Cold atoms

Lecture 2.

4th October, 2006

Preliminary plan for the whole fall term

Lecture 1 …	Something about everything (see next slide) The textbook version of BEC in extended systems	Sep 22
Lecture 2 …	thermodynamics, grand canonical ensemble, extended gas: ODLRO, nature of the BE phase transition	Oct 4
Lecture 3 …	atomic clouds in the traps – theory. Confined independent bosons, what is BEC?, interactions, GP equation	Oct 18
Lecture 4 …	atomic clouds in the traps – experiment. Cooling, trapping, monitoring and measuring the clouds	???
Lecture 5 …	Infinite systems: Bogolyubov-de Gennes theory, BEC and symmetry breaking, coherent states	
Lecture 6 …	Time dependent GP theory Finite systems: BEC theory preserving the particle number	

Back to Lecture 1.

A few important points from the last class

⌘ Why extreme low temperature physics: new phenomena connected with freezing out the thermal noise and with quantum coherence

⌘ Example of NDR in rhodium: temperature record and nuclear antiferromagnetism. Details in two attached documents

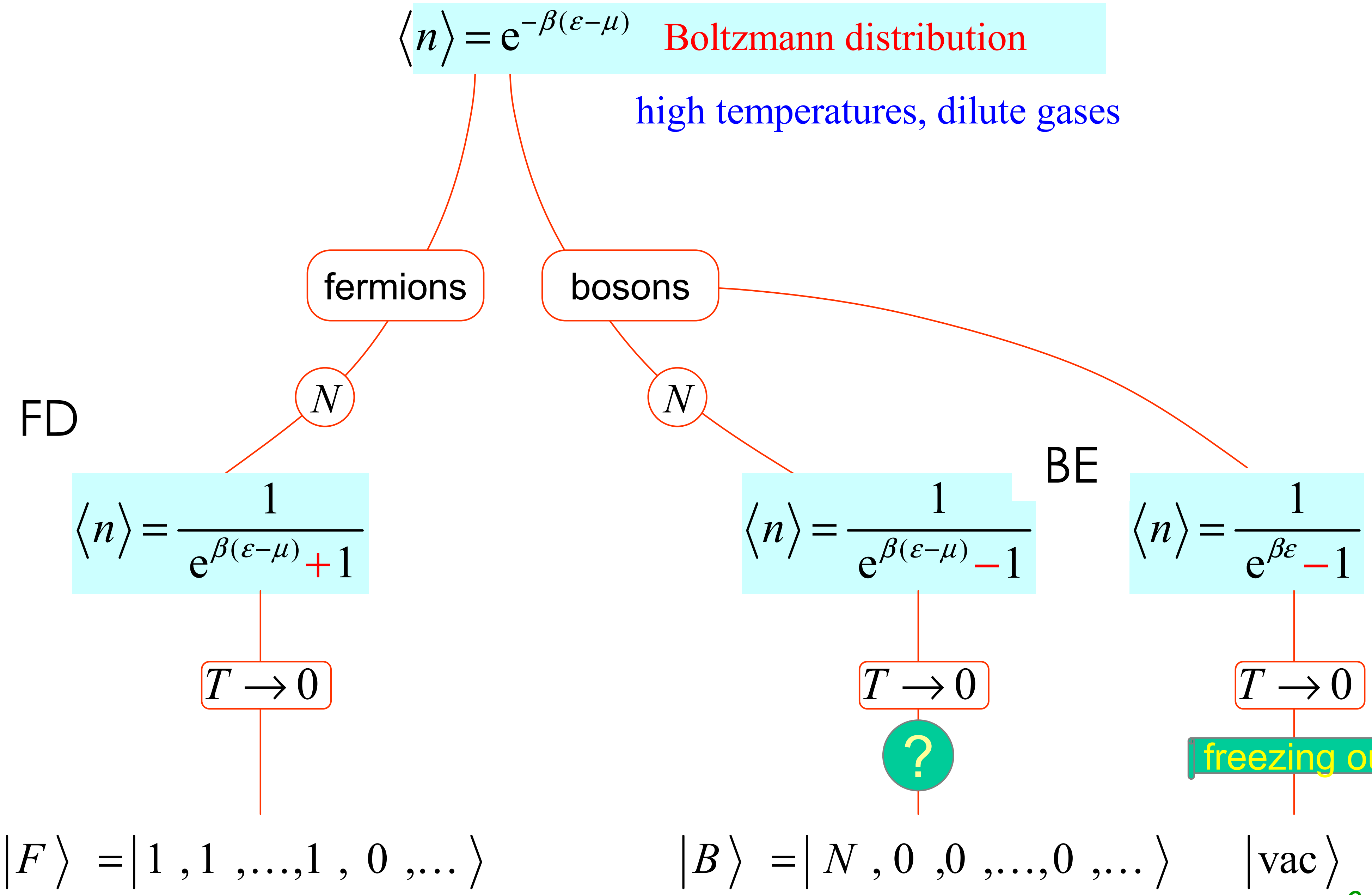
⌘ BEC in atomic clouds – a multidisciplinary task: cryogenics&LT physics, atomic physics, laser physics& spectroscopy, …

⌘ Crucial point: identical particles are quantum correlated. This changes statistics even for non-interacting particles

⌘ BEC in an extended system according to Einstein: below a critical temperature a macroscopic occupancy of the lowest one-particle level

Bose-Einstein condensation: elementary approach

L1: Ideal quantum gases at a finite temperature



$$\langle n \rangle = \mathrm{e}^{-\beta(\varepsilon-\mu)}$$ Boltzmann distribution

high temperatures, dilute gases

fermions

bosons

N

N

FD

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}+1}$$

BE

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}-1}$$

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta\varepsilon}-1}$$

$T \to 0$

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?

freezing out

$$|F\rangle = |1, 1, \ldots, 1, 0, \ldots\rangle$$

$$|B\rangle = |N, 0, 0, \ldots, 0, \ldots\rangle$$

$$|\mathrm{vac}\rangle$$

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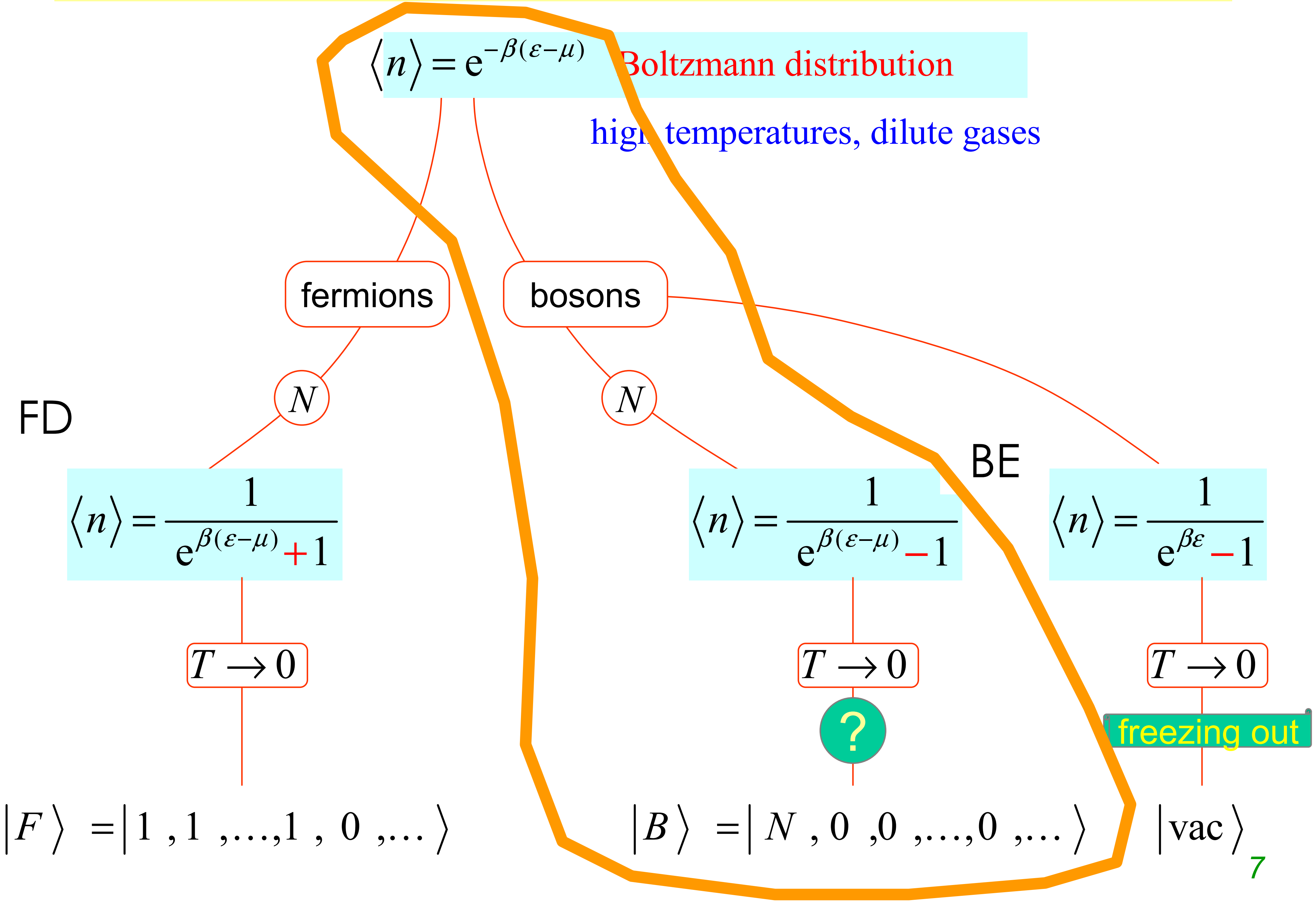

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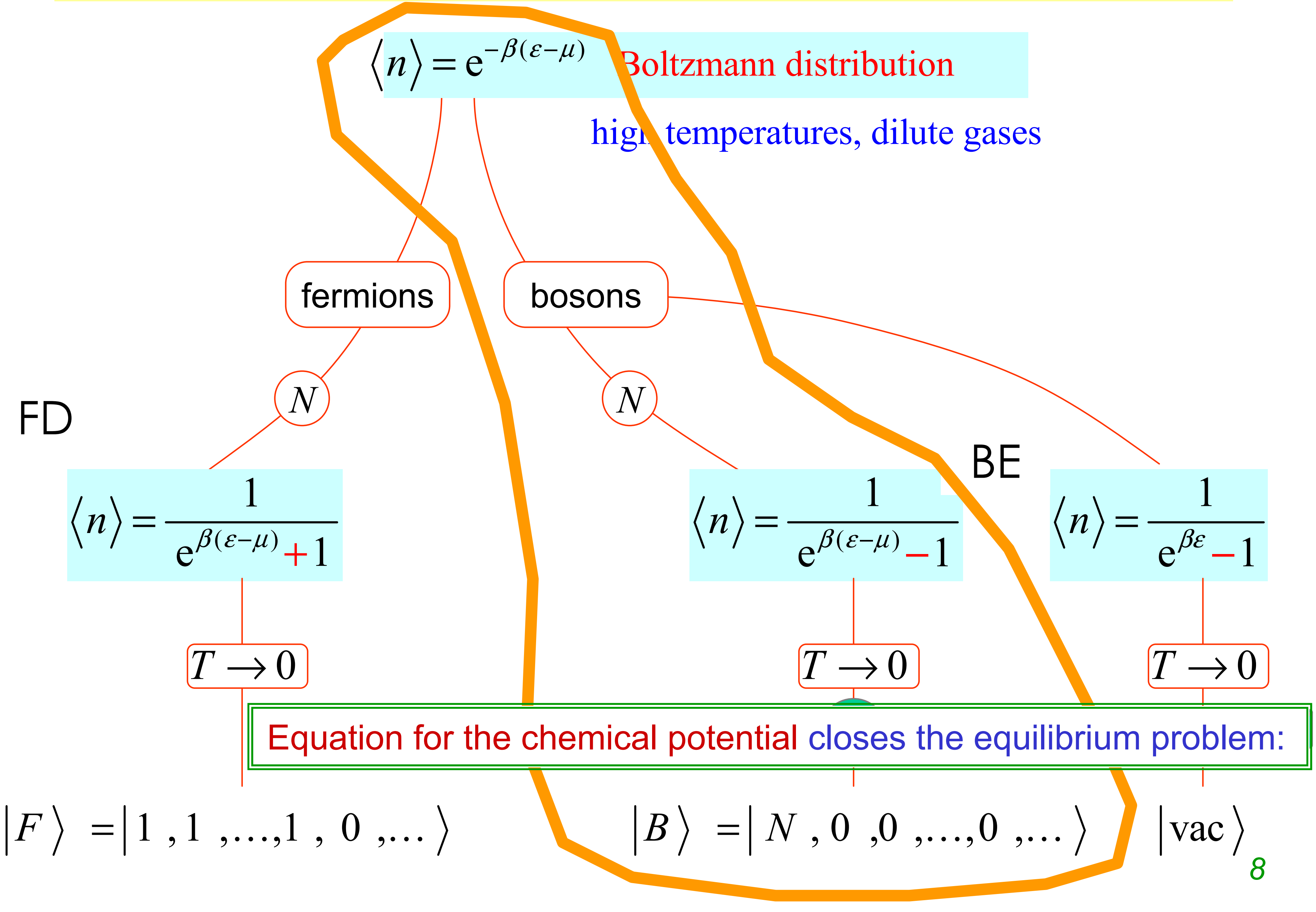

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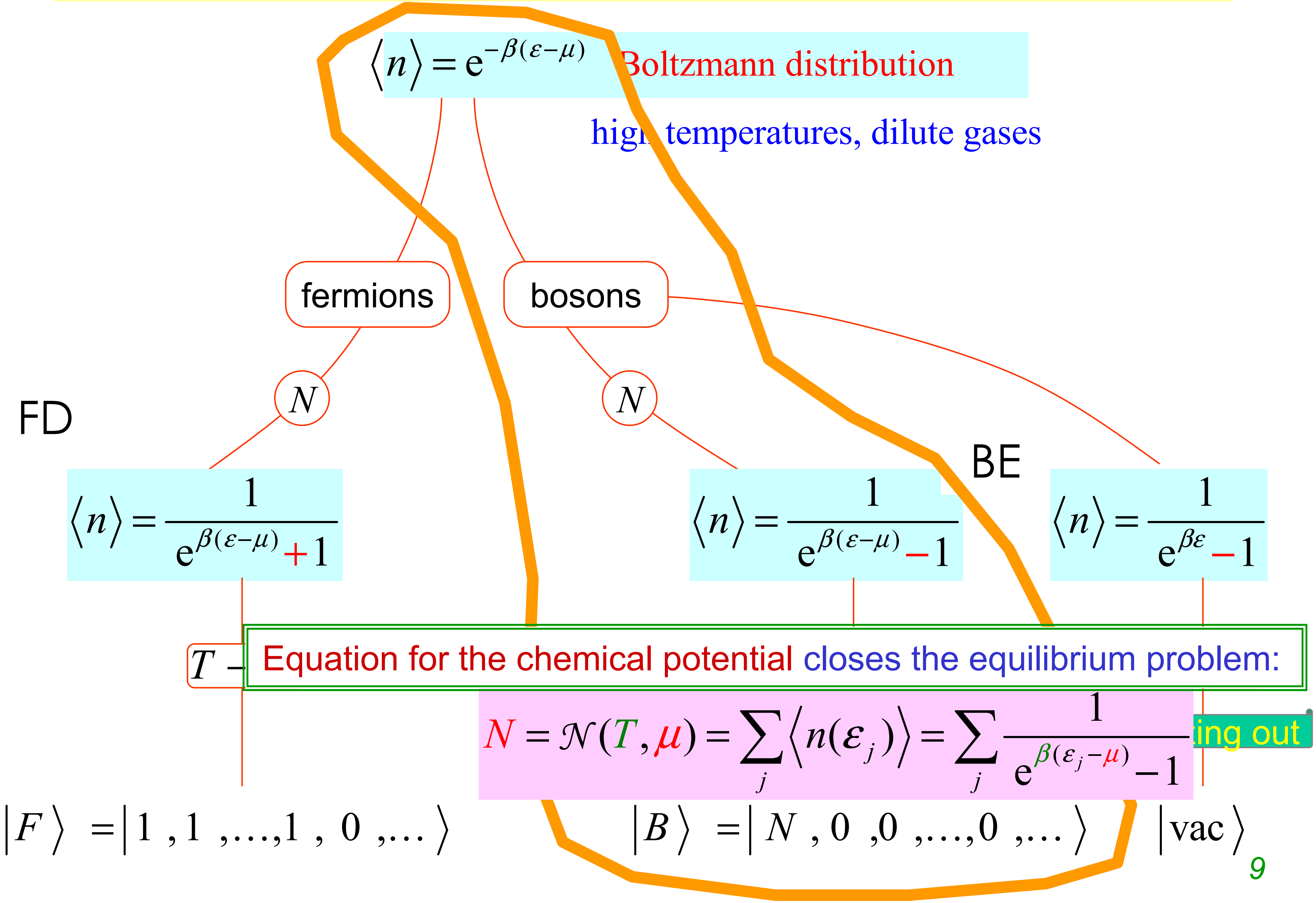

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T –

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L1: A gas with a fixed average number of atoms

Ideal boson gas (macroscopic system)

atoms: mass m, dispersion law $\varepsilon(p) = \dfrac{p^2}{2m}$

system as a whole:

volume V, particle number N, density $n = N/V$, temperature T.

Equation for the chemical potential closes the equilibrium problem:

$$N = \mathcal{N}(T,\mu) = \sum_j \langle n(\varepsilon_j) \rangle = \sum_j \frac{1}{\mathrm{e}^{\beta(\varepsilon_j - \mu)} - 1}$$

Always $\mu < 0$. At high temperatures, in the thermodynamic limit, the continuum approximation can be used:

$$N \approx V \int_0^\infty \mathrm{d}\varepsilon \frac{1}{\mathrm{e}^{\beta(\varepsilon - \mu)} - 1} \mathcal{D}(\varepsilon) \equiv \tilde{\mathcal{N}}(T,\mu)$$

$$T > T_C = \frac{h^2}{4\pi m k_B} \cdot \left(\frac{N}{2{,}612\, V} \right)^{\frac{2}{3}}$$

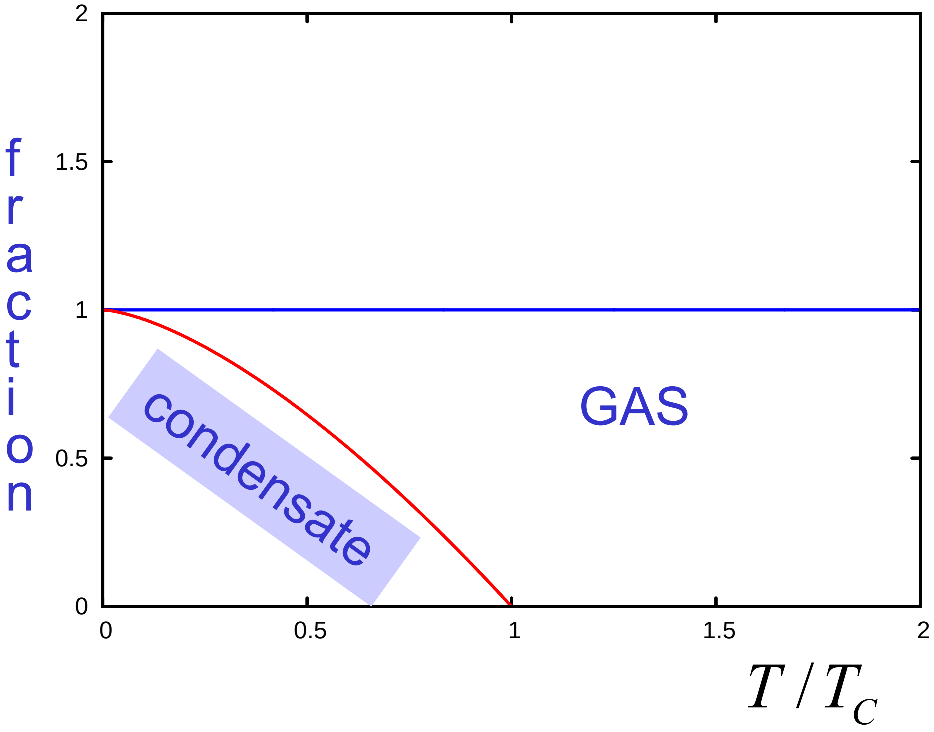
The balance equation for $T < T_C$ is

$$N = \mathcal{N}(T,\mu) = \frac{1}{\mathrm{e}^{\beta(\varepsilon_0 - \mu)} - 1} + V \int_0^\infty \mathrm{d}\varepsilon \frac{1}{\mathrm{e}^{\beta(\varepsilon - 0)} - 1} \mathcal{D}(\varepsilon)$$

L1: Condensate concentration

$$n_G = \frac{\tilde{\mathcal{N}}(T_C,0)}{V} = B\,T^{\frac{3}{2}} = n\left(\frac{T}{T_C}\right)^{\frac{3}{2}} \quad \text{for } \; T < T_C$$

$$n \equiv n_G + n_{BE} = n\left(\frac{T}{T_C}\right)^{\frac{3}{2}} + n\left[1 - \left(\frac{T}{T_C}\right)^{\frac{3}{2}}\right]$$



L1: Closer look at BEC

- Thermodynamically, this is a real phase transition, although unsual
- Pure quantum effect
- There are no real forces acting between the bosons, but there **IS** a real correlation in their motion caused by their identity (symmetrical wave functions)
- BEC has been so difficult to observe, because other (classical G/L or G/S) phase transitions set on much earlier
- BEC is a "condensation in the momentum space", unlike the usual liquefaction of classical gases, which gives rise to droplets in the coordinate space.
- This is somewhat doubtful, especially now, that the best observed BEC takes place in traps, where the atoms are significantly localized
- What is valid on the "momentum condensation": BEC gives rise to quantum coherence between very distant places, just like the usual plane wave
- BEC is a **macroscopic quantum phenomenon** in two respects:
  - ♠ it leads to a correlation between a macroscopic fraction of atoms
  - ♠ the resulting coherence pervades the whole macroscopic sample

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Off-Diagonal Long Range Order

Analysis on the one-particle level

Coherence in BEC: ODLRO

***O**ff-**D**iagonal **L**ong **R**ange **O**rder*

Without field-theoretical means, the coherence of the condensate may be studied using the **one-particle density matrix.**

Definition of OPDM for non-interacting particles: Take an additive observable, like local density, or current density. Its average value for the whole assembly of atoms in a given equilibrium state:

$$\langle X\rangle = \sum_{\alpha} \langle \alpha | X | \alpha \rangle \langle n_{\alpha} \rangle \qquad \text{double average, quantum and thermal}$$

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$$= \mathrm{Tr}\,\rho X \qquad \rho = \sum_\alpha |\alpha\rangle\langle n_\alpha\rangle\langle\alpha|$$

OPDM for homogeneous systems

In coordinate representation

$$\rho(\boldsymbol{r},\boldsymbol{r}') = \sum_{\boldsymbol{k}} \langle \boldsymbol{r} | \boldsymbol{k} \rangle \langle n_{\boldsymbol{k}} \rangle \langle \boldsymbol{k} | \boldsymbol{r}' \rangle$$

$$= \frac{1}{V} \sum_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')} \langle n_{\boldsymbol{k}} \rangle$$

- depends only on the relative position (transl. invariance)
- Fourier transform of the occupation numbers
- isotropic … provided thermodynamic limit is allowed
- in systems without condensate, the *momentum distribution* is smooth and the density matrix has a finite range.

CONDENSATE lowest orbital with $\boldsymbol{k}_0$

OPDM for homogeneous systems: ODLRO

CONDENSATE lowest orbital with $\boldsymbol{k}_0 = O(V^{-\frac{1}{3}}) \approx 0$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \underbrace{\frac{1}{V}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_0(\boldsymbol{r}-\boldsymbol{r}')}\langle n_0\rangle}_{\text{coherent across the sample}} + \underbrace{\frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle}_{FT\text{ of a smooth function has a finite range}}$$

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DISTANT OFF-DIAGONAL ELEMENT $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$

$$\rho_{\mathrm{BE}}(\boldsymbol{r}-\boldsymbol{r}') \xrightarrow{|\boldsymbol{r}-\boldsymbol{r}'|\to\infty} n_{\mathrm{BE}}$$

$$\rho_{\mathrm{G}}(\boldsymbol{r}-\boldsymbol{r}') \xrightarrow{|\boldsymbol{r}-\boldsymbol{r}'|\to\infty} 0$$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') \xrightarrow{|\boldsymbol{r}-\boldsymbol{r}'|\to\infty} n_{\mathrm{BE}}$$

Off-Diagonal Long Range Order

ODLRO

From OPDM towards the macroscopic wave function

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$$= \underbrace{\Psi(\boldsymbol{r})\Psi^*(\boldsymbol{r}')}_{\text{dyadic}} + \frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle$$

MACROSCOPIC WAVE FUNCTION

$$\Psi(\boldsymbol{r}) = \sqrt{n_{BE}}\cdot\mathrm{e}^{\mathrm{i}(\boldsymbol{k}_0\boldsymbol{r}+\varphi)}, \quad \varphi\ldots \text{ an arbitrary phase}$$

- expresses ODLRO in the density matrix
- measures the condensate density
- appears like a pure state in the density matrix, but macroscopic
- expresses the notion that the condensate atoms are in the same state
- is the order parameter for the BEC transition

From OPDM towards the macroscopic wave function

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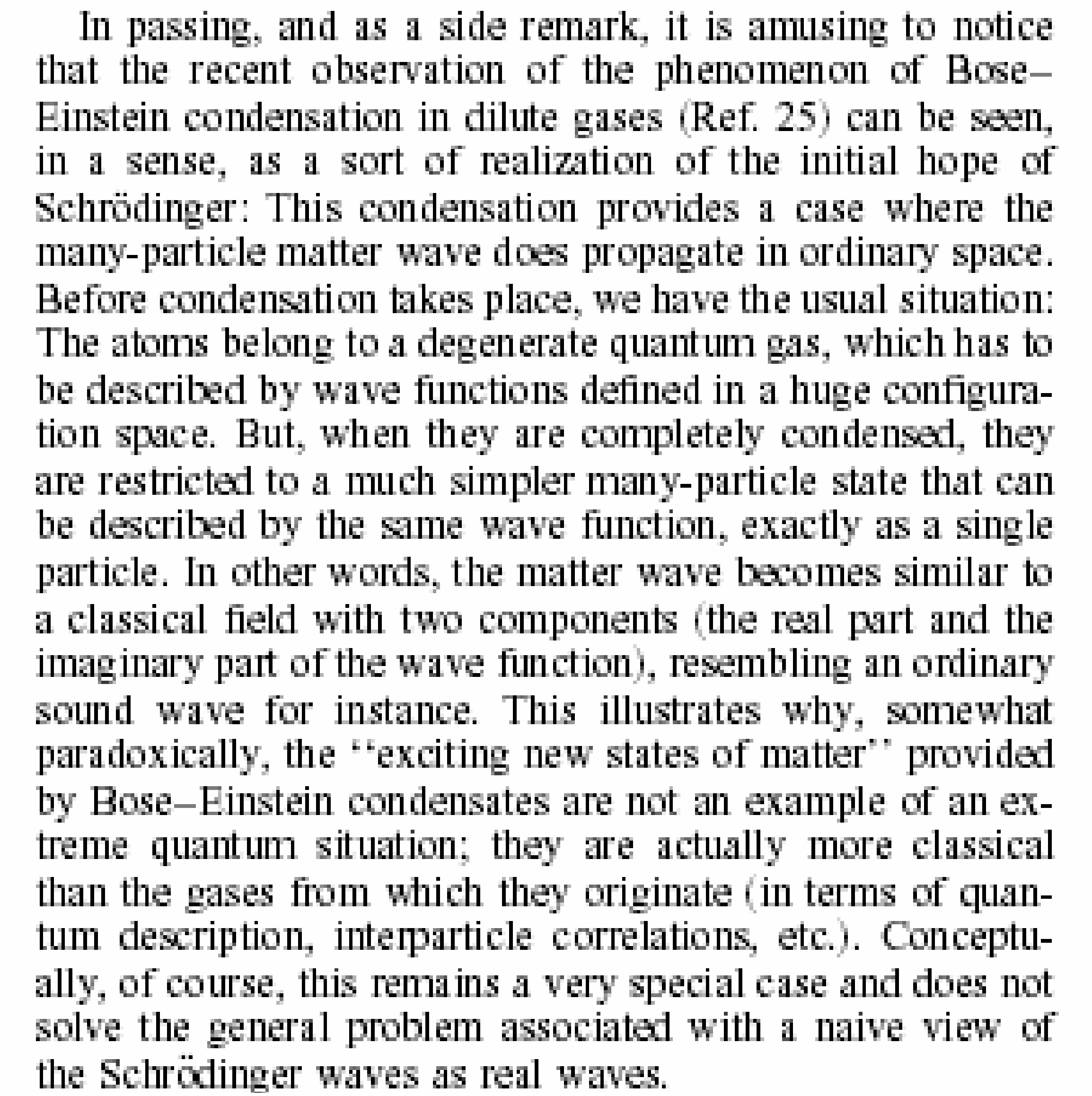
MACROSCOPIC WAVE FUNCTION

$\Psi(\boldsymbol{r}) = \sqrt{n_{BE}}\cdot\mathrm{e}^{\mathrm{i}(\boldsymbol{k}_0\boldsymbol{r}+\varphi)}, \quad \varphi\ldots$ an arbitrary phase ? **why bother?**

- expresses ODLRO in the density matrix ✓
- measures the condensate density ✓
- appears like a pure state in the density matrix, but macroscopic ✓
- expresses the notion that the condensate atoms are in the same state ? **how?**
- is the order parameter for the BEC transition ? **what is it?**

F.Laloë: Do we really understand Quantum mechanics, Am.J.Phys.**69**, 655 (2001)



In passing, and as a side remark, it is amusing to notice that the recent observation of the phenomenon of Bose–Einstein condensation in dilute gases (Ref. 25) can be seen, in a sense, as a sort of realization of the initial hope of Schrödinger: This condensation provides a case where the many-particle matter wave does propagate in ordinary space. Before condensation takes place, we have the usual situation: The atoms belong to a degenerate quantum gas, which has to be described by wave functions defined in a huge configuration space. But, when they are completely condensed, they are restricted to a much simpler many-particle state that can be described by the same wave function, exactly as a single particle. In other words, the matter wave becomes similar to a classical field with two components (the real part and the imaginary part of the wave function), resembling an ordinary sound wave for instance. This illustrates why, somewhat paradoxically, the ‘‘exciting new states of matter’’ provided by Bose–Einstein condensates are not an example of an extreme quantum situation; they are actually more classical than the gases from which they originate (in terms of quantum description, interparticle correlations, etc.). Conceptually, of course, this remains a very special case and does not solve the general problem associated with a naive view of the Schrödinger waves as real waves.

Thermodynamics of BEC

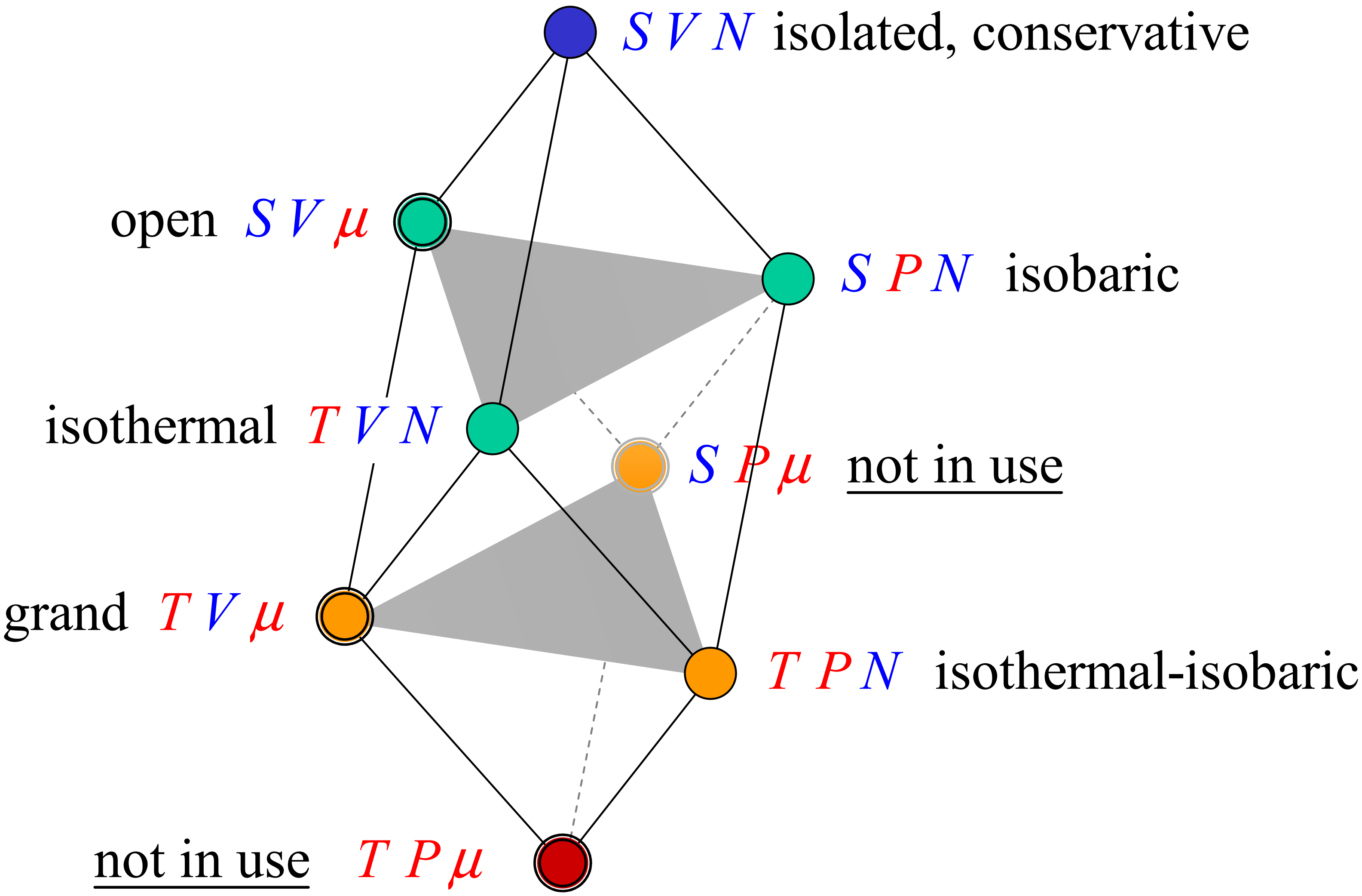
Capsule on thermodynamics
Grand canonical ensemble
Thermodynamic functions of an ideal gas
BEC in an ideal gas
Comparison with real gases/vdW equation

Homogeneous one component phase:
boundary conditions (environment) and state variables

$S\ V\ N$ additive variables, have densities $s = S/V$ $n = N/V$ "extensive"

↕ ↕ ↕

$T\ P\ \mu$ dual variables, intensities "intensive"



$S\ V\ N$ isolated, conservative

open $S\ V\ \mu$

$S\ P\ N$ isobaric

isothermal $T\ V\ N$

$S\ P\ \mu$ not in use

grand $T\ V\ \mu$

$T\ P\ N$ isothermal-isobaric

not in use $T\ P\ \mu$

Homogeneous one component phase: boundary conditions (environment) and state variables

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$\updownarrow \updownarrow \updownarrow$

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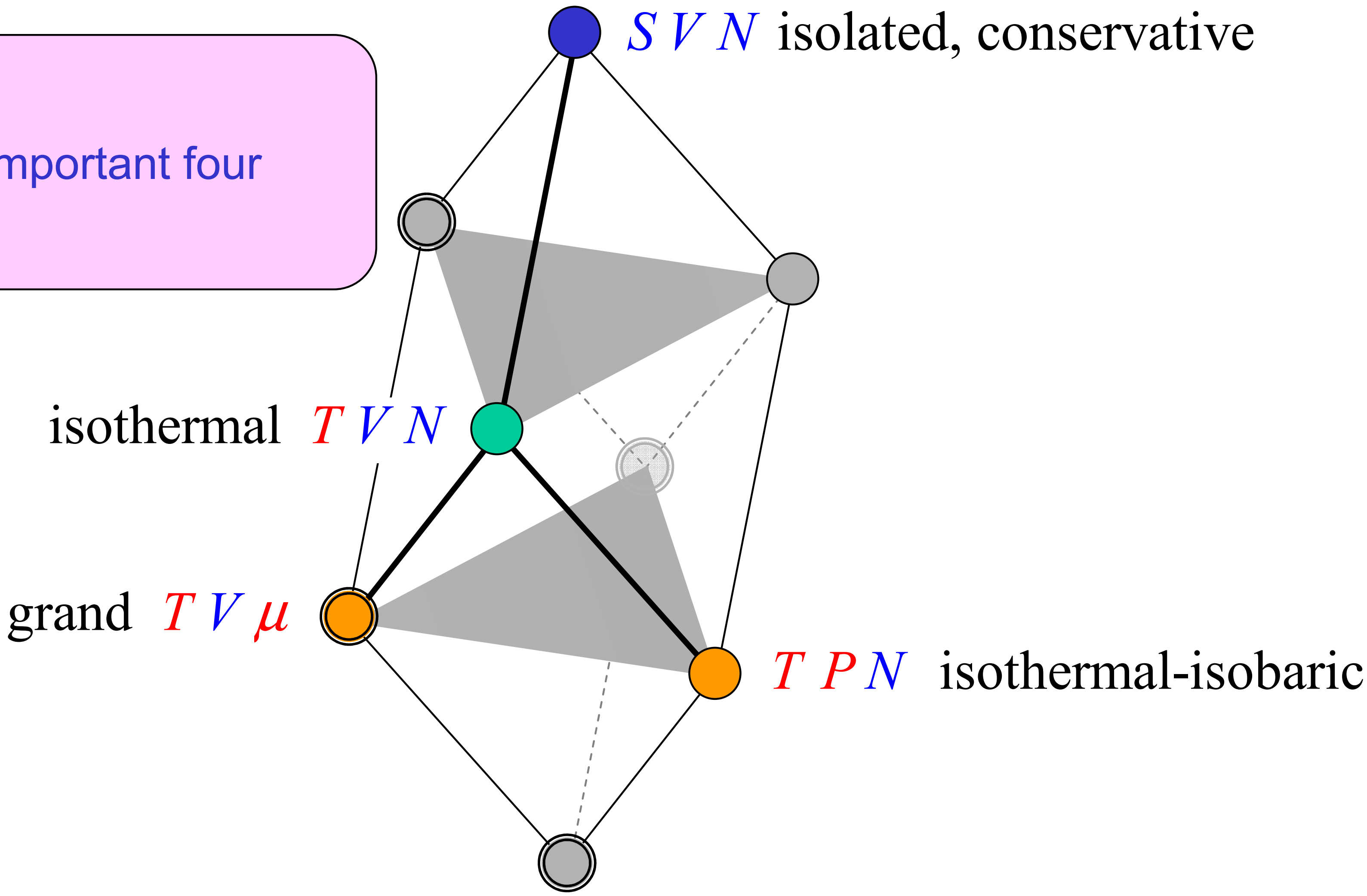
The important four



Thermodynamic potentials and all that

Basic thermodynamic identity (for equilibria)

$$\boxed{\mathrm{d}U = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N}$$

For an isolated system, $T = T(S,V,N) = \left(\frac{\partial U}{\partial S}\right)_{V,N}$, etc.

For an isothermic system, the independent variables are T, V, N.

The change of variables is achieved by means of the **Legendre transformation**. Define ***Free Energy***

$$F = U - TS,\ U = U(T,V,N),\ S = S(T,V,N), \cdots$$

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perform the substitution everywhere; this shows in the Maxwell identities (partial derivatives)

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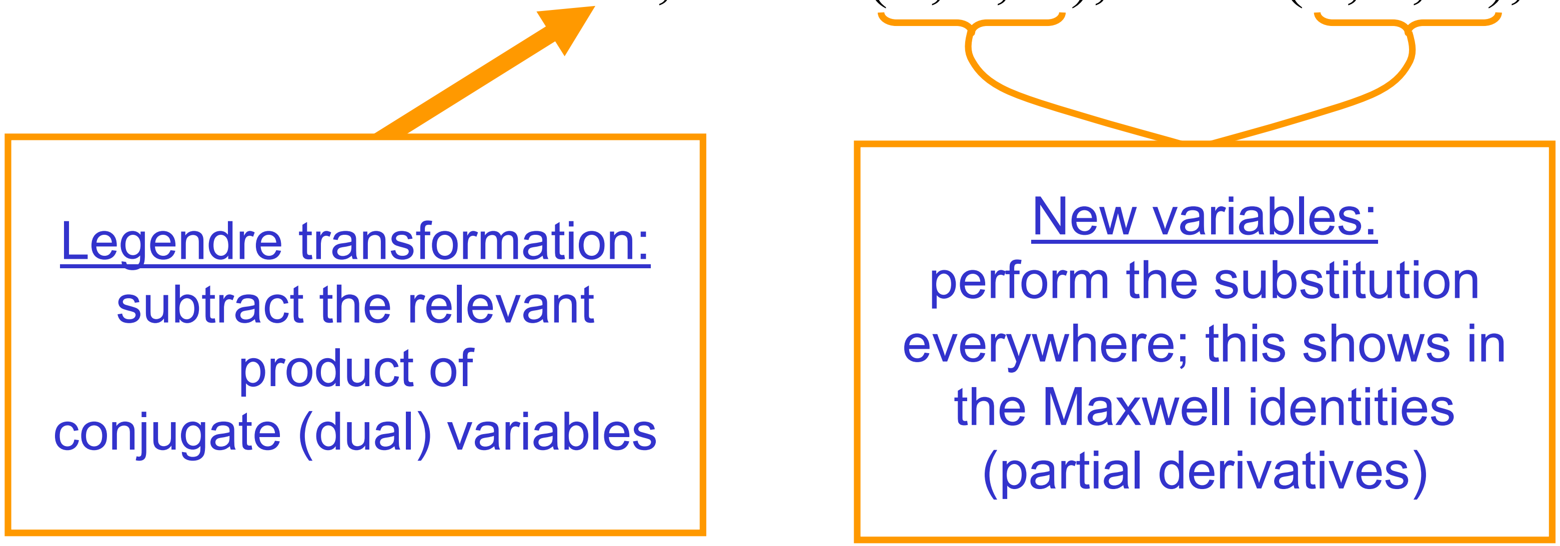

Legendre transformation:
subtract the relevant
product of
conjugate (dual) variables

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For an isolated system, $T = T(S,V,N) = \left(\frac{\partial U}{\partial \mathrm{S}}\right)_{V,N}$, etc.

For an isothermic system, the independent variables are T, S, V.

The change of variables is achieved by means of the **Legendre transformation**. Define ***Free Energy***

$$F = U - TS,\ U = U(T,V,N),\ S = S(T,V,N), \cdots$$

$$\mathrm{d}F = -S\,\mathrm{d}T - P\,\mathrm{d}V + \mu\,\mathrm{d}N$$

$$S = \left(\frac{\partial F}{\partial \mathrm{T}}\right)_{V,N},\ \text{etc.}$$

A table

isolated system	microcanonical ensemble	S, V, N
internal energy	U	$\mathrm{d}U = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N$

isothermic system	canonical ensemble	T, V, N
free energy	$F = U - TS$	$\mathrm{d}F = -S\,\mathrm{d}T - P\,\mathrm{d}V + \mu\,\mathrm{d}N$

isothermic-isobaric system	isothermic-isobaric ensemble	T, P, N
free enthalpy	$\Phi = U - TS + PV \equiv \mu N$	$\mathrm{d}\Phi = -S\,\mathrm{d}T + V\,\mathrm{d}P + \mu\,\mathrm{d}N$

isothermic open system	grand canonical ensemble	T, V, μ
grand potential	$\Omega = U - TS - \mu N \equiv -PV$	$\mathrm{d}\Omega = -S\,\mathrm{d}T - P\,\mathrm{d}V - N\,\mathrm{d}\mu$

How comes $\Omega = -PV$? Ω is additive, V is the only additive independent variable. Thus,

$$\Omega = \omega(T, \mu) \times V, \quad \omega(T, \mu) = \left(\frac{\partial \Omega}{\partial V}\right)_{T,\mu} = -P$$

Similar consideration holds for $\Phi = \varphi(T, P) \cdot N$

Digression: which environment to choose?

THE ENVIRONMENT IN THE THEORY SHOULD CORRESPOND
TO THE EXPERIMENTAL CONDITIONS

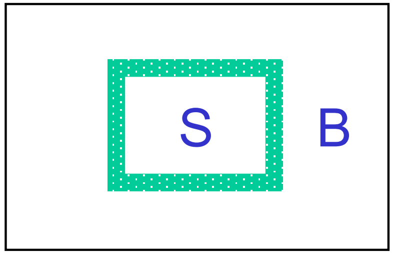
… a truism difficult to satisfy

❶ For large systems, this is not so sensitive for two reasons

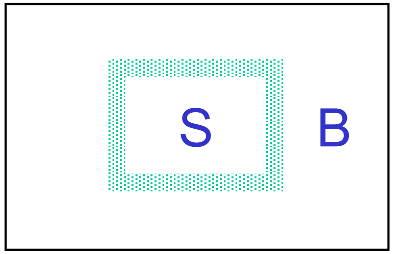
- System serves as a thermal bath or particle reservoir all by itself
- Relative fluctuations (distinguishing mark) are negligible

❷

	<u>Adiabatic system</u>	<u>Real system</u>	<u>Isothermal system</u>
SB heat exchange –	the slowest	medium fast process	the fastest



- temperature lag
- interface layer



❸ Atoms in a trap: ideal model … isolated. In fact: unceasing energy exchange (laser cooling). A small number of atoms may be kept (one to, say, 40). With 10^7, they form a bath already. Besides, they are cooled by evaporation and they form an open (albeit non-equilibrium) system.

❹ Sometime, $N=\text{const.}$ crucial (persistent currents in non-SC mesoscopic rings)

Grand canonical ensemble

Definition following Gibbs
General treatment for independent particles
Thermodynamic functions of an ideal gas
BEC in an ideal gas
Comparison with real gases/vdW equations

Grand canonical ensemble - definition

Grand canonical ensemble admits both energy and particle number exchange between the system and its environment.

The statistical operator (many body density matrix) $\hat{\rho}$ acts in the Fock space

External variables are T, V, μ. They are specified by the conditions

$$\left\langle \hat{H} \right\rangle \equiv \mathrm{Tr}\,\hat{\rho}\hat{H} = U \qquad V = \text{ sharp} \qquad \left\langle \hat{N} \right\rangle \equiv \mathrm{Tr}\,\hat{\rho}\hat{N} = N$$

$$S = -k_{\mathrm{B}} \cdot \mathrm{Tr}\,\hat{\rho} \ln \hat{\rho} = \max$$

Grand canonical statistical operator has the Gibbs' form

$$\boxed{\hat{\rho} = Z^{-1}\,\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}$$

$$Z(\beta,\mu,V) = \mathrm{Tr}\,\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} \equiv \mathrm{e}^{-\beta\Omega(\beta,\mu,V)} \quad \text{statistical sum}$$

$$\Omega(\beta,\mu,V) = -k_{\mathrm{B}}T \ln Z(\beta,\mu,V) \quad \text{grand canonical potential}$$

Grand canonical ensemble – general definition

Grand canonical ensemble admits both energy and particle number exchange between the system and its environment.

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volume … for an extended homogeneous system

V … generic for generalized coordinates of external fields whose change is connected with the mechanical work done by the system

Grand canonical ensemble – finite systems

Grand canonical ensemble admits both energy and particle number exchange between the system and its environment.

The statistical operator (many body density matrix) $\hat{\rho}$ acts in the Fock space

External variables are $T, \{\Xi\}, \mu$ They are specified by the conditions

$$\left\langle \hat{H} \right\rangle \equiv \mathrm{Tr}\,\hat{\rho}\hat{H} = U \qquad \{\Xi\} = \text{ sharp} \qquad \left\langle \hat{N} \right\rangle \equiv \mathrm{Tr}\,\hat{\rho}\hat{N} = N$$

$$S = -k_{\mathrm{B}} \cdot \mathrm{Tr}\,\hat{\rho} \ln \hat{\rho} = \max$$

In fact, the external variables T, μ are properties of the bath/reservoir. They are *imposed* on the system and have meaning even for small systems .

. ***one particle has a temperature – that of the bath***

Fluctuations I. – global quantities

Fluctuations of the total number of particles around the mean value

First derivative of the grand potential

$$\frac{\partial \Omega}{\partial \mu} = \frac{\partial}{\partial \mu}\left(-k_\mathrm{B} T \ln Z\right) = -k_\mathrm{B} T \frac{\partial}{\partial \mu} \ln \mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} = -\frac{\mathrm{Tr}\, \hat{N}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}} = -\left\langle \hat{N} \right\rangle$$

Second derivative of the grand potential

$$\frac{\partial^2 \Omega}{\partial \mu^2} = -\frac{\partial}{\partial \mu}\left\langle \hat{N} \right\rangle = -\frac{\partial}{\partial \mu}\frac{\mathrm{Tr}\, \hat{N}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}} =$$

$$= -\frac{\mathrm{Tr}\, \hat{N}^2\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}} + \frac{(\mathrm{Tr}\, \hat{N}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})})^2}{(\mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})})^2} = -\left\langle \hat{N}^2 \right\rangle + \left\langle \hat{N} \right\rangle^2$$

Final estimate for the relative fluctuation

$$\boxed{\frac{\left\langle \hat{N}^2 \right\rangle - \left\langle \hat{N} \right\rangle^2}{\left\langle \hat{N} \right\rangle^2} = \frac{\frac{\partial}{\partial \mu}\left\langle \hat{N} \right\rangle}{\left\langle \hat{N} \right\rangle^2} = O\left(\left\langle \hat{N} \right\rangle^{-1}\right)}$$

Useful identities

Calculate $\frac{\partial \Omega}{\partial T}$ in two ways.

$$\frac{\partial \Omega}{\partial T} = \frac{\partial}{\partial T}\left(-k_{\mathrm{B}} T \ln Z\right) = -k_{\mathrm{B}} \ln Z - k_{\mathrm{B}} T \frac{\partial}{\partial T} \ln Z$$

$$= -k_{\mathrm{B}} \ln Z - k_{\mathrm{B}} T \frac{1}{Z} \frac{\partial}{\partial T} Z = -k_{\mathrm{B}} \ln Z - k_{\mathrm{B}} T \frac{\partial \beta}{\partial T} \frac{1}{Z} \cdot \frac{\partial}{\partial \beta} Z =$$

$$= \frac{1}{T} \Omega - \frac{1}{T} \mathrm{Tr}\, \hat{\rho} (\hat{H} - \mu \hat{N}) = \begin{cases} \dfrac{1}{T}\left(\Omega - \left\langle \hat{H} \right\rangle + \mu \left\langle \hat{N} \right\rangle\right) \\ +k_{\mathrm{B}}\, \mathrm{Tr}\, \hat{\rho} \left\{ \underbrace{-\ln Z - \dfrac{1}{k_{\mathrm{B}} T} (\hat{H} - \mu \hat{N})}_{\boxed{\ln \hat{\rho}}} \right\} \equiv -S \end{cases}$$

$$\Omega = \left\langle \hat{H} \right\rangle - TS - \mu \left\langle \hat{N} \right\rangle, \quad S = -\left(\frac{\partial \Omega}{\partial T} \right)_{\mu, V}$$

Grand canonical statistical sum for independent bosons

Recall

$$\left|\underline{Z(\beta,\mu,V)} = \underline{\mathrm{Tr}\,\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}\right| \equiv \mathrm{e}^{-\beta\Omega(\beta,\mu,V)} \quad \text{statistical sum}$$

$$= \sum_{\ell} \mathrm{e}^{-\beta(E_\ell - \mu N_\ell)} \qquad \ell \ldots \text{ eigenstate label } \ell \equiv \{n_\alpha\} \text{ with } \sum_{\alpha} n_\alpha = N_\ell$$

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$$=\sum_{\ell}\mathrm{e}^{-\beta(E_\ell-\mu N_\ell)}$$ $\ell\ldots$ eigenstate label $\ell\equiv\{n_\alpha\}$ with $\sum_\alpha n_\alpha = N_\ell$

$$=\sum_{\{n_\alpha\}}\mathrm{e}^{-\beta\sum_\alpha(\varepsilon_\alpha-\mu)n_\alpha} = \sum_{\{n_\alpha\}}\prod_\alpha\left(\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}\right)^{n_\alpha}$$ up to here trivial

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TRICK!! $$= \prod_\alpha \sum_{n_\alpha} \left(\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}\right)^{n_\alpha} = \prod_\alpha \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}}$$

$\mathrm{e}^{\beta\mu} \equiv z$ activity

fugacity

Grand canonical statistical sum for independent bosons

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$$Z(\beta,\mu,V) = \prod_\alpha\frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}} \equiv \prod_\alpha\frac{1}{1-z\,\mathrm{e}^{-\beta\varepsilon_\alpha}}$$

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Grand canonical statistical sum for independent bosons

Recall

$$\underline{\left| Z(\beta,\mu,V) \right.} = \underline{\left. \mathrm{Tr}\,\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} \right|} \equiv \mathrm{e}^{-\beta\Omega(\beta,\mu,V)}$$ statistical sum

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$$Z(\beta,\mu,V) = \prod_\alpha \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}} \equiv \prod_\alpha \frac{1}{1-z\,\mathrm{e}^{-\beta\varepsilon_\alpha}}$$

$$\Omega(\beta,\mu,V) = -k_{\mathrm{B}}T \ln Z(\beta,\mu,V)$$ grand canonical potential

$$= +k_{\mathrm{B}}T \sum_\alpha \ln\left(1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}\right)$$

$$= +k_{\mathrm{B}}T \sum_\alpha \ln\left(1-z\,\mathrm{e}^{-\beta\varepsilon_\alpha}\right)$$

Grand canonical statistical sum for independent bosons

Recall

$$Z(\beta,\mu,V)=\mathrm{Tr}\,\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\equiv\mathrm{e}^{-\beta\Omega(\beta,\mu,V)}$$

statistical sum

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up to here trivial

TRICK!!

$$=\prod_{\alpha}\sum_{n_\alpha}\left(\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}\right)^{n_\alpha}=\prod_{\alpha}\frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}}$$

$\mathrm{e}^{\beta\mu}\equiv z$ activity

fugacity

$$Z(\beta,\mu,V)=\prod_{\alpha}\frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}}\equiv\prod_{\alpha}\frac{1}{1-z\,\mathrm{e}^{-\beta\varepsilon_\alpha}}$$

$$\Omega(\beta,\mu,V)=-k_{\mathrm{B}}T\ln Z(\beta,\mu,V)$$

grand canonical potential

$$=+k_{\mathrm{B}}T\sum_{\alpha}\ln\left(1-\mathrm{e}^{-\beta(\varepsilon_\alpha-\mu)}\right)$$

$$=+k_{\mathrm{B}}T\sum_{\alpha}\ln\left(1-z\,\mathrm{e}^{-\beta\varepsilon_\alpha}\right)$$

valid for
- extended "infinite" gas
- parabolic traps
just the same

Thermodynamic functions for an extended Bose gas

For Born-Karman periodic boundary conditions, the lowest level is

$$\varepsilon(\boldsymbol{k}=\boldsymbol{0})=0$$

Its contribution has to be singled out, like before:

$$e^{\beta\mu} \equiv z$$

activity

fugacity

① $$\beta\Omega(T,\mu,V)=\ln(1-z)+V\int_0^\infty \mathrm{d}\varepsilon\,\ln(1-z\,e^{-\beta\varepsilon})\,\mathcal{D}(\varepsilon)$$

② $$N(T,\mu,V)=\frac{z}{1-z}+V\int_0^\infty \mathrm{d}\varepsilon\,\frac{1}{z^{-1}\,e^{\beta\varepsilon}-1}\,\mathcal{D}(\varepsilon)$$

③ $$U(T,\mu,V)=+V\int_0^\infty \mathrm{d}\varepsilon\,\frac{\varepsilon}{z^{-1}\,e^{\beta\varepsilon}-1}\,\mathcal{D}(\varepsilon)$$

3D DOS

$$\mathcal{D}(\varepsilon)=2\pi\left(\frac{2m}{h^2}\right)^{\frac{3}{2}}\cdot\sqrt{\varepsilon}$$

HOW TO PROCEED

Start from ②. This we **did** already. Below *TC*,

$$\frac{z}{1-z}=N_{\mathrm{BE}} \Rightarrow z\approx 1-0,\ \ln\left(1-z\right)\approx \ln N_{\mathrm{BE}}=\mathrm{O}\left(\ln V\right)$$

Thus, the singular term in ① **is negligible** for $V \to \infty$, there is none in ③

Thermodynamic functions for an extended Bose gas

The following equation of state results

①* $$P(T,\mu,V) = -2\pi\left(2mh^{-2}\right)^{\frac{3}{2}} k_{\mathrm{B}}T \int_0^\infty \mathrm{d}\varepsilon \ln(1 - z\,\mathrm{e}^{-\beta\varepsilon}) \cdot \varepsilon^{\frac{1}{2}}$$

Integrating by parts, Eqs. ① and ③ are found as nearly identical

③* $$PV = \tfrac{2}{3}U$$

This is an extension of the result known for classical gases

Series expansion

$$P = -2\pi\left(2mh^{-2}\right)^{\frac{3}{2}} k_{\mathrm{B}}T \int_0^\infty \mathrm{d}\varepsilon \ln(1 - z\,\mathrm{e}^{-\beta\varepsilon}) \cdot \varepsilon^{\frac{1}{2}} = \cdots \int_0^\infty \mathrm{d}\varepsilon \sum \frac{1}{n}(z\,\mathrm{e}^{-\beta\varepsilon})^n \cdot \varepsilon^{\frac{1}{2}}$$

$$= \cdots \sum \frac{z^n}{n} \int_0^\infty \mathrm{d}\varepsilon (\mathrm{e}^{-\beta\varepsilon})^n \varepsilon^{\frac{1}{2}}$$

①** $$\boxed{\boxed{\frac{P}{k_{\mathrm{B}}T} = \lambda^{-3} g_{5/2}(z)} \quad \lambda = h(2\pi m k_{\mathrm{B}}T)^{-\frac{1}{2}} \quad g_{5/2}(z) = \sum_1^\infty \frac{z^p}{p^{5/2}}}$$

Thermodynamic functions for an extended Bose gas

Similar expansions:

$$\boxed{\frac{N}{V} = \frac{z}{1-z} + \lambda^{-3} g_{3/2}(z)} \qquad \lambda = h(2\pi m k_B T)^{-\frac{1}{2}} \qquad g_{3/2}(z) = \sum_1^\infty \frac{z^p}{p^{3/2}}$$

$$\boxed{\frac{U}{V} = \frac{3}{2} k_B T \cdot \lambda^{-3} g_{5/2}(z)} \qquad \lambda = h(2\pi m k_B T)^{-\frac{1}{2}} \qquad g_{5/2}(z) = \sum_1^\infty \frac{z^p}{p^{5/2}}$$

Suitable for numerical studies above the critical temperature

Results simplify in the condensation region: $z = 1,\ \lambda^{-3} = \Lambda \cdot \left(k_B T\right)^{3/2}$

and all temperature dependences are explicit.

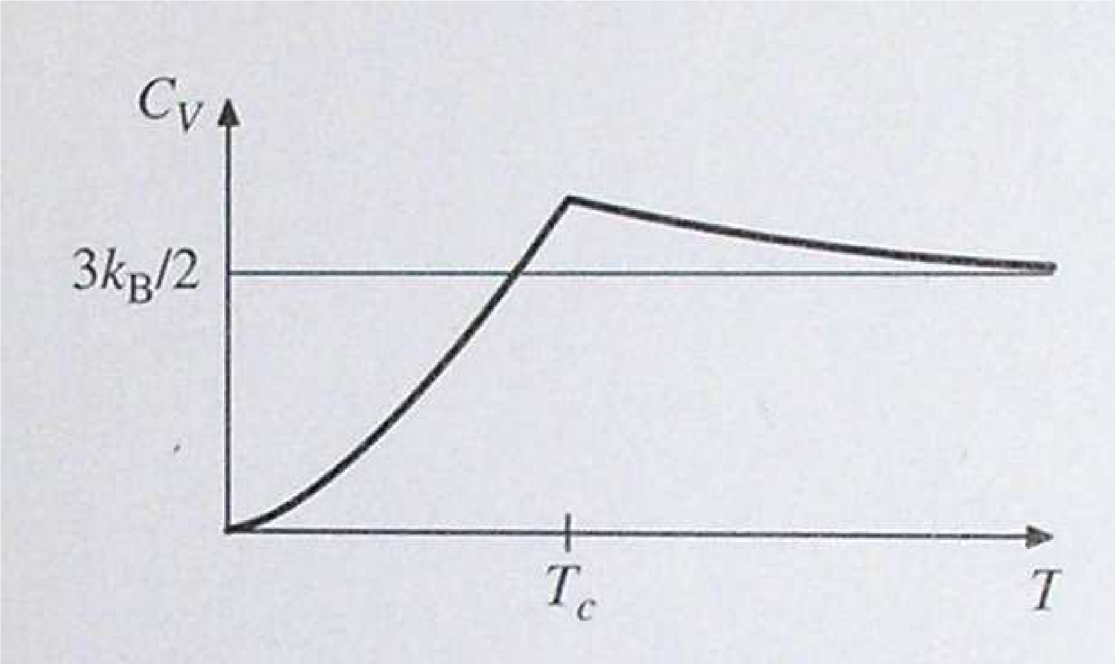
$$\frac{N}{V} = \frac{N_{BE}}{V} + \Lambda g_{3/2}(1) \cdot \left(k_B T\right)^{3/2}$$

$$\frac{U}{V} = \frac{3}{2} \Lambda g_{5/2}(1) \cdot \left(k_B T\right)^{5/2}$$

$$P = \Lambda g_{5/2}(1) \cdot \left(k_B T\right)^{5/2}$$

Specific heat

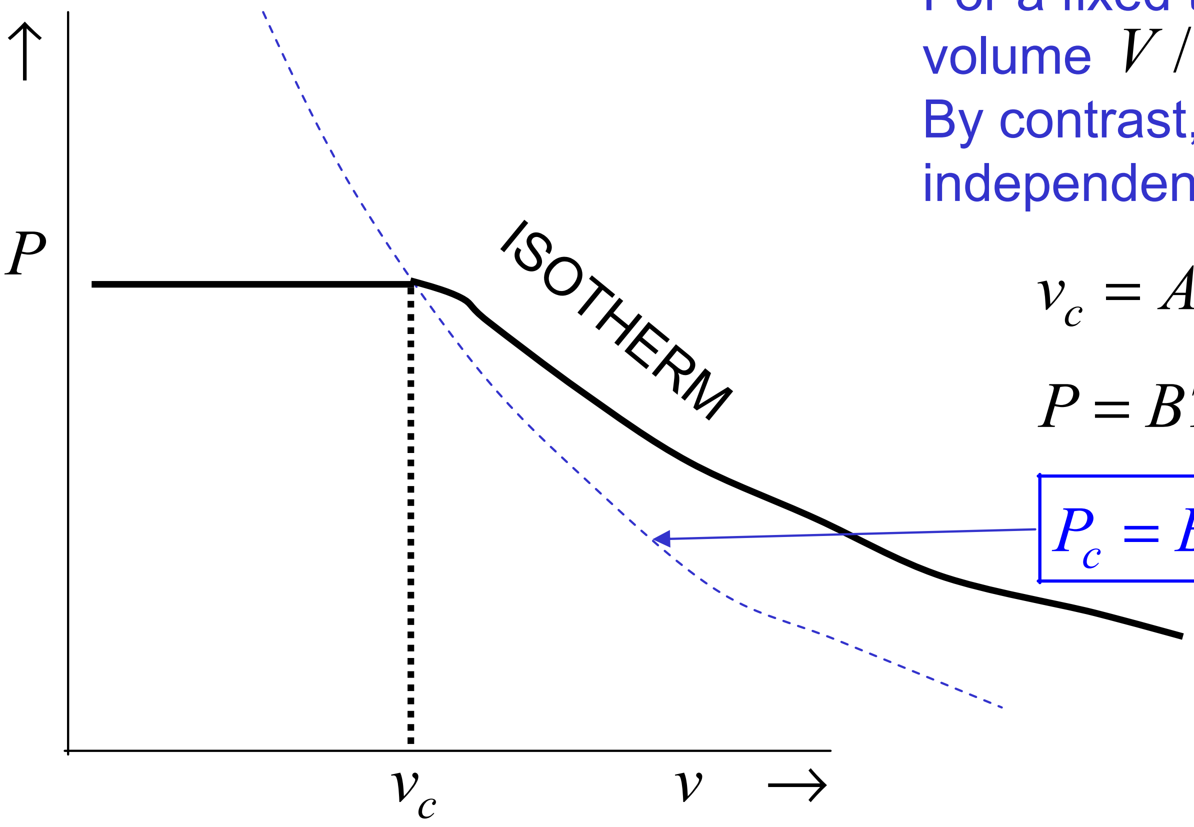
$$C_V = \left.\frac{\partial(U/N)}{\partial T}\right|_{V,N}$$



A weak singularity …

what decides is the coexistence of two phases

Isotherms in the P-V plane



For a fixed temperature, the specific volume V/N can be arbitrarily small. By contrast, the pressure is volume independent …typical for condensation

$$v_c = AT^{-3/2} \qquad T = \left(v_c / A\right)^{-2/3}$$

$$P = BT^{5/2}$$

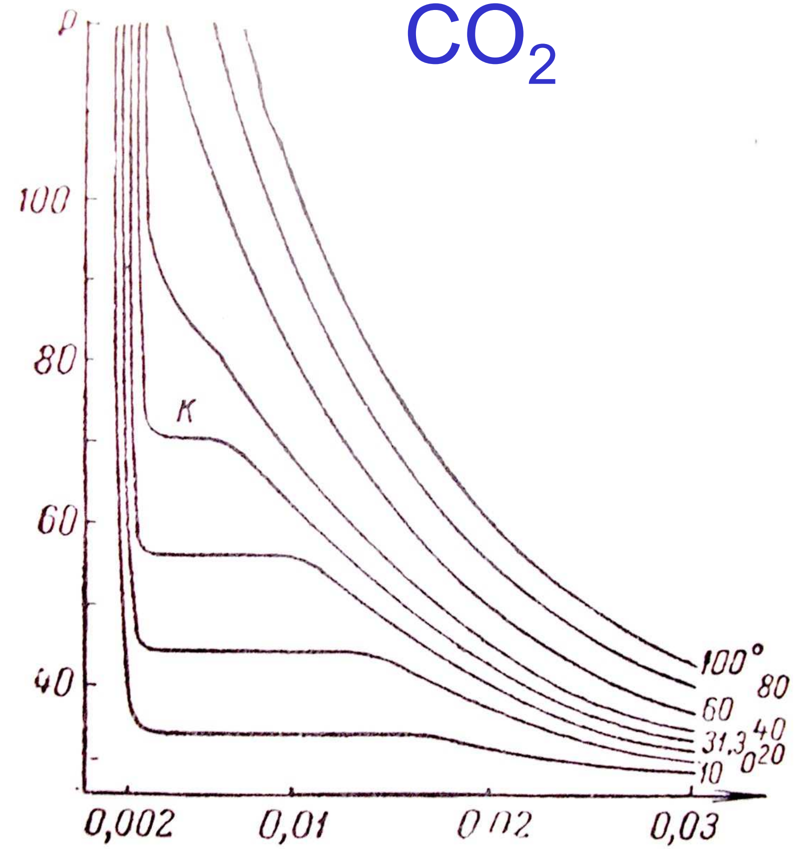
$$\boxed{P_c = BA^{5/3} \cdot v_c^{-5/3}}$$

$$\frac{N}{V} = \frac{N_{\mathrm{BE}}}{V} + \Lambda g_{3/2}(1) \cdot \left(k_{\mathrm{B}}T\right)^{3/2}$$

$$P = \Lambda g_{5/2}(1) \cdot \left(k_{\mathrm{B}}T\right)^{5/2}$$

Compare with condensation of a real gas

CO_2



Obr. 151. Pokusně získané isothermy kysličníku uhličitého (CO_2).

Basic similarity:

increasing pressure with compression

critical line

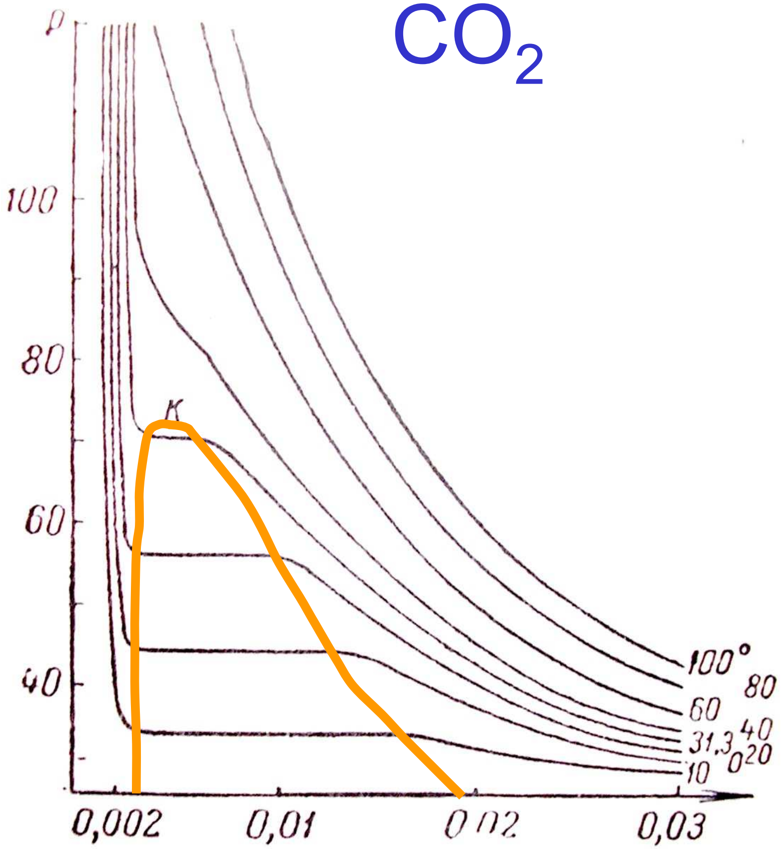
beyond is a plateau

Differences:

at high pressures

at high compressions

Compare with condensation of a real gas



CO_2

Obr. 151. Pokusně získané isothermy kysličníku uhličitého (CO_2).

Basic similarity:

increasing pressure with compression

critical line

beyond is a plateau

Differences:

no critical point

⇒ at high pressures

⇒at high compressions

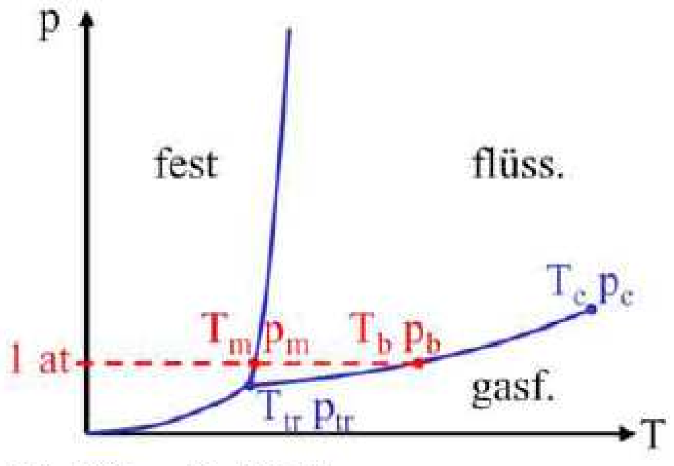
Conclusion:

BEC in a gas is a phase transition

of the first order

What will be the analogue for BEC?

Cryogenic Liquids



Substance	T_b [K]	T_m [K]	T_{tr} [K]	P_{tr} [bar]	T_c [K]	P_c [bar]
	@ 1 bar					
H_2O	373.15	273.15	273.16	0.06	647.3	220
Xe	165.1	161.3	161.4	0.82	289.8	58.9
Kr	119.9	115.8	114.9	0.73	209.4	54.9
O_2	90.2	54.4	54.36	0.016	154.3	50.4
Ar	87.3	83.8	83.81	0.67	150.9	48.7
N_2	77.4	63.3	63.15	0.12	126.0	33.9
Ne	27.1	24.5	24.56	0.43	44.5	27.2
D_2	23.7	18.7	18.72	0.17	38.3	16.6
H_2	20.3	14.0	13.80	0.07	33.3	13.0
^{4}He	4.21	--	--	--	5.20	2.28
^{3}He	3.19	--	--	--	3.32	1.16

The end

Problems

Problems to Lecture 1.

Some problems are expanding on the presented subject matter and are voluntary… (*)

The other ones are directly related to the theme of the class and are to be worked out within a week. The solutions will be presented on the next seminar and posted on the web.

(1.1*) Problems with metastable states and quasi-equilibria in defining the temperature and applying the 3rd law of thermodynamics T_c

(1.2*) Relict radiation and the Boomerang Nebula

(1.3) Work out in detail the integral defining

(1.4) Extend the resulting series expansion to the full balance equation (BE integral)

(1.5) Modify for a 2D gas and show that the BE condensation takes never place

(1.6) Obtain an explicit procedure for calculating the one-particle density matrix for an ideal boson gas [*difficult*]

Problems to Lecture 2.

Some problems are expanding on the presented subject matter and are voluntary… (*)

The other ones are directly related to the theme of the class and are to be worked out within a week. The solutions will be presented on the next seminar and posted on the web.

(2.1*) How was measured the record temperature of the order of 100 pK?

(2.2*) The BE distribution can be obtained from a combinatorial analysis of microstates of the system with the subsequent use of the Stirling formula. Which is the least number of the particles, for which the limit makes sense? (see the example for Boltzmann in *Blatt*).

(2.3) Extend the integrals from problem (1,4) to all thermodynamic quantities

(2.4) Obtain the entropy for BE gas. Below the transition, it should display the two phases

(1.5) Fluctuations of $\langle n_\alpha \rangle$

(1.6) Phase diagram in $p - V$ coordinates for BEC [*difficult*]

* * *