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### Outline

- Ideal quantum gas in the grand canonical ensemble
- Ideal Bose gas
- Bose Einstein condensation

• Scope: analysis of the ideal gas in the quantum degenerate limit; understanding how quantum statistics affect thermodynamic properties (e.g. pressure)

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# The ideal quantum gas

- As a first concrete application of quantum statistics we want to calculate the properties of an ideal gas of (non-relativistic) indistinguishable bosons
- One has to expect that the ideal Bose gas becomes the ideal Boltzmann gas (classical ideal gas) at high temperatures and low densities. The largest deviations in thermodynamic properties should therefore occur if the condition

the condition  $n\lambda_{\tau}^{3} = \frac{N}{V} \left( \frac{2\pi \hbar^{2}}{m k_{B} T} \right)^{3/2} << 1 \quad \text{for the purisible}$ In the condition  $n\lambda_{\tau}^{3} = \frac{N}{V} \left( \frac{2\pi \hbar^{2}}{m k_{B} T} \right)^{3/2} << 1 \quad \text{in the purisible}$ In the condition  $n\lambda_{\tau}^{3} = \frac{N}{V} \left( \frac{2\pi \hbar^{2}}{m k_{B} T} \right)^{3/2} << 1 \quad \text{in the purisible}$ 

is <u>no longer</u> fulfilled. In applications to real systems, however, the parameter  $n(\lambda_T)^3$  must not become too large, since for very small temperatures (small mean kinetic energy per particle) as well as for high densities (small mean distance between particles) the interactions in real systems are no longer negligible.

• The ideal Bose gas is thus a model system, where the influence of quantum effects can be very well studied, but which can only approximately describe real systems. For diluted (meta-stable) Bose gases this model is better suited!

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# The occupation number representation

- Note that one can specify a state with particles in state  $v_1$  ...  $v_N$  in terms of occupation numbers  $n_v$  for each state of the basis  $|v\rangle$ ; this corresponds to write the basis state  $|v_1$  ...  $|v_N\rangle$  of the Fock space as a tensor product of eigenstates of the occupation number operator:  $|v_1$  ...  $|v_N\rangle = |n_{v_1}$  ...  $|n_{v_N}\rangle = |n_{v_1}$  ...  $|n_{v_N}\rangle = |n_{v_1}| |n_{v_N}\rangle$
- For Bosons, the occupation numbers are a priori not restricted, whereas for Fermions they can take only the value 0 or 1
- In both cases, the sum of the occupation numbers, which counts the total number of occupied states, must be equal to the number of particles  $N=\Sigma n_v$

 The basis states for an N-particle system in the occupation number representation are obtained simply by listing the occupation numbers of each basis state

N	fermion basis states $ n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, \ldots\rangle$
0	0,0,0,0,⟩
1	$ 1,0,0,0,\rangle,  0,1,0,0,\rangle,  0,0,1,0,\rangle,$
2	$  \  1,1,0,0,\rangle, \  0,1,1,0,\rangle, \  1,0,1,0,\rangle, \  0,0,1,1,\rangle, \  0,1,0,1,\rangle, \  1,0,0,1,\rangle, \$
:	i i i
N	boson basis states $ n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, \ldots \rangle$
N 0	boson basis states $ n_{\nu_1},n_{\nu_2},n_{\nu_3},\dots\rangle$ $ 0,0,0,0,\dots\rangle$
1	
	0,0,0,0, angle

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- In the following the quantum statistical description of the ideal quantum gas in the context of the grand canonical ( $\mu$ VT) ensemble (where the formalism becomes particularly simple) will be introduced.
- Let us consider now a system described by the independent particle
   Hamiltonian H=Σ<sub>i</sub>H<sub>i</sub><sup>(1)</sup>. In this case, the eigenstates |k⟩ of H are defined by
   specifying the set {n<sub>i</sub>} of the occupation numbers n<sub>i</sub> of the single particle states, obtained by solving the Schrödinger equation:

$$\begin{split} \hat{\pmb{\mathcal{H}}}^{(1)}\varphi_{_{i}}(\vec{\pmb{r}}) &= \varepsilon_{_{i}} \; \varphi_{_{i}}(\vec{\pmb{r}}) \\ \left| n_{_{0}}n_{_{1}}\cdots \right\rangle &= \left(a_{_{o}}^{_{+}}\right)^{n_{_{0}}} \left(a_{_{1}}^{_{+}}\right)^{n_{_{1}}} \cdots \left| vac \right\rangle \quad ; \quad \left[a_{_{i}},a_{_{j}}^{^{+}}\right]_{_{-\mathcal{E}}} &= \delta_{_{ij}} \end{split}$$

 For this Hamiltonian the grand canonical function can be worked out exactly; in the occupation number representation we have (see supplementary material)

$$\hat{n}_{i} | n_{0} n_{1} \cdots \rangle = a_{i}^{+} a_{i} | n_{0} n_{1} \cdots \rangle = n_{i} | n_{0} n_{1} \cdots \rangle \Rightarrow \hat{N} | n_{0} n_{1} \cdots \rangle = \left( \sum_{i} n_{i} \right) | n_{0} n_{1} \cdots \rangle$$

$$\hat{H}^{(1)} | n_{0} n_{1} \cdots \rangle = \varepsilon_{i} | n_{0} n_{1} \cdots \rangle \Rightarrow \hat{H} | n_{0} n_{1} \cdots \rangle = \left( \sum_{i} \varepsilon_{i} n_{i} \right) | n_{0} n_{1} \cdots \rangle$$
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Thus the grand partition function can be written as

$$Z(T,V,z) = \text{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})}) = \sum_{N=0}^{\infty} \sum_{\substack{\{n_i\}\\ (\sum n_i = N)}} e^{-\beta \sum_i n_i \varepsilon_i + \beta \mu \sum_i n_i} = \sum_{N=0}^{\infty} \sum_{\substack{\{n_i\}\\ (\sum n_i = N)}} z^{\sum_i n_i} e^{-\beta \sum_i n_i \varepsilon_i} =$$

$$=\sum_{N=0}^{\infty}\sum_{\substack{\left\{n_{i}\right\}\\\left(\sum n_{i}=N\right)}}\prod_{i}\left(\boldsymbol{z}\boldsymbol{e}^{-\beta\varepsilon_{i}}\right)^{n_{i}}=\sum_{\substack{\left\{n_{i}\right\}=\left\{\begin{array}{c}0,1,2,3,\cdots\text{Bose}\\0,1\end{array}\right\}\\\text{Fermi}}}\prod_{i}\left(\boldsymbol{z}\boldsymbol{e}^{-\beta\varepsilon_{i}}\right)^{n_{i}}=\prod_{i}\sum_{n_{i}}\left(\boldsymbol{z}\boldsymbol{e}^{-\beta\varepsilon_{i}}\right)^{n_{i}}$$

that for the Bose case gives rise to a geometric series:

$$\mathcal{Z}(T,V,z) = \prod_{i} \frac{1}{1 - ze^{-\beta \varepsilon_{i}}}$$

with the condition

$$ze^{-\beta\varepsilon_i} = e^{\beta(\mu-\varepsilon_i)} < 1$$
 \(\forall \text{for amore conveyed to } \)
$$= \mu < \varepsilon_0 \qquad \qquad \left( \mu < \varepsilon_0 < \varepsilon_1 . . . \varepsilon \)$$

 One can straightforwardly evaluate the thermodynamic behaviour of the system via the grand (canonical) potential

$$\Omega(T,V,z) = -k_B T \ln \mathcal{Z}(T,V,z) = \frac{1}{\beta} \sum_{i} \ln(1-ze^{-\beta\varepsilon_i})$$

• For example, the average total number of particles

$$\left\langle \hat{\boldsymbol{N}} \right\rangle = \operatorname{Tr}(\hat{\boldsymbol{\rho}}\hat{\boldsymbol{N}}) = \frac{1}{\mathcal{Z}} \sum_{N=0}^{\infty} N e^{\beta \mu N} Q(T, V, N) = \frac{k_{B}T}{\mathcal{Z}} \frac{\partial}{\partial \mu} \left[ \mathcal{Z}(T, V, z) \right]_{T, V} = -\frac{\partial \Omega(T, V, z)}{\partial \mu}$$

It follows that

$$\widehat{\langle \hat{\mathbf{N}} \rangle} = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \sum_{i} \ln(1 - \mathbf{e}^{\beta \mu} \mathbf{e}^{-\beta \varepsilon_{i}}) = \sum_{i} \frac{\mathbf{z} \mathbf{e}^{-\beta \varepsilon_{i}}}{1 - \mathbf{z} \mathbf{e}^{-\beta \varepsilon_{i}}} = \sum_{i} \frac{1}{\mathbf{e}^{\beta (\varepsilon_{i} - \mu)} - 1} = \sum_{i} \langle \mathbf{n}_{i} \rangle$$

· For the energy:

$$\left\langle \hat{H} \right\rangle = \frac{\partial}{\partial \beta} \left[ \beta \Omega(T, V, z) \right]_{V, z} = \sum_{i} \varepsilon_{i} \left\langle n_{i} \right\rangle = \sum_{i} \frac{\varepsilon_{i}}{e^{\beta(\varepsilon_{i} - \mu)} - 1}$$

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- From now on, for simplicity, we will write N, N<sub>0</sub>, N<sub>T</sub>, n<sub>i</sub> in place of their average values, but remember, we have used the grand canonical ensemble thus such numbers fluctuate
- Consider the case  $\varepsilon_0$ =0, the condition that the chemical potential of an ideal Bose gas must be  $< \varepsilon_0$  is equivalent to the fact that bosons seem to feel an attractive potential, and that adding further bosons to the system is energetically favorable. When  $\mu \rightarrow \varepsilon_0$  the average occupation number  $\langle n_0 \rangle = 1/\{ \exp[\beta(\varepsilon_0 \mu)] 1 \}$  becomes increasingly large. This is actually the mechanism at the origin of Bose-Einstein condensation
- Let us write the total number of particles as

$$N = N_0 + N_T = \frac{ze^{-\beta\varepsilon_0}}{1 - ze^{-\beta\varepsilon_0}} + \sum_{i \neq 0} \langle n_i(T, \mu) \rangle$$

 $N_0$  is always of order 1, except when  $\mu$  is close to  $\epsilon_0$  where  $N_0$  diverges

# The ideal Bose gas

- Let us apply this to the problem of an ideal Bose gas confined in a box of volume V=L3
- In this case the single particle Hamiltonian has the simple form  $H^{(1)}=p^2/2m$ , whose solutions, using periodic boundary conditions  $\varphi(x,y,z)=\varphi(X+L,y,z)$ , etc. are plane waves

$$\varphi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \quad \text{with energy} \quad \frac{\hbar^2 \vec{k}^2}{2m} \quad \text{and momentum} \quad \begin{vmatrix} \vec{p} = \hbar \vec{k} = \hbar \frac{2\pi}{L} \vec{n} \\ = \hbar \frac{2\pi}{L} [n_x, n_y, n_z] \end{vmatrix}$$

- $\epsilon_0$ =0 so that the chemical potential must always be negative.
- By making the replacement  $\Sigma_k = V/(2\pi)^3 \int dk$  (see supplementary material), to evaluate the sum over the states with  $k\neq 0$  , the number of atoms out of the condensate can be written in the form

$$N_{T} = \sum_{\vec{k} \neq 0} \frac{1}{e^{\beta \left(\hbar^{2} k^{2} / 2m - \mu\right)} - 1} = \frac{V}{(2\pi)^{3}} \int d\vec{k} \frac{1}{e^{\beta \left(\hbar^{2} k^{2} / 2m - \mu\right)} - 1} = \frac{V}{\lambda_{T}^{3}} g_{3/2}(z)$$
 where  $g_{p}(z) := \sum_{l=1}^{\infty} \frac{z^{l}}{l^{p}}$  is obtained expanding the integrand and integrating term by term

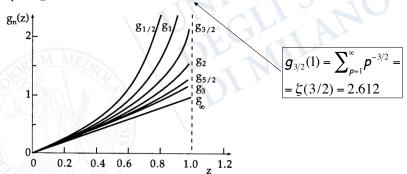
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Note that given

$$g_p(z) := \sum_{l=1}^{\infty} \frac{z^l}{l^p}$$

we have  $g_n(1) = \sum_{p=1}^{\infty} p^{-n} = \zeta(n)$  which is the Riemann's Zeta function

The functions  $g_n(z)$  all start at the origin with slope 1 and diverge for z → 1 , if n ≤ 1



For n > 1 they have a finite value at z=1, which becomes steadily smaller with increasing n. For  $n\rightarrow\infty$ ,  $g_n(z)\approx z$ .

- Notice also that the above results have been derived in 3D and that the behaviour of the corresponding functions is very different in lower dimensions
- We start now from the eq. for the particle number, from which we have to determine the fugacity z for given (N), V, and T:

$$N = N_0 + N_T = \frac{z}{1-z} + \frac{V}{\lambda_T^3} g_{3/2}(z)$$

of course, N>1, and for temperatures which are not too small, in general  $N_T$  > 1. On the other hand,  $0 \le g_{3/2}(z) \le \zeta(3/2) = 2.612$ .

For a given V and T the second term in the equation can at most assume the value

when the fugacity z for given (N), V, and I: 
$$N = N_0 + N_T = \frac{z}{1-z} + \frac{V}{\lambda_T^3} g_{3/2}(z)$$
which is make fear the proof of the

- $N_T$  is extensive, but for fixed V we have that  $N_T \rightarrow 0$  when  $T \rightarrow 0$
- We now study the thermodynamic limit of the previous equation:  $N\rightarrow\infty$ ,  $V\rightarrow\infty$ , N/V=cost.

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When N >  $N_T^{max}$  the excited states are not enough to contain all of the particles. Then  $z \rightarrow 1$ , and the excess

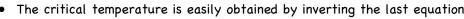
$$N_0 = N - N_T^{\text{max}} = N - \frac{V}{\lambda_T^3} \zeta(3/2) = N - V \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2} \zeta(3/2)$$

condenses in the ground state: this is the phenomenon called Bose-Einstein condensation (BEC)

This happens just when we reach the (critical) density:

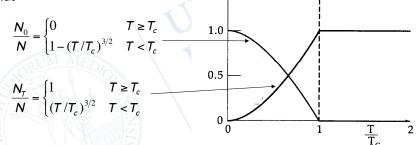
$$n_c = \frac{N}{V} = \frac{\zeta(3/2)}{\lambda_T^3} = \zeta(3/2) \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}$$

- For larger temperatures and lower densities the thermal energy is sufficiently large to excite (nearly) all particles into higher levels.
- On the contrary, if the temperature becomes very small or the density sufficiently high, the positive statistical correlation of the bosons becomes strongly noticeable: the bosons try to gather in the ground state. It becomes more probable for the system to no longer distribute the thermal excitation energy homogeneously over all particles, but only over the fraction N<sub>T</sub>max/N, and to put the rest, into the ground state



$$T_c = \left(\frac{N}{V}\right)^{2/3} \frac{1}{\xi^{2/3}(3/2)} \frac{2\pi\hbar^2}{mk_B}$$
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If one expresses  $N_0$  and  $N_T$  in terms of the critical temperature, one



These functions are illustrated in the figure. One quickly realizes how, from  $T = T_c$  on, the ground state has to contain more and more particles as the system is further cooled down. However, this picture actually holds only in the thermodynamic limit. For finite particle numbers, no kinks occur at  $T = T_c$ 13

for ToTc perpre To=0



# TEB

# The equation of state

• Consider now the grand potential

$$\Omega(T, V, z) = \frac{1}{\beta} \sum_{i} \ln(1 - ze^{-\beta \varepsilon_{i}}) = \frac{1}{\beta} \left( \frac{V}{(2\pi)^{3}} \int d\vec{k} \ln(1 - ze^{-\beta \hbar^{2} \vec{k}^{2}/2m}) + \ln(1 - z) \right) = \frac{1}{\beta} \left( \frac{V}{(2\pi)^{3}} \int d\vec{k} \ln(1 - ze^{-\beta \hbar^{2} \vec{k}^{2}/2m}) + \ln(1 - z) \right)$$

$$= \frac{1}{\beta} \left[ -\frac{V}{\lambda^3} \left( -\frac{4}{\sqrt{\pi}} \int_0^\infty dx \, x^2 \ln(1 - z e^{-x^2}) \right) + \ln(1 - z) \right] = \frac{1}{\beta} \left( -\frac{V}{\lambda_\tau^3} g_{5/2}(z) + \ln(1 - z) \right)$$

Expanding the integrand and integrating term by term

Eulero's equation for a simple fluid, TS-pV+µN=E, tells us that the grand potential function  $\Omega$  reduces to  $\Omega=E-TS-\mu N=-pV$  where p is the pressure acting on the system, and hence directly provides the equation of state

$$p = -\frac{1}{V}\Omega(T, V, z) = \frac{k_B T}{\lambda_T^3} g_{5/2}(z) - \frac{k_B T}{V} \ln(1 - z)$$

Here it is also convenient to first consider the thermodynamic limit...

- One readily observes that the last term can be always neglected:
  - if z < 1,  $\ln(1-z)$  is finite and this term goes to zero for  $V \rightarrow \infty$ .
  - Furthermore, 1–z=z/N $_{\!0}$  can at most decrease as 1/N , so that the product of V $^{\!-1}$  with the logarithmically divergent term ln(N) vanishes in the thermodynamic limit.
- This simply means that the particles in the ground state having no kinetic energy do not contribute to the pressure
- Below the critical temperature we may set z=1, in this region the pressure

 $p = \frac{k_B T}{\lambda_T^3} \zeta(5/2)$ 

becomes independent of volume and particle number, and is solely a function of temperature

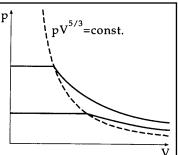
The equation for N yields a critical density at given temperature (or if the particle number is given as well, a critical volume), above (below) which Bose condensation sets in:

 $\frac{N}{V} = \frac{\zeta(3/2)}{\lambda_T^3} \implies V_C = \frac{\lambda_T^3 N}{\zeta(3/2)}$ 

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One concludes that the isotherms of the Bose gas are horizontal lines in the pV diagram for volumes V<Vc , just like a van der Waals gas in the coexistence region of gas and liquid



One could try to interpret Bose condensation as a kind of phase transition in a system where "coexist" two phases: one phase is represented by the particles in the excited

states, while the other is formed by the particles in the ground state

- However, Bose condensation is not a condensation in coordinate space, as in the phase transition gas-liquid, but a condensation in momentum space, in which particles gather in a certain momentum state
- If one eliminates the temperature from the previous equations, one obtains the limiting curve in the pV diagram where Bose condensation sets in:

 $pV^{5/3} = \cos t. = \frac{h^2}{2\pi m} \frac{\zeta(5/2)}{\left[\zeta(3/2)\right]^{5/3}} N^{5/3}$ 

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 Finally, we want to consider the internal energy, the specific heat and the entropy of the Bose gas:

$$\left\langle \hat{H} \right\rangle = \frac{\partial}{\partial \beta} \left[ \beta \Omega(T, V, z) \right]_{Vz} = \frac{\partial}{\partial \beta} \left[ -\frac{V}{\lambda_{\tau}^{3}} g_{5/2}(z) + \ln(1-z) \right]_{Vz} = \frac{3}{2} k_{B} T \frac{V}{\lambda_{\tau}^{3}} g_{5/2}(z)$$

• Comparison with the equation for the pressure yields

$$p = \frac{2}{3} \frac{\langle \hat{H} \rangle}{V} = \frac{2}{3} \frac{E}{V}$$

This relation is already well known to us from the classical ideal gas. With the pressure we thus also know the energy density of the system

- To calculate the specific heat at constant volume C<sub>V</sub>, we proceed as follows:
  - for  $T < T_c$  we have z = 1, independent of temperature, so that

$$\frac{C_{V}}{Nk_{B}} = \frac{1}{Nk_{B}} \frac{\partial E}{\partial T}\Big|_{N,V} = \frac{3}{2} \frac{V}{N} \zeta(5/2) \frac{\partial}{\partial T} \left(\frac{T}{\lambda_{T}^{3}}\right) = \frac{15}{4} \frac{\zeta(5/2)}{\lambda_{T}^{3}} \frac{V}{N} \propto T^{3/2}$$

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- For T ≥ T<sub>c</sub>, z is no longer independent of T. However, since now  $N_0 \approx 0$ , we can eliminate the term  $V\lambda^{-3}$  with the help of

$$N = \frac{V}{\lambda_{\tau}^{3}} g_{3/2}(z) \implies E = \frac{3}{2} k_{B} T \frac{V}{\lambda_{\tau}^{3}} g_{5/2}(z) = \frac{3}{2} N k_{B} T \frac{g_{5/2}(z)}{g_{3/2}(z)}$$

One readily recognizes the classical limit:  $E = \frac{3}{2} N k_{_B} T \frac{g_{_{5/2}}(z)}{g_{_{3/2}}(z)} \underset{_{z<<1}}{\rightarrow} \frac{3}{2} N k_{_B} T$ 

For the specific heat, one obtains (see supplementary material)

$$\frac{C_{V}}{Nk_{B}} = \frac{1}{Nk_{B}} \frac{\partial E}{\partial T}\Big|_{N,V} = \frac{3}{2} \frac{g_{5/2}(z)}{g_{3/2}(z)} + \frac{3}{2} T \frac{\partial}{\partial T} \left( \frac{g_{5/2}(z)}{g_{3/2}(z)} \right) = \dots = \frac{15}{4} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4} \frac{g_{3/2}(z)}{g_{1/2}(z)}$$

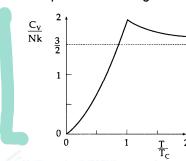
• The classical limit (z $\rightarrow$ 0,  $g_n(z)\approx z \ \forall n)$  can be easily read off; it holds that

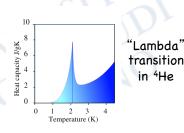
$$C_V = \left(\frac{15}{4} - \frac{9}{4}\right)Nk_B = \frac{3}{2}Nk_B$$
 (ideal gas)

• For  $z\rightarrow 1$  ( $T\rightarrow T_c$ ),  $g_{1/2}$  is divergent, and the second term in the equation vanishes, so that the specific heat tends to the value

$$C_V(T_C) = \frac{15}{4} \frac{\zeta(5/2)}{\zeta(3/2)} N k_B = 1.925 N k_B > C_V^{ideal}$$
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One consequently obtains the following picture of the specific heat, which is depicted in the figure:





- in the region of Bose condensation,  $T/T_{\text{C}} <\!\! 1$  , the specific heat increases like  $T^{3/2}$  to the maximum value,
- At T = T<sub>C</sub> a spike appears, and for  $T\rightarrow\infty$ ,  $C_V$  approaches the value of the ideal gas.
- This is not however a general rule of the ideal Bose gas; for example, in the harmonic trap the specific heat predicted by the ideal Bose gas model exhibits a discontinuity at T=T<sub>C</sub>

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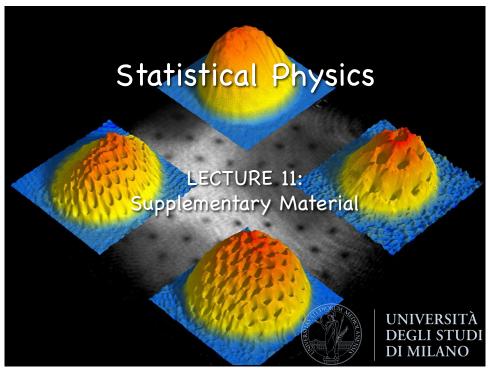
- Let's now consider the entropy; Eulero's equation, TS-PV+ $\mu$ N=E, tells us that  $S = \frac{E + pV \mu N}{T} \implies \frac{S}{Nk_o} = \frac{E + pV}{Nk_o T} \frac{\mu}{k_o T}$
- We had earlier that pV=2E/3 and  $E = \frac{3}{2}k_BT\frac{V}{\lambda_T^3}g_{5/2}(z)$
- It follow that  $\frac{S}{Nk_{B}} = \frac{5}{3} \frac{E}{Nk_{B}T} \ln z = \frac{5}{2} \frac{g_{5/2}(z)}{n \lambda_{T}^{3}} \ln z = \begin{cases} \frac{5}{2} \frac{g_{5/2}(z)}{g_{3/2}(z)} \ln z & T > T_{c} \\ \frac{5}{2} \frac{g_{5/2}(1)}{g_{3/2}(z)} \ln z & T > T_{c} \end{cases}$   $\left( n = \frac{N}{V} = \frac{g_{3/2}(z)}{\lambda_{T}^{3}} \right)$
- Note that for  $T \le T_C$  in the condensate we have a density  $n_0$  and  $n_n$  in the excited states ("normal" state) related by
- Thus for T $\leq$ T<sub>C</sub> we have  $\frac{S}{Nk_{p}} = \frac{5}{2} \frac{n_{n}}{n_{n}} \frac{g_{5/2}(1)}{g_{3/2}(1)} \xrightarrow{T \to 0} 0$
- Entropy proportional to the fraction of "normal" particles; we can imagine that each "normal" particle carries entropy:  $\frac{5}{2}k_B\frac{g_{5/2}(1)}{g_{-1}(1)}$
- $\Rightarrow$  "normal" particles carry the entropy, condensate has zero entropy

### Lecture 11: Suggested books

- L. Peliti, "Appunti di meccanica statistica", Bollati Boringhieri
- R. K. Pathria, "Statistical mechanics", II ed., Oxford
- L. Pitaevskii, S. Stringari "Bose Einstein Condensation", Clarendon Press, Oxford

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# The Thermodynamic Limit

What happens to the various momentum summations in the thermodynamic limit,  $V\rightarrow \infty$ ?



- When the allowed momenta become arbitrarily close together, the discrete summations over momentum must be replaced by continuous integrals. For each dimension, the increment in momentum appearing inside the discrete summations is:  $\Delta q=2\pi/L$  ... so that  $L\Delta q/2\pi = 1$ .
- Thus in 1D, the summation over the discrete values of q can be formally  $\sum_{q} \left\{ \cdots \right\} = L \sum_{q} \frac{\Delta q}{2\pi} \left\{ \cdots \right\} \quad \text{where } q_n = 2\pi n/L \text{ and } n \in \mathbb{Z}$
- When we take  $L\rightarrow\infty$ , q becomes a continuous variable, so that the summation can now be replaced by a continuous integral:

$$\sum_{q} \left\{ \cdots \right\} \to L \int_{-\infty}^{\infty} \frac{dq}{2\pi} \left\{ \cdots \right\}$$

$$\sum_{q_n} \left\{ \cdots \right\} \to L \int_{-\infty}^{\infty} \frac{dq}{2\pi} \left\{ \cdots \right\}$$
Similarly, in in d-dimensions: 
$$\sum_{\bar{q}_n} \left\{ \cdots \right\} \to L^d \int \frac{d\bar{q}}{(2\pi)^d} \left\{ \cdots \right\} = \frac{V}{(2\pi)^d} \int d\bar{q} \left\{ \cdots \right\}$$

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# Ideal Bose gas specific heat

• For T ≥ T<sub>c</sub> the specific heat reads

$$\frac{C_{V}}{NK_{B}} = \frac{3}{2} \frac{g_{5/2}(z)}{g_{3/2}(z)} + \frac{3}{2} T \frac{\partial}{\partial T} \left( \frac{g_{5/2}(z)}{g_{3/2}(z)} \right) \Big|_{NV}$$

Employing the series expansion, one immediately anticipates the following recursion relation:  $q'_n(z)=q_{n-1}(z)/z$ . With this one obtains

$$\frac{\partial}{\partial T} \left( \frac{g_{5/2}(z)}{g_{3/2}(z)} \right) = \frac{\partial z}{\partial T} \frac{1}{z} \left( 1 - \frac{g_{5/2}(z)g_{1/2}(z)}{g_{3/2}^2(z)} \right)$$

but the expression  $\partial z/\partial T$  can be derived as follow

$$\frac{\partial \mathbf{z}}{\partial T} \frac{1}{\mathbf{z}} \mathbf{g}_{1/2}(\mathbf{z}) = \frac{\partial}{\partial T} \mathbf{g}_{3/2}(\mathbf{z}) = \frac{\partial}{\partial T} \left( \frac{\mathbf{N} \lambda_{\tau}^{3}}{\mathbf{V}} \right) = -\frac{3}{2T} \left( \frac{\mathbf{N} \lambda_{\tau}^{3}}{\mathbf{V}} \right) = -\frac{3}{2T} \mathbf{g}_{3/2}(\mathbf{z}) \implies \frac{\partial \mathbf{z}}{\partial T} = -\frac{3\mathbf{z}}{2T} \frac{\mathbf{g}_{3/2}(\mathbf{z})}{\mathbf{g}_{1/2}(\mathbf{z})}$$

If one uses this and the previous equation one obtains

$$\frac{C_V}{Nk_B} = \frac{15}{4} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4} \frac{g_{3/2}(z)}{g_{1/2}(z)} \qquad T > T_C$$