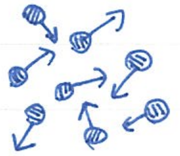
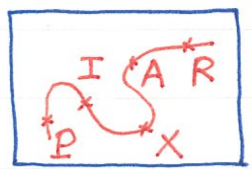
HH0005 Fermi and Bose Distributions



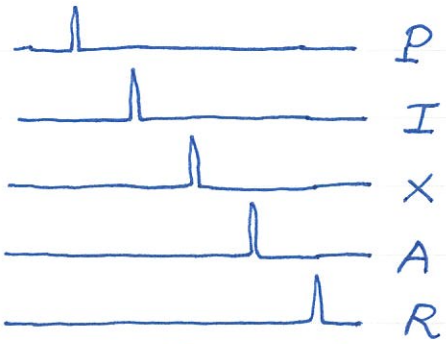
What's the best way to describe a system of many particles? Think about a particle trajectory on the computer screen.

Two ways to describe it:

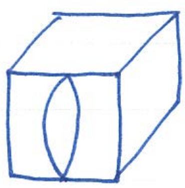
$$\boxed{\begin{array}{l}(1)\ \text{particle view: } X(t). \\ (2)\ \text{field view: } \psi(x,t).\end{array}}$$



Both views are equivalent but the field view is better when many particles are present.



Thus, we stop aking about the trajectories. In stead, we are interested in the distribution of particles in a particular state. Consider non-interacting particles in a box



diff. modes.

$$k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{L}, \quad k_z = \frac{n_z \pi}{L}$$

$\boxed{(k_x, k_y, k_z) \text{ labels different orbitals}}$

single-particle state.

$$\sum_n \longrightarrow \frac{1}{8}\int 4\pi n^2 dn = \frac{\pi}{2}\int_0^\infty n^2 dn$$

(I) Fermi Distribution:

For simplicity, consider a system with just one orbital for fermions. The Gibbs sum is rather simple,

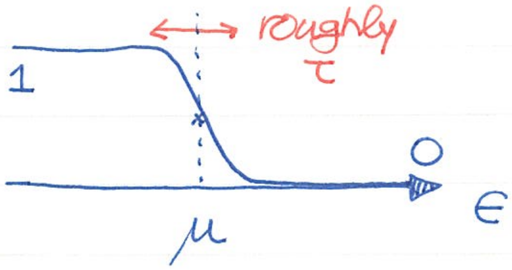
$$\mathcal{Z} = 1 + \lambda e^{-\epsilon/\tau} \longrightarrow f = \frac{\lambda e^{-\epsilon/\tau}}{1+\lambda e^{-\epsilon/\tau}}$$

prob. to find one particle

The distribution can be rewritten in the familiar form,

$$\boxed{f = \frac{1}{e^{(\epsilon-\mu)/\tau}+1}} \quad \text{because } \lambda = e^{\mu/\tau}$$

$\leftarrow$ Fermi distribution



$$\begin{cases} \text{For } (\epsilon-\mu)/\tau < 0, & f \approx 1. \\ \text{For } (\epsilon-\mu)/\tau > 0, & f \approx 0. \end{cases}$$

The value of f is between 0 and 1, reflecting Fermi statistics.

Now, we can generalize the calculations to $N_s = 2$ orbitals.

There are 4 possible states

ϵ_2, ϵ_1 $\longrightarrow$ vacant, ϵ_1, ϵ_2, $\epsilon_2 \, \epsilon_1$

$E=0$ $\quad E=\epsilon_1$ $\quad E=\epsilon_2$ $\quad E=\epsilon_1+\epsilon_2$

Gibbs Sum

$$\mathcal{Z} = 1 + \lambda e^{-\epsilon_1/\tau} + \lambda e^{-\epsilon_2/\tau} + \lambda^2 e^{-(\epsilon_1+\epsilon_2)/\tau}$$

$$= \boxed{\left(1+\lambda e^{-\epsilon_1/\tau}\right)\left(1+\lambda e^{-\epsilon_2/\tau}\right)} \rightarrow \mathcal{Z}_1 \times \mathcal{Z}_2$$

Similarly, one can compute the occupation probability,

$$f_1 = \frac{1}{\mathcal{Z}}\left(\lambda e^{-\epsilon_1/\tau} + \lambda^2 e^{-(\epsilon_1+\epsilon_2)/\tau}\right)$$

$$= \frac{\lambda e^{-\epsilon_1/\tau}}{1+\lambda e^{-\epsilon_1/\tau}} \; \frac{\cancel{1+\lambda e^{-\epsilon_2/\tau}}}{\cancel{1+\lambda e^{-\epsilon_2/\tau}}} = \frac{1}{\frac{1}{\lambda}e^{\epsilon_1/\tau}+1}$$

the same form!

Of course, the occupation probability for the other orbital is

$$f_2 = \frac{1}{\frac{1}{\lambda}e^{\epsilon_2/\tau}+1}.$$

The calculations can be generalized to many orbitals without any trouble.

(II) Bose distribution:

Now we turn to a simple system with just one orbital for bosons. There are infinite states with $E = 0, \epsilon, 2\epsilon, 3\epsilon, \cdots$

Gibbs sum $\mathcal{Z} = 1 + \lambda e^{-\epsilon/\tau} + \lambda^2 e^{-2\epsilon/\tau} + \cdots\cdots$

$$= \frac{1}{1-\lambda e^{-\epsilon/\tau}} \quad \text{if } \lambda e^{-\epsilon/\tau} < 1$$

The average number of particles is

$$f(\epsilon) = \lambda \frac{\partial}{\partial \lambda}(\log \mathcal{Z}) = -\lambda \frac{\partial}{\partial \lambda}\left[\log\left(1-\lambda e^{-\epsilon/\tau}\right)\right]$$

$$= (-\lambda)\frac{-e^{-\epsilon/\tau}}{1-\lambda e^{-\epsilon/\tau}}$$

The above expression can be rewritten as

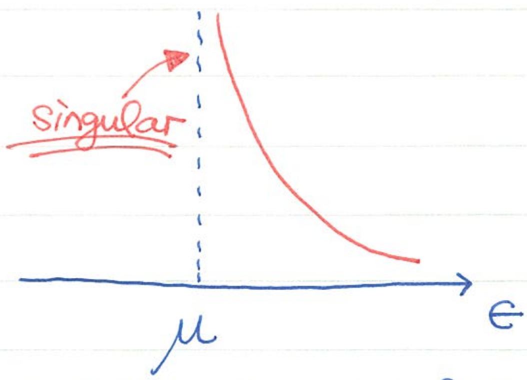
$$\boxed{f(\epsilon) = \frac{1}{\frac{1}{\lambda}e^{\epsilon/\tau} - 1}}$$

± 1 difference for fermions and bosons.

Now we come back to the criterion $\lambda e^{-\epsilon/\tau} < 1$.

$$\lambda e^{-\epsilon/\tau} = e^{-(\epsilon-\mu)/\tau} < 1 \longrightarrow \boxed{\mu < \epsilon}$$

Chemical potential μ must be less than the energy ϵ so that the particle number is bounded. Note that the average particle number diverges as $\epsilon \to \mu^+$. We will learn later that this divergence is the origin of Bose-Einstein condensate.



Follow the same spirit, let's work out the 2-orbital case.

Gibbs sum $\mathcal{Z} = 1 + \left(\lambda e^{-\epsilon_1/\tau} + \lambda e^{-\epsilon_2/\tau}\right)$ ← 1 particle

$$+ \left(\lambda^2 e^{-2\epsilon_1/\tau} + \lambda^2 e^{-2\epsilon_2/\tau} + \lambda^2 e^{-(\epsilon_1+\epsilon_2)/\lambda}\right)$$

↑ 2 particles

$$+ \cdots$$

The above sum can be regrouped into the following form

$$\mathcal{Z} = \left(1 + \lambda e^{-\epsilon_1/\tau} + \lambda^2 e^{-2\epsilon_1/\tau} + \cdots\right)\left(1 + \lambda e^{-\epsilon_2/\tau} + \lambda^2 e^{-2\epsilon_2/\tau} + \cdots\right),$$

just the same as in the fermion case. After some algebra, the average particle number in a particular orbital is

$$\boxed{f(\varepsilon_i) = \frac{1}{e^{(\varepsilon_i - \mu)/\tau} - 1}}$$

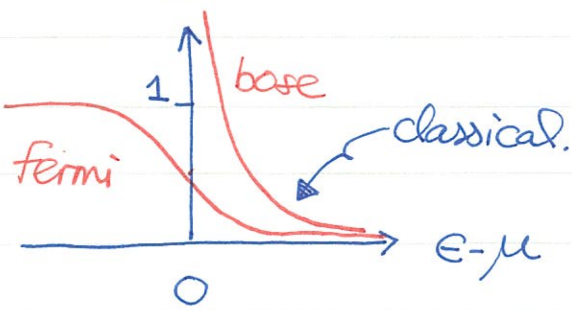
It is very important to emphasize that the convergent criterion changes a bit....

$$e^{(\varepsilon_i - \mu)/\tau} > 1 \longrightarrow \boxed{\min(\varepsilon_i) > \mu \quad \text{OR} \quad \mu < \min(\varepsilon_i)}$$

Generalization to many orbitals is straightforward.

(III) Fermi, Bose and classical.

Plotting Fermi and Bose functions together. Several important features are clear.



(1) When $\epsilon \approx \mu$, distributions have some features.

(2) For fermions, μ can be viewed as "on-off" switch for occupation of the orbital.

(3) For bosons, μ gives rise to a strange singularity. The average particle number in the orbital $\epsilon \approx \mu$ is huge!

(4) The distribution functions are approximately the same in high-temperature limit,

$$\boxed{f(\varepsilon) = \frac{1}{e^{(\epsilon-\mu)/\tau} \pm 1} \approx e^{-(\epsilon-\mu)/\tau}}$$

This is more than Boltzmann dist. !!

In the classical regime, $f(\varepsilon) \ll 1$. This is in fact what we mean by "dilute" in previous studies. That is to say, the occupation number in each orbital is much less than one.

Pauli exclusion principle almost puts no constraint. (fermions).

☆ rarely find two particles in one orbital. (bosons)

Thus, quantum statistics does not show up in the high-T limit. The difference between fermions and bosons vanishes, leaving us with the so-called "ideal gas" in classical regime.

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