5 3) BOSE-EINSTEIN CONDENSATES

~~3.1. Bose-Einstein Condensation~~

3.1. Quantum statistical physics

For large systems, we cannot know all microscopic detail
⇒ describe with density-matrix (see 1.3.2)

All essential postulates take a very similar form to classical statistical physics.

Quantum statistical ensembles

Microcanonical ensemble
(fixed N, V, E)

$$\hat{\rho} = \frac{1}{\Gamma(E)} \sum_{\substack{k \\ E_k \approx E}} |\Psi_k\rangle\langle\Psi_k| \qquad (3.1)$$

- the sum runs over all many-body states k in energy range $E \leq E_k \leq E+\Delta E$ for a small ΔE. See Eq. (1.10) for $|\Psi_k\rangle$, E_k. i.e they are many-body states

Canonical ensemble
(fixed N, V, T)

$$\hat{\rho} = \frac{1}{Z} \exp^{-\beta \hat{H}} \qquad Z = \mathrm{Tr}\left[\exp[-\beta\hat{H}]\right] \qquad (3.2)$$

power series

$\beta = 1/k_B T$

Partition function

- In eigenbasis of $\hat{H}$ can write

$$\hat{\rho} = \frac{1}{Z}\sum_k e^{-\beta E_k} |\Psi_k\rangle\langle\Psi_k| \qquad (3.3)$$

- (3.2) is more general. We may not know the eigenbasis. (Finding it is hard for interacting many-body systems)

Grand-canonical ensemble

(fixed μ, V, T)

μ = chemical potential

$\hat{N}$ = total number operator for system

$$\hat{\rho} = \frac{1}{Z_G} \exp\left[-\beta(\hat{H} - \mu\hat{N})\right] \qquad (3.4)$$

$$Z_G = \mathrm{Tr}\left[\exp\left[-\beta(\hat{H} - \mu\hat{N})\right]\right]$$

really WANT $\hat{H}$ in second-quant. now

- In eigenbasis of $\hat{H}$ AND $\hat{N}$ can write: (3.5)

$$\hat{\rho} = \frac{1}{Z_G} \sum_k e^{-\beta(E_k - \mu N_k)} |\psi_k\rangle\langle\psi_k|$$

N_k = # particles in $|\psi_k\rangle$

Consequences for Indistinguishable particles

~~If demand:~~ (ask if seen deriv of BE/FD or want again, Might skip details)

Consider single particle basis $H_0|\varphi_k\rangle = \varepsilon_k|\varphi_k\rangle$ and non-interacting many-body Hamiltonian (3.6)

$$\hat{H} = \sum_k \varepsilon_k \hat{a}^\dagger_k \hat{a}_k$$

- Convince yourself that Fock-states $|\vec{N}\rangle$ (3.14) are eigenstates of

$$\hat{H}|\vec{N}\rangle = E_{\vec{N}}|\vec{N}\rangle \quad \text{with } E_{\vec{N}} = \sum_k N_k \varepsilon_k$$

(define $N_{\vec{N}} = \sum_k N_k$)

- From (3.5)

$$\hat{\rho} = \sum_{\vec{N}} P_{\vec{N}} |\vec{N}\rangle\langle\vec{N}| \quad \text{with}$$

$$P_{\vec{N}} = \frac{e^{-\beta(E_{\vec{N}} - \mu N_{\vec{N}})}}{\sum_{\vec{N}} e^{-\beta(E_{\vec{N}} - \mu N_{\vec{N}})}} = \frac{\exp\left[-\beta\left(\sum_k N_k \varepsilon_k\right) + \beta\mu\left(\sum_k N_k\right)\right]}{\sum_{N_1 N_2 N_3 \ldots} \exp\left[-\beta\left(\sum_k N_k \varepsilon_k\right) + \beta\mu\left(\sum_k N_k\right)\right]}$$

$$= \frac{\prod_k \exp\left[\beta N_k(\mu - \varepsilon_k)\right]}{\prod_k \left[\sum_{N_k} \exp\left[\beta N_k(\mu - \varepsilon_k)\right]\right]} = \prod_k P_k(N_k)$$

keep on board

with $$P_k(N_k) = \frac{\exp\left(\beta N_k(\mu - \varepsilon_k)\right)}{\sum_{N_k} \exp\left[\beta N_k(\mu - \varepsilon_k)\right]}$$ the "probability to have N_k particles in state k" (3.7)

(* to see via math $P_k(N_k) = \sum_{\vec{N}'} P_{\vec{N}'}$ with $\sum$ running over all $\vec{N}'$ with $N_k' = N_k$)

Now: what is the mean number of particles in state $|\varphi_b\rangle$?
(with energy ε_b)

$$\overline{m}_b = \langle \underset{\hat{a}_b^+ \hat{a}_b}{\underset{\shortparallel}{\hat{N}_b}} \rangle = \mathrm{Tr}\left[\hat{\rho}\,\hat{N}_b\right] = \sum_{\vec{N}} P_{\vec{N}}\, \mathrm{Tr}\left[N_b |\vec{N}\rangle\langle\vec{N}|\right]$$

$$= \sum_{\vec{N}} P_{\vec{N}} N_b \overset{\text{as } \circledast}{=} \sum_{N_b} P_b(N_b) N_b \qquad (3.8)$$

Fermions | Allowed values of $N_b = 0, 1$

$$\Rightarrow \overline{m}_b = 0 + P_b(1) \times 1 = \frac{\exp\left(\beta(\mu - \varepsilon_b)\right)}{1 + \exp\left(\beta(\mu - \varepsilon_b)\right)} \Rightarrow$$

Fermi-Dirac distribution | Mean number of particles in a given state b with energy ε_b:

$$\boxed{\overline{m}_b = \frac{1}{1 + \exp\left(\beta(\varepsilon_b - \mu)\right)}} \quad \text{(Fermions)} \qquad (3.9)$$

Bosons | All values of $N_b = 0, 1, 2, \ldots \infty$ are allowed

- define $a = \exp\left[\beta(\mu - \varepsilon_b)\right]$ and note

$$\overline{m}_b = \sum_{N_b} P_b(N_b) N_b = \frac{a \frac{d}{da}\left(\sum_{N_b} a^{N_b}\right)}{\sum_{N_b} a^{N_b}}$$

(μ<0 (see later) hence a<1)

- Use geometric series $\sum_n a^n = \frac{1}{1-a}$ to reach

Bose-Einstein distribution |

$$\boxed{\overline{m}_b = \frac{1}{\exp\left(\beta(\varepsilon_b - \mu)\right) - 1}} \quad \text{(Bosons)} \qquad (3.10)$$

- Classical limit $\overline{m}_b \ll 1 \Rightarrow \exp \gg 1$

$$\Rightarrow \overline{m}_b = \exp\left(-\beta(\varepsilon_b - \mu)\right)$$

- For given system (ε_K), & temperature, chemical potential controls mean total particle number via $N = \sum_K \overline{m}_K$

3.2 Bose-Einstein condensation

Consider non interacting bosonic atoms in a harmonic trap

$$\varepsilon_{\vec{n}} = \hbar\omega\left(n_x + n_y + n_z + \tfrac{3}{2}\right)$$

In 3.2 $n_x\ n_y\ n_z$ label oscillator states NOT occupation numbers

total atom number

$$N = \sum_{n_x n_y n_z} \bar{m}_{n_x n_y n_z} \overset{(3.10)}{\underset{\text{B.E. dist}}{=}} \sum_{n_x n_y n_z} \frac{1}{\exp\left[\beta\left[\hbar\omega\left(n_x+n_y+n_z+\tfrac{3}{2}\right)-\mu\right]\right]-1}$$

- Define $\tilde{\mu} = \mu - \frac{3}{2}\hbar\omega$ We need $\tilde{\mu} < 0$ for sensible results ($\bar{m}_{\vec{n}} > 0$)
- For given state $\vec{n} = (n_x n_y n_z)$, if $T\downarrow$ then $\bar{m}_{\vec{n}}\downarrow$

  — " — $\vec{n}$ and T, if $\tilde{\mu}\uparrow$ then $\bar{m}_{\vec{n}}\uparrow$
- To keep N fixed as we lower T, need to increase μ (
- But $\tilde{\mu} < 0$, what happens at $\tilde{\mu} = 0$? $\bar{m}_{000} = \frac{1}{e^{\beta\cdot 0}-1} \to \infty$

  for all other states still OK. Groundstate occupation

- Seperately write:

$$N = N_0 + \sum_{\vec{n}\neq(000)} \bar{m}_{\vec{n}} \qquad (3.11)$$

Let us find the lowest temperature T_c where $N_0 \approx 0$ is possible. This will be for $\tilde{\mu} = 0$. Hence:

$$N = \sum_{\vec{n}\neq(0,0,0)} \frac{1}{\exp\left[\beta\left(\hbar\omega(n_x+n_y+n_z) - \tilde{\mu}\right)\right]-1}, \quad \tilde{\mu} = 0 \qquad \beta_c = \frac{1}{k_B T_c}$$

$$\approx \int dn_x\, dn_y\, dn_z \frac{1}{\exp\left[\beta_c\left(\hbar\omega(n_x+n_y+n_z)\right)\right]-1} \qquad n_x' = \hbar\omega\beta_c n_x$$

$$N_{CT} \approx \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \int_0^\infty dn_x'\, dn_y'\, dn_z' \frac{1}{e^{(n_x'+n_y'+n_z')}-1} = \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^{\infty} \int d^3\vec{n}\; e^{-p(n_x'+n_y'+n_z')}$$

$$\boxed{\sum_{p=1}^{\infty} e^{-p\alpha} = \frac{1}{e^{\alpha}-1} \quad \text{(via geometric series)}}$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^{\infty} \underbrace{\left(\int_0^\infty dn_x'\, e^{-pn_x'}\right)}_{=\frac{1}{p}} \left(\int_0^\infty dn_y'\, e^{-pn_y'}\right)\left(\int_0^\infty dn_z'\, e^{-pn_z'}\right) = \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^{\infty} \frac{1}{p^3}$$

$$= \left(\frac{k_B T_C}{\hbar\omega}\right)^3 \zeta(3)$$

Riemann-Zeta function

$\Rightarrow$

Critical temperature for <u>Bose-Einstein condensation</u> in a 3D isotropic harmonic trap

$$k_B T_c = \hbar\omega \, N^{\frac{1}{3}} \zeta(3)^{-\frac{1}{3}} = 0.94 \, N^{\frac{1}{3}} \hbar\omega \qquad (3.12)$$

- depends on dimensions & trap details
- numeric estimate! $N = 10\,000$ $\quad \omega = (2\pi)\cdot 100\,\mathrm{Hz}$

  $\Rightarrow T_c = 97\,\mathrm{nK}$ (nano Kelvin)

Now let $T < T_c$. From (3.11) $\Rightarrow$

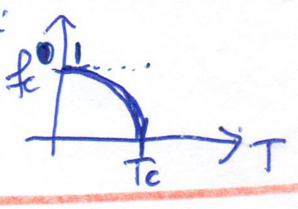
$$N = N_0(T) + \sum_{\vec{n} \neq (0,0,0)} \overline{m}_{\vec{n}} \underset{\text{as before}}{=} N_0(T) + \int dn_x dn_y dn_z \frac{1}{\exp[\beta\hbar\omega(n_x+n_y+n_z)] - 1}$$

$\beta = \frac{1}{k_B T}$ (not T_c now)

$$= N_0(T) + \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) = N_0(T) + \left(\frac{k_B T}{k_B T_c}\right)^3 N \Rightarrow$$

Fraction of Bose condensed atoms:

$$f_c = \frac{N_0(T)}{N} = \left[1 - \left(\frac{T}{T_c}\right)^3\right] \qquad (3.13)$$



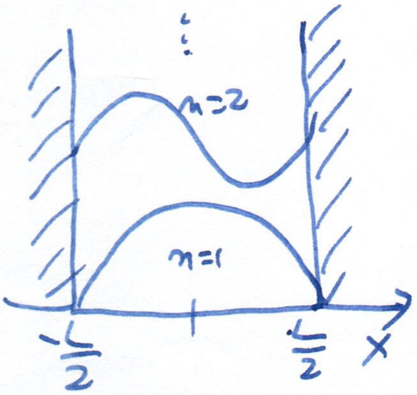
- Bose Einstein condensation has the properties of a <u>second order phase transition</u>
- unlike most of those, it does not require interactions (except indirectly, for thermalisation)
- At $T=0$, the system is in the state $N_0 = N$, with

$$\hat{\rho} = |N\,000\ldots\rangle\langle N\,000\ldots| \Leftrightarrow |\Psi_0\rangle = |N\,000\rangle \qquad (3.14)$$

Fock-state with all N atoms in the ground-state

3.2.1: De-Broglie Wave overlapp

To work out one more aspect of condensation, for Bosons in let us redo the derivation in 3.2, a 3D infinite square (cubic) well (of volume $L^3 = V$)



$$E_n = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \qquad k_n = \frac{n\pi}{L}$$

n_x, n_y, n_z.

Using a similar calculation as in 3.2 (bit harder due to $E \sim n^2$) one can show:

$$T_C \approx \frac{\hbar^2}{2m\pi k_B}\left(\frac{N}{2.6 \cdot V}\right)^{\frac{2}{3}}$$

Let us define the thermal de-Broglie wavelength

$$\lambda_T \approx \hbar \sqrt{\frac{2\pi}{m k_B T}} \qquad (3.136)$$

as wavelength of a particle with kinetic energy $E_{kin} \approx k_B T$

? why not $\frac{3}{2}$

Mean nearest neighbor distance of randomly distributed atoms at density $\rho = \frac{N}{V}$ is $\bar{d} = \frac{1}{3}\left(\frac{3}{4\pi\rho}\right)^{\frac{1}{3}} \Gamma(1/3) \approx 0.5\, \rho^{-\frac{1}{3}}$

Thus

$$\lambda_{T_c} = \hbar \sqrt{\frac{1}{m k_B}\left(\frac{2\pi m k_B}{\hbar^2}\left(\frac{2.6\, V}{N}\right)^{\frac{2}{3}}\right)} = \frac{\sqrt{2\pi\,(2.6)^{\frac{2}{3}}}}{\rho^{\frac{1}{3}}} = 3\, \rho^{-\frac{1}{3}}$$

Thus at T_c, atomic de-Broglie waves begin to overlapp.