UNIVERSITY OF WARSAW

2. BEC in ideal gas

2.1. BE distribution

•) recall, gas of noninteracting/ideal bosons

$$H = \sum_p p^2 a_p^* a_p \quad \leftrightsquigarrow \quad H_N = \sum_{j=1}^{N} (-\Delta_{x_j})$$

on $L^2_{sym}(\Omega^N)$ in the latter case (canonical) or
on $F(L^2(\Omega))$ in former (grand-canonical)
$\Omega = [0,L]^3$ with p.b.c.

•) we now stick to the grand canonical ensemble and let us compute $\langle a_p^* a_p \rangle \equiv \langle n_p \rangle$
By definition

$$\langle n_p \rangle = \mathrm{Tr}\left(n_p \frac{e^{-\beta(H-\mu N)}}{Z} \right)$$

$$-\beta(H-\mu N) = -\beta \sum_p (p^2-\mu) a_p^* a_p \equiv \sum_p \varepsilon(p)\, n_p$$

Note that $\mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right) = \prod_p \sum_{n_p=0}^{\infty} e^{\varepsilon(p) n_p}$

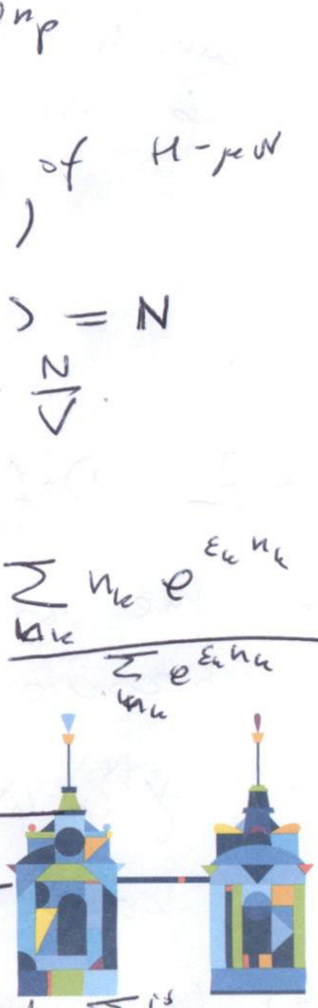
This is because plain waves are eigenstates of $H-\mu N$ (or rather form the Fock space basis)

<u>Remark</u>: $\mu < 0$ is chosen such that $\langle N \rangle = N$
i.e. to make sense of density $\rho = \frac{N}{V}$.

Thus we can compute (exercise)

$$\langle n_k \rangle = \frac{\sum_k n_k e^{\varepsilon_k n_k} \prod_{q \neq k} \sum_{n_q} e^{\varepsilon_q n_q}}{\prod_q \sum_{n_q} e^{\varepsilon_q n_q}} = \frac{\sum_{n_k} n_k e^{\varepsilon_k n_k}}{\sum_{n_k} e^{\varepsilon_k n_k}}$$

$$= -\frac{\partial}{\partial x} \log \sum_n e^{-nx} \Big|_{x=\beta(\varepsilon_k - \mu)} = \frac{1}{e^{\beta(p^2-\mu)} - 1}$$



Bose-Einstein distribution:

$$\gamma^{id}(p) = \frac{1}{\exp\left(\frac{p^2-\mu}{T}\right) - 1}, \quad \mu < 0 \text{ s.t. } \sum_p \gamma^{id}(p) = N$$

Properties of $\gamma^{id}(p)$

-) for every $p \neq 0$ $\gamma^{id}(p) \to 0$ as $T \to 0$

-) thermodynamic limit: $N, L^3 \to \infty$, $\rho = \frac{N}{L^3} = \text{const}$

$$\rho = \frac{\langle N \rangle}{L^3} = \frac{1}{V} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \gamma^{id}(p) \xrightarrow[L \to \infty]{\substack{\text{Riemann} \\ \text{Sum}}} \frac{1}{(2\pi)^3} \int \gamma^{id}(p)\, dp$$

$$\leq \int \gamma^{id}(p)\Big|_{\mu=0} dp =: \rho_{cr}(T)$$

-) however, $\rho_{cr}(T) \xrightarrow[T \to 0]{} 0$ which implies $\rho \to 0$

-) what went wrong?

  setting $L \to \infty$ and $\mu = 0$ do not commute,

  in particular: $\mu \to 0$ as $L \to \infty$

  which leads to a macroscopic ocapation of the $p=0$ mode.

$$\gamma^{id}(0) = \frac{1}{\exp(-\beta\mu) - 1} \sim \mathcal{O}(N)$$

$$\sim \frac{-1}{\beta\mu} \Rightarrow \mu \sim L^{-3}$$

2.2. Definition of BEC

-) the computation of the BE distribution possible because there was no interaction

-) $\gamma^{id}(p)$ was the Fourier transform of the kernel of one-body reduced density matrix

-) for a general state $\gamma_\Gamma^{(1)}(x,y) = \mathrm{Tr}\,(a_x^* a_y \Gamma)$

•) $\gamma^{id}(0)$ is a macroscopic eigenvalue of $\gamma^{id}(x,y)$

Def (Penrose, Onsager 1956)

We say that a sequence of states Γ_N (canonical) displays BEC iff

$$\liminf_{N\to\infty} \sup_{\|\varphi\|=1} \frac{\langle \varphi, \gamma^{(1)}_{\Gamma_N} \varphi\rangle}{N} > 0$$

•) in other words: the 1-pdm has an eigenvalue of order N

Example: ideal gas ground state:

$$\Gamma_N = |\varphi_N\rangle\langle\varphi_N| \quad , \quad \gamma^{(1)}_{\varphi_N}(x,y) = N\int dx_2 \dots dx_N\, \varphi_N(x, x_2, \dots x_N)\overline{\varphi_N(y, x_2, \dots x_N)}$$

↳ we know $\varphi_N := u_0^{\otimes N} = u_0(x_1)\dots u_0(x_N)$
where $u_0(x)$ is the ground state of the one-body Hamiltonian $-\Delta + V(x)$ (in the case of box with p.b.c $V \equiv 0$ $u_0(x) = \frac{1}{L^{3/2}}$.)

↳ we compute $\gamma^{(1)}_{u_0^{\otimes N}}(x,y) = N u_0(x)\overline{u_0}(y)$

$$\Downarrow$$

$$\gamma^{(1)}_{(u_0^{\otimes N})} = \underset{\uparrow}{N} |u_0\rangle\langle u_0|$$

eigenvalue of order N

The BEC conjecture

Consider an interacting system ($w \not\equiv 0$) in the thermodynamic limit $N, L \to \infty$, $N/L^3 = \rho = \text{const}$. Show its ground / Gibbs state displays BEC.

Let us stress: even in the ground state...

Why difficult?

-) ground state of interacting systems is not a product state ⇝ correlations play a crucial role
-) no analytical solutions (computer simulations do not help)
-) large volume ⇒ gap of Laplacian closes ($\frac{1}{L^2}$)
  ⇒ loss of coercivity

To make progress:

-) consider toy models
-) test methods on them, understand those
-) extend to more difficult models

⇝ simpler scaling regimes than TL

3. Scaling regimes

idea: 1) change, rescale the interaction to make it weak
 2) keep volume fixed ⇝ spectral gap

$$H_N = \sum_{i=1}^{N} \left(-\Delta_{x_i} + V(x_i)\right) + \lambda_N \sum_{i<j} w_N(x_i - x_j)$$

-) $\lambda_N \geq 0$ coupling constant
  weaken the interaction $\lambda_N \sim \frac{1}{N}$
-) the gap in the spectrum is fixed by $V(x)$ on a fixed box. ($L = 1$)
-) macroscopic parameter $N \to \infty$
-) with $\lambda_N \sim \frac{1}{N}$ both terms in H_N are $O(N)$

•) we can tune the range of interaction

$$w_N(x) = N^{3\alpha} w(N^\alpha x) \qquad \alpha \in [0,1]$$

notice $\int w_N(x) = \int w(x)$

↳ $\alpha = 0$ range of interaction $O_N(1)$
"long range" as the size of the system is $O_N(1)$, all particles interact with each other

mean-field scaling

↳ $\alpha > 0$ $\quad w_N \rightharpoonup \delta$ - point interaction

range of interaction $\sim N^{-\alpha}$
average distance between the particles $N^{-1/3}$ $(\rho^{-1/3})$
dilute system $N^{-\alpha} \ll N^{-1/3}$

↳ $\alpha = 1$ ultra-dilute regime relevant for cold atom experiments

$$w_N(x) = \underbrace{N^3}_{\text{strong interactions}} w(Nx)$$

→ rare interaction due to diluteness

Gross-Pitaevski scaling (comment later)

4. BEC in the mean-field Bose gas

$$H_N^{MF} = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1} \sum_{i<j} w(x_i - x_j)$$

•) as before $V(x) \to \infty$ as $|x| \to \infty$, $w \geq 0$, $\hat{w} \geq 0$

4.1. Ground state energy of the MF gas

$$E_0^{MF}(N) = \inf_{\|\psi_N\|=1} \langle \psi_N, H_N^{MF} \psi_N \rangle$$

4.1.1 Upper bound

•) idea: weakly interacting system - maybe, at least energetically, a product trial state is good?

trial state: $\Psi_N^{trial}(x_1, \dots, x_N) = u(x_1)\dots u(x_N)$ for some normalized u.

Then:

$$E_0^{MF}(N) \leq N \langle u, (-\Delta + V) u \rangle + \frac{1}{N-1} \frac{N(N-1)}{2} \iint \overline{u(x)}\,\overline{u(y)}\, w(x-y)\, u(x) u(y)$$

$$= N \int (|\nabla u|^2 + V|u|^2) + \frac{N}{2} \iint w(x-y) |u(x)|^2 |u(y)|^2 \, dx\, dy$$

$$= N \int |\nabla u|^2 + V|u|^2 + \frac{N}{2} \int w * |u|^2(x) |u(x)|^2 \, dx$$

We define $\mathcal{E}_H(u) = \int (|\nabla u|^2 + V|u|^2) + \frac{1}{2} \int (w * |u|^2)|u|^2$

Then $$\frac{E_0^{MF}(N)}{N} \leq \underbrace{\inf_{\|u\|_2 = 1} \mathcal{E}_H(u)}_{= e_H}$$ — Hartree functional

<u>Thm</u> The assumptions on V and w imply that the $\mathcal{E}_H$ admits a pointwise positive minimizer u_H which is unique up to phase and which satisfies the Euler-Lagrange equation

$$(-\Delta + V + w * |u_H|^2) u_H = \varepsilon_0 u_H$$

<u>Hartree equation</u>

$\uparrow$ Lagrange multiplier due to the condition $\|u\| = 1$

where

$$\varepsilon_0 = \mathcal{E}_H(u_H) + \frac{1}{2} \langle u_H, w * |u_H|^2 u_H \rangle = e_H + \frac{1}{2} \langle u_H, w * |u_H|^2 u_H \rangle$$