{+\infty} e^{p\beta\mu} \left(\frac{2\pi}{p\lambda_{\text{th}}}\right)^3$$

$$= \left(\frac{L}{\lambda_{\text{th}}}\right)^3 g_{3/2}(z)$$

We used

$$\frac{1}{1-x} = \sum_{p=0}^{+\infty} x^p,$$

$$\int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}.$$

Polylogarithm functions

The statistical mechanics of ideal quantum gases involves integrals of the form

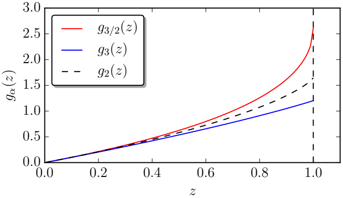
$$\int_{t=0}^{\infty} \frac{t^{\alpha-1}}{z^{-1}e^t \mp 1}\,dt = \pm\Gamma(\alpha)\mathrm{Li}_\alpha(\pm z)$$

Li_α is a member of a family of special functions known as polylogarithm functions.

We prefer to define separately (*not* a universal convention) the

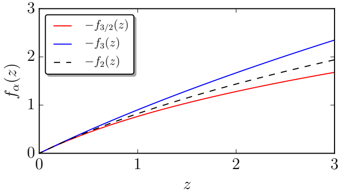
Bose-Einstein functions :

$$g_\alpha(z) = \sum_{l=1}^{+\infty} \frac{z^l}{l^\alpha} = \Gamma(\alpha)\mathrm{Li}_\alpha(z),$$



Fermi-Dirac functions :

$$f_\alpha(z) = \sum_{l=1}^{+\infty} \frac{(-z)^l}{l^\alpha} = -\Gamma(\alpha)\mathrm{Li}_\alpha(-z),$$



Useful limits :

$$\mathrm{Li}_\alpha(\pm z) \underset{z\to 0}{\to} \frac{\pm z}{\Gamma(\alpha)} \text{ (Boltzmann gas)}, \qquad \mathrm{Li}_\alpha(-e^{\beta\mu}) \underset{\beta\to\infty}{\to} -\frac{(\beta\mu)^\alpha}{\Gamma(\alpha+1)} \text{ } (T = 0 \text{ Fermi gas})$$

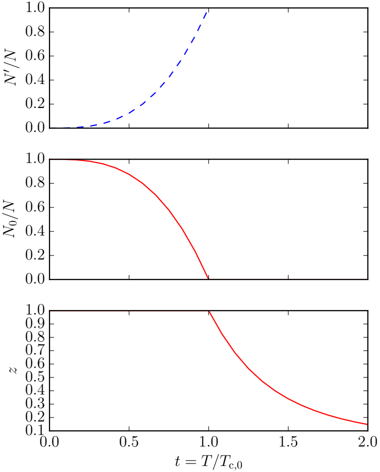
Bosons in a harmonic trap

Energy levels : $\epsilon_{\boldsymbol{n}} = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right) = \left(n + \frac{3}{2}\right)\hbar\omega$

Degeneracy $g_{\boldsymbol{n}} = \frac{(n+1)(n+2)}{2}$

Excited states population :

$$N' = \sum_n \frac{g_n}{z^{-1}e^{-\beta n\hbar\omega} - 1}$$
$$\approx \frac{1}{2}\int_1^\infty \frac{n^2}{z^{-1}e^{-\beta n\hbar\omega} - 1}dn$$
$$= \left(\frac{k_B T}{\hbar\omega}\right)^3 g_3(z)$$



Discrete sum replaced by an integral, valid if $k_B T \gg \hbar\omega$.

Saturation of excited states:

$$N'_{\max} = \left(\frac{k_B T}{\hbar\omega}\right)^3 \underbrace{g_3(1)}_{\approx 1.202}$$

$$T_{c,0} \approx \hbar\omega\left(\frac{N}{1.202}\right)^{1/3}$$

NB: $T_{c,0} \gg \hbar\omega$

NB2: thermodynamic limit in a harmonic trap : $N \to \infty$, $\omega \to 0$, $N\omega^3 \to$cst.

Semi-classical approximation - I

- Consider the particles as classical, with energy $\epsilon(\boldsymbol{r},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2M} + U(\boldsymbol{r})$.
- However include their statistics in the determination of the phase-space density f.

$$f(\boldsymbol{r},\boldsymbol{p}) = n_{\mathrm{BE}}(\epsilon(\boldsymbol{r},\boldsymbol{p})) = \frac{1}{z^{-1}e^{\beta\epsilon(\boldsymbol{r},\boldsymbol{p})} \mp 1}$$

Excited states population :

$$N' = \int \frac{d^3\boldsymbol{r}d^3\boldsymbol{p}}{(2\pi\hbar)^3} f(\boldsymbol{r},\boldsymbol{p})$$

$$N' = \int dE \int \frac{d^3\boldsymbol{r}d^3\boldsymbol{p}}{(2\pi\hbar)^3}\, n_{\mathrm{BE}}(E)\, \delta\Big[E - \epsilon(\boldsymbol{r},\boldsymbol{p})\Big] = \int dE\, \rho(E)\, n_{\mathrm{BE}}(E)$$

Semi-classical density of states:

$$\rho(E) = \int \frac{d^3\boldsymbol{r}d^3\boldsymbol{p}}{(2\pi\hbar)^3}\, \delta\Big[E - \epsilon(\boldsymbol{r},\boldsymbol{p})\Big]$$

Semi-classical approximation - II

- Consider the particles as classical, with energy $\epsilon(\boldsymbol{r},\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2M} + U(\boldsymbol{r})$.
- However include their statistics in the determination of the phase-space density f.

$$f(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{z^{-1}e^{\beta\epsilon(\boldsymbol{r},\boldsymbol{p})} \mp 1}$$

Excited states population :

$$N' = \int \frac{d^3\boldsymbol{r}d^3\boldsymbol{p}}{(2\pi\hbar)^3} f(\boldsymbol{r},\boldsymbol{p})$$

- Same result as before for bosons in harmonic trap in the limit $k_B T \gg \hbar\omega$
- Simpler to derive certain physical observables, *e.g.* the spatial density of thermal bosons is given by

$$n'(\boldsymbol{r}) = \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} f(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{\lambda_{\rm th}^3} g_{3/2}\left(ze^{-\beta U(\boldsymbol{r})}\right)$$

BEC occurs when the phase space density in the center is

$$\mathcal{D}(0) = n'(0)\lambda_{\rm th}^3 = g_{3/2}(1)$$

Semi-classical approximation = Local density approximation

Another point of view on the semi-classical approximation:

Local density approximation: Treat the non-uniform system (with smoothly varying density) locally as a uniform one, with "cells" of size $d_{\rm cell}$ large compared to some microscopic length l but small compared to the cloud size R,

$$l \ll d_{\rm cell} \ll R$$

Within each cell, the system is considered as uniform with a local chemical potential

$$\mu_{\rm loc}(\mathbf{r}) = \mu - U(\mathbf{r}),$$

offset by the trap potential. Here μ : global chemical potential fixed by constraining the total atom number to N.

The density in each cell (or other thermodynamic quantities) is then given by the same function as for the uniform gas $n[\mu_{\rm loc}(\mathbf{r})]$.

Very useful approximation for interacting systems

Validity of the LDA: $|\boldsymbol{\nabla}\mu_{\rm loc}| d_{\rm cell} \ll |\mu_{\rm loc}|$

Check for the Bose gas:

$$l = \lambda_{\rm th} = \sqrt{\frac{2\pi\hbar^2}{Mk_BT}}, R = \sqrt{\frac{k_BT}{m\omega^2}}, \frac{R}{\lambda_{\rm th}} \sim \frac{k_BT}{\hbar\omega} \gg 1$$

Bose-Einstein condensation in coordinate space

Back to the Bose gas and to the harmonic trap, which we take now to be anisotropic as most experiments ($\omega_\perp \gg \omega_x$),

$$U(\boldsymbol{r}) = \frac{1}{2} M\omega_x^2 x^2 + \frac{1}{2} M\omega_\perp^2 (y^2 + z^2).$$

Spatial density : $n(\boldsymbol{r}) = n_0(\boldsymbol{r}) + n'(\boldsymbol{r})$

Condensate density n_0:
$n_0(\boldsymbol{r}) = N_0|\phi_0(\boldsymbol{r})|^2$
with ϕ_0 the single-particle ground state wavefunction given by

$$\phi_0(\boldsymbol{r}) = \frac{1}{\pi^{3/4} a_\perp a_x^{1/2}} e^{-\frac{x^2}{2a_x^2} - \frac{y^2+z^2}{2a_\perp^2}}$$

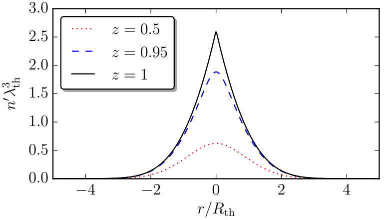
Here $a_{\perp/x} = \sqrt{\frac{\hbar}{M\omega_{\perp/x}}}$ are the respective oscillator lengths.

$$\frac{R_\perp}{a_\perp} = \frac{k_B T}{\hbar\omega_\perp} \gg 1$$

Non-condensate density n':

$$n'(\boldsymbol{r}) = \frac{1}{\lambda_{\rm th}^3} g_{3/2}\left(z e^{-\frac{x^2}{2R_{x,\rm th}^2} - \frac{y^2+z^2}{2R_{\perp,\rm th}^2}} \right)$$

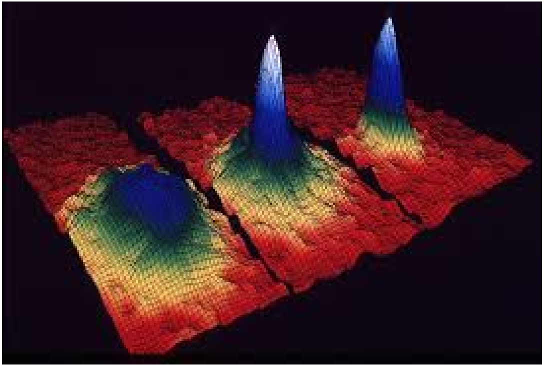
with $R_{\perp/x} = \sqrt{\frac{k_B T}{M\omega_{\perp/x}^2}}$.



The condensate shows up as a narrow peak in the density in the trap center.

First observation of BEC

First observation at JILA 1995 (Wieman/Cornell group, M. Anderson *et al.*, Science 269, 198 (1995)).



Observed not in position space but in "momentum space", *i.e.* after a time of flight.

Time-of-flight experiment (quantum mechanical version)

Time-of-flight experiment : suddenly switch off the trap potential at $t = 0$ and let the cloud expand for a time t.

General formulation for a single particle: The wave-function $\psi(\mathbf{r}, t)$ is proportional (for long times) to the initial *momentum space wavefunction* $\tilde{\psi}_0(\mathbf{k})$ evaluated at $\mathbf{k} = \frac{m\mathbf{r}}{\hbar t}$.

$$\psi(\mathbf{r}, t) \approx \left(\frac{M}{\hbar t}\right)^{3/2} \tilde{\psi}_0\left(\mathbf{k} = \frac{M\mathbf{r}}{\hbar t}\right) e^{i\frac{M\mathbf{r}^2}{2\hbar t} + i\chi}$$

with χ a uniform phase.

Proof using stationary phase approximation :

$$\psi(\mathbf{r}, 0) = \int \frac{d^3\boldsymbol{k}}{(2\pi\hbar)^{3/2}} \tilde{\psi}_0(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}},$$

$$\psi(\mathbf{r}, t) = \int \frac{d^3\boldsymbol{k}}{(2\pi\hbar)^{3/2}} \tilde{\psi}_0(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{r} - i\frac{\hbar\boldsymbol{k}^2 t}{2M}}$$

$$\approx \tilde{\psi}_0\left(\mathbf{k} = \frac{M\mathbf{r}}{\hbar t}\right) e^{i\frac{M\mathbf{r}^2}{2\hbar t}} \int \frac{d^3\delta\boldsymbol{k}}{(2\pi\hbar)^{3/2}} e^{-i\frac{\hbar\delta\boldsymbol{k}^2 t}{2M}}, \delta\boldsymbol{k} = \boldsymbol{k} - \frac{m\boldsymbol{r}}{\hbar t}.$$

- Analogous to Fraunhofer regime of optical diffraction, requires $\frac{\hbar\Delta k_0 t}{M} \gg \Delta x_0$ with $\Delta x_0, \Delta k_0$ the spread of ψ_0 in real and in momentum space.
- for a condensate : N atoms behaving identically, density profile $\rho(\boldsymbol{r}, t) \approx N|\psi(\mathbf{r}, t)|^2$ with Ψ the condensate wavefunction.

Bose-Einstein condensation in momentum space

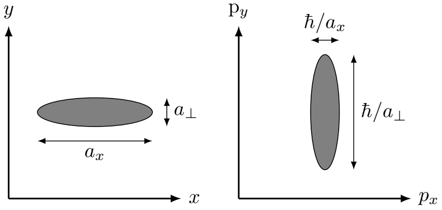
Momentum distribution (accessible after a time-of-flight) also features a condensed and an uncondensed component :

$$\mathcal{P}(\boldsymbol{p}) = N_0|\tilde{\phi}_0(\boldsymbol{p})|^2 + \mathcal{P}'(\boldsymbol{p})$$

$$\tilde{\phi}_0(\boldsymbol{r}) \propto e^{-\frac{p_x^2}{2\Delta p_x^2}-\frac{p_y^2+p_z^2}{2\Delta p_\perp^2}}, \qquad \Delta p_{\perp/x} = \sqrt{M\hbar\omega_{\perp/x}},$$

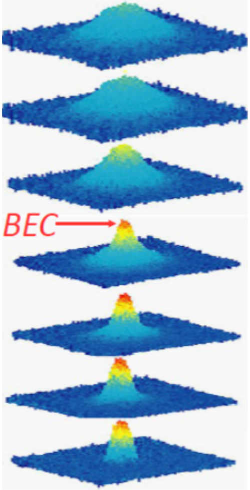
$$\mathcal{P}'(\boldsymbol{p}) \propto g_{3/2}\left(z e^{-\frac{p_x^2+p_y^2+p_z^2}{2\Delta p_{\rm th}^2}}\right) \qquad \Delta p_{\rm th} = \sqrt{M k_B T}.$$

- the condensate expands much more slowly than the thermal component (by a factor $\sqrt{\hbar\omega_i/k_B T}$ for direction i),
- the thermal component expands isotropically,
- the condensate expands anisotropically and undergoes an inversion of ellipticity :

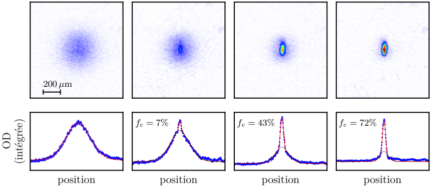


Experiments with bosons : observation and condensate fraction

Rb BEC, Institut d'optique



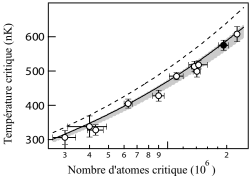
Ytterbium BEC, LKB :



Fit of the thermal component by a Bose function g_2

[figure from A. Dareau's PhD thesis]

Critical temperature :



- ideal gas theory (dashed)
- small but measurable shift due to interactions

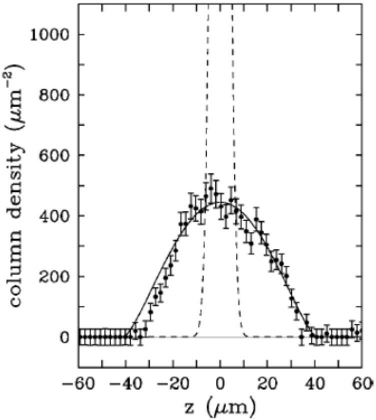
F. Gerbier *et al.*, PRL 2003.

Experiments with bosons: "pure BEC" in real space

"Almost pure" condensates : no discernible thermal pedestal ($N_0/N \geq 80\,\%$)

Unlike for thermal bosons, the ideal gas theory fails to describe the condensate properties.

in-situ density profile: Dashed line shows the expected Gaussian density profile of the harmonic oscillator ground state.

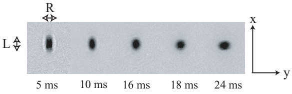


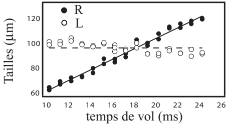
Hau *et al.*, PRA 1998

Experiments with bosons: “pure BEC” in momentum space

Anisotropic expansion in a cigar-shaped trap ($\omega_\perp \gg \omega_x$) For an ideal gas:

- in the trap, $R_y = a_\perp \ll R_x = a_x$
  $\Longrightarrow \quad \frac{R_x}{R_y} = \sqrt{\frac{\omega_y}{\omega_x}} \gg 1,$
- for long time of flights,
  $\frac{R_x}{R_y} \approx \sqrt{\frac{\omega_x}{\omega_y}} \ll 1.$

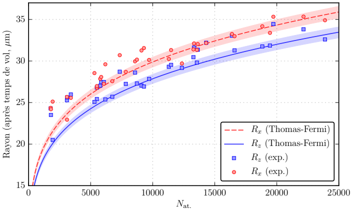




BUT

- Expect Gaussian distribution : not the case
- BEC size depend on atom number

Ideal gas theory describes reasonably well a gas bosons above T_c, or the thermal component below T_c, but fails to describe the condensate properties.



[figure from A. Dareau’s PhD thesis]

Essential to include interactions between the condensed atoms.

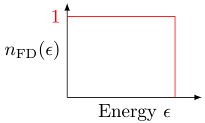
Ideal Fermi gases in a trap : zero temperature limit

Semi-classical description :

$$n(\boldsymbol{r}) = \frac{1}{\lambda_{\rm th}^3} f_{3/2}\left(z e^{-\beta U(\boldsymbol{r})}\right)$$

At zero temperature, the Fermi-Dirac distribution becomes a Heaviside step function Step, centered at the Fermi energy $\mu = E_F$

$$n(\boldsymbol{r}) = \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \mathrm{Step}\left(E_F - \frac{\mathbf{p^2}}{2M} - U(\boldsymbol{r})\right)$$
$$= \frac{k_F^2}{6\pi^2}\left[1 - \left(\frac{r}{R_F}\right)^2\right]^{3/2}$$

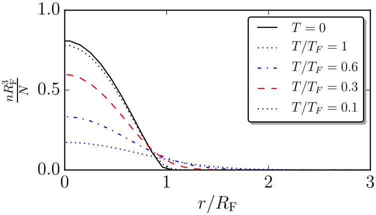


Fermi wavevector : $k_F = \sqrt{\frac{2M\mu}{\hbar^2}}$, with $E_F = \mu$ the Fermi energy

Fermi radius : $R_F = \sqrt{\frac{2E_F}{M\omega^2}}$

From $N = \int d^3\boldsymbol{r} n(\boldsymbol{r})^a$, one finds

Fermi energy : $E_F = \mu = \hbar\omega\,(6N)^{1/6}$



[a] $\int_0^1 x^2(1-x^2)^{3/2}dx = \frac{\pi}{32}$.

Low temperature limit : the "Fermi lake"

Fugacity z (chemical potential μ) for given N, T, ω found from

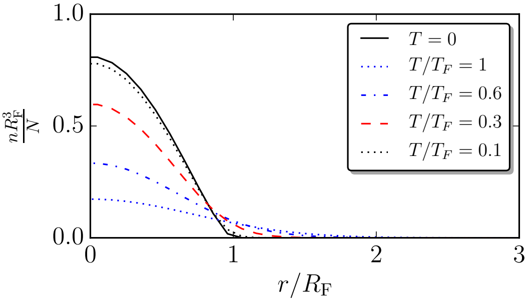
$$N = \left(\frac{k_B T}{\hbar\omega}\right)^3 f_3\left(-z\right)$$

Density:

$$n(\boldsymbol{r}) = \frac{1}{\lambda_{\text{th}}^3} f_{3/2}\left(z e^{-\beta U(\boldsymbol{r})}\right)$$

Dimensionless form : $\tilde{r} = \frac{r}{R_F}$, $t = \frac{T}{T_F}$

$$\frac{n(\boldsymbol{r}) R_F^3}{N} = \frac{6 t^{3/2}}{\pi^2} f_{3/2}\left(z e^{-\frac{\tilde{r}^2}{t}}\right)$$



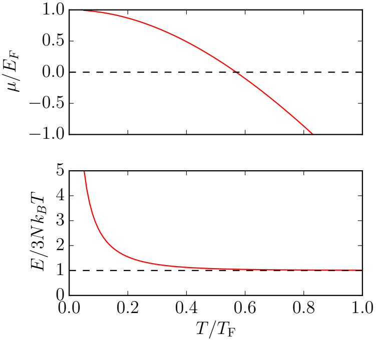
DeMarco and Jin, Science 1999

Internal energy :

$$E = 3\frac{(k_B T)^4}{(\hbar\omega)^3} f_4(z)$$

$$= 3Nk_B T \frac{f_4(z)}{f_3(z)}$$

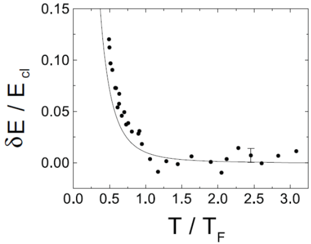
$$E_{\text{kin}} = E_{\text{pot}} = \frac{E}{2} \quad \text{(harmonic potential)}$$



Observation in a two-component gas of Potassium :

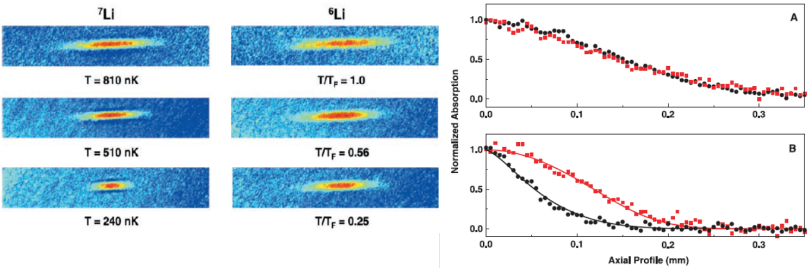
Measurement of “release energy” $E_{\text{kin}} = \frac{E}{2}$ after time of flight

Extra energy when cooling down when compared to a classical gas

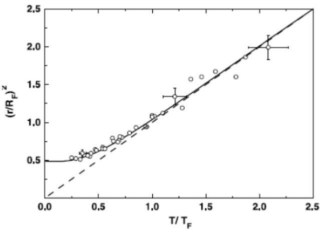


Experiments with Bose-Fermi mixtures : case of Lithium

Spatial profiles of coexisting BEC and Fermi sea after forced evaporation in a magnetic trap :



Evidence for Fermi pressure keeping the cloud size from shrinking further down once T is substantially below T_F



Truscott *et al.*, Science 2001; see also Schreck *et al.*, PRL 2001