

# 12. Quantum gases

## N as a function of $\mu$



- Grand canonical distribution applies to an "open" system in equilibrium with a reservoir of energy and particles
- Microstates of all energies and particle numbers are possible

$$\overline{N} = \sum_{r} N_{r} P_{r} = \frac{1}{\mathscr{Z}} \sum_{r} N_{r} \exp\left(\beta \left[N_{r} \mu - E_{r}\right]\right)$$

$$\overline{N} = \frac{1}{\beta} \frac{\partial \ln \mathscr{Z}}{\partial \mu}$$

• Find  $\frac{\left(\Delta \overline{N^2}\right)^{1/2}}{\overline{N}} \sim \frac{1}{N^{1/2}}$ 

• Key point 16: choose  $\mu$  to fix  $\overline{N} = N(\mu)$  (eg by varying density of particles in the reservoir)

• ie. N is sharp about  $\overline{N}$ 

## Indistinguishable particles



- Recall that for **Distinguishable particles**: A microstate is specified by  $i_1, i_2, ..., i_N$ , i.e., the quantum state of each particle and has energy  $E = \sum_{m=1}^{N} \varepsilon_{i_m}$
- For **Indistinguishable particles**: A microstate is specified by  $n_1, n_2, ...$ , where  $n_i$  is the occupation number, i.e., the number of particles in single-particle state i.
- Thus, for indistinguishable particles in microstate r specified by the set  $\{n_i\}$ :

$$N_r = \sum_i n_i$$
 and  $E_r = \sum_i n_i \epsilon_i$ 

where  $e_i$  is the energy of single-particle state i.

• Hence 
$$\beta(N_r\mu - E_r) = \beta \sum_i n_i(\mu - \epsilon_i)$$

# Microstates: localised versus non-localised particles

Feature	Localised Particles	Non-localised Particles
Particle Identity	Distinguishable	Indistinguishable
Microstate Specified	Individual particle states	Occupation numbers per state
Framework	Canonical Ensemble (ie Boltzmann distribution)	Grand Canonical Ensemble (Gibbs-Boltzmann distribution)

### Indistinguishable particles



$$\mathcal{Z} = \sum_{r} \exp\left(\beta \left[N_{r}\mu - E_{r}\right]\right)$$

$$= \left[\sum_{n_{1}} \sum_{n_{2}} \cdots \right] \exp\left(\beta \sum_{i} n_{i}(\mu - \epsilon_{i})\right)$$

$$= \left[\sum_{n_{1}} \exp\left(\beta n_{1}(\mu - \epsilon_{1})\right)\right] \times \left[\sum_{n_{2}} \exp\left(\beta n_{2}(\mu - \epsilon_{2})\right)\right] \times \cdots$$

$$= \mathcal{Z}_{1} \times \mathcal{Z}_{2} \times \cdots = \prod_{i} \mathcal{Z}_{i}$$

where  $\mathcal{Z}_i = \sum_{n_i} e^{\beta n_i (\mu - \epsilon_i)}$  is the (grand canonical) partition function for single particle state i

Thus, a factorization into single-state partition functions occurs.



- **Fermions**: spin is a half-integral multiple of  $\hbar$ ; there are 2s + 1 spin states. Eg. electrons, neutrons, protons, and composite particles etc,
- **Bosons**: spin is an integral multiple of  $\hbar$  (including spin zero). Eg. photons and composite particles made up of an even number of fermions, e.g.,  $He^4$
- Pauli Exclusion Principle

There can be at most one fermion in any quantum state.

Single state partition function for Fermions

$$\mathcal{Z}_i = \sum_{\substack{n_i = 0, 1 \\ \text{Pauli}}} \exp\left(\beta n_i (\mu - \epsilon_i)\right) = 1 + \exp\left(\beta (\mu - \epsilon_i)\right)$$

(See chapter 12 of year 1 Quantum Physics)

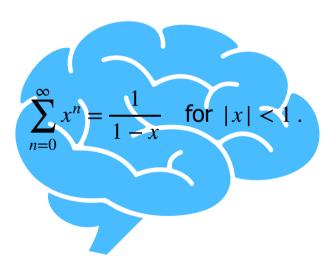


Single state partition function for Bosons

$$\mathcal{Z}_{i} = \sum_{n_{i}=0}^{\infty} \exp\left(\beta n_{i}(\mu - \epsilon_{i})\right) = \frac{1}{1 - \exp\left(\beta(\mu - \epsilon_{i})\right)}$$

No restriction

For 
$$\exp(\beta(\mu - \epsilon_i)) < 1$$





• If we know  $\mathcal{Z}_i$  we can calculate the average number of particles in state i

$$\overline{n_i} = \frac{1}{\beta} \frac{\partial \ln \mathcal{Z}_i}{\partial \mu}$$

Derivation

$$\mathcal{Z}_{i} = \sum_{n_{i}} e^{\beta n_{i}(\mu - \epsilon_{i})}$$

$$\frac{\partial \ln \mathcal{Z}_{i}}{\partial \mu} = \frac{1}{\mathcal{Z}_{i}} \frac{\partial \mathcal{Z}_{i}}{\partial \mu}$$

$$= \frac{1}{\mathcal{Z}_{i}} \sum_{n_{i}} \beta n_{i} e^{\beta n_{i}(\mu - \epsilon_{i})}$$

$$= \beta n_{i} p(n_{i})$$

$$= \beta \overline{n_{i}}$$



- Now calculate  $\overline{n}_i$ , the average number of particles in quantum state i (having energy  $\epsilon_i$ ) for the specific case of Bosons and Fermions
- Write:  $\mathcal{Z}_i = \left[1 \pm \exp\left(\beta(\mu \epsilon_i)\right)\right]^{\pm 1}$  where +refers to fermions, and refers to Bosons.

$$\overline{n}_{i} = \sum_{n_{i}} n_{i} P(n_{i}) = \frac{1}{\beta} \frac{\partial \ln \mathcal{Z}_{i}}{\partial \mu}$$

$$= \pm \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \left[ 1 \pm \exp \left( \beta(\mu - \epsilon_{i}) \right) \right]$$

$$= \pm \frac{1}{\beta} (\pm \beta) \frac{\exp \left( \beta(\mu - \epsilon_{i}) \right)}{1 \pm \exp \left( \beta(\mu - \epsilon_{i}) \right)}$$

$$= \frac{\exp \left( \beta(\mu - \epsilon_{i}) \right)}{1 \pm \exp \left( \beta(\mu - \epsilon_{i}) \right)}$$

$$= \frac{1}{\exp \left( \beta(\mu - \epsilon_{i}) \right)}$$

$$= \frac{1}{\exp \left( \beta(\epsilon_{i} - \mu) \right)}$$



• Key point 17: 
$$\overline{n}_i = f_{\pm}(\epsilon_i) = \frac{1}{\exp(\beta(\epsilon_i - \mu)) \pm 1}$$

where + refers to fermions, and - refers to Bosons.

• Thus  $N(\mu)$  is determined via

$$N = \sum_{i} \overline{n}_{i} = \sum_{i} f_{\pm}(\epsilon_{i})$$