Week2-Review of Fermi-Dirac and Bose-Einstein Statistics

ECE 695-O Semiconductor Transport Theory

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Contents

Phase space

- a multidimensional space in which each axis corresponds to one of the coordinates required to specify the state of a physical system, all the coordinates being thus represented so that a point in the space corresponds to a state of the system.

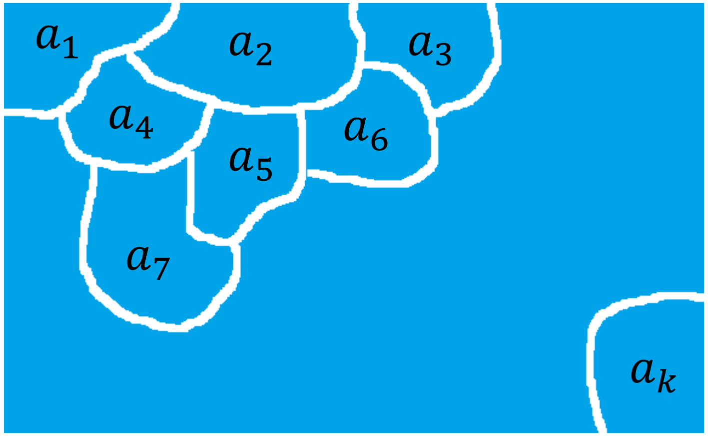
- The state of a system of particles can be specified classically at a particular moment if the position and momentum of each particles are known: x, y, z, p_x, p_y, p_z.
- This combined position and momentum space is called ***phase space***.

- A point (x_i, y_i, z_i, p_{xi}, p_{yi}, p_{zi}) in phase space corresponds to a particular position and momentum.

- However, from the uncertainty principle, momentum and position cannot be specified as a single point simultaneously. The point is actually a cell with a volume of h^3.

$$\tau = dxdydzdp_x dp_y \,\mathrm{d}p_z \qquad dx\,\mathrm{d}p_x \geq \hbar \qquad \tau = h^3 \geq \hbar^3$$

The Probability of a Distribution(1)



- Let's assume we toss a coin on a board with the area A.
- The board is divided by k sections and the area of each section is a_i .
- The probability of the coin fall into the ith cell is

$$g_i = \frac{a_i}{A} .$$

- Naturally, $A = a_1 + a_2 + \cdots + a_k$ and $\Sigma g_i = g_1 + y_2 + \cdots + g_k = 1$.
- The probability that two coins fall in the ith cell is g_i^2. n_i balls in the ith cell is, then, g_i^{ni}.
- The probability G of any particular distribution of the N balls among k cells is the product of g_i^{ni} s.

$$G = (g_1)^{n_1}(g_2)^{n_2}(g_3)^{n_3} \ldots (g_k)^{n_k}$$

- And, of course, the total number of balls equal N:

$$\Sigma n_i = n_1 + n_2 + \cdots + n_k = N$$

The Probability of a Distribution(2)

- Total number of permutations possible for N balls is N!.
- When more than one ball is in a cell, permuting them has no significance.
  → We do not care in which sequence n_i balls fall into ith cell.
- The thermodynamic probability M of distribution is the total number of possible permutations N! divided by the total number of irrelevant permutations, so

$$M = \frac{N!}{n_1!\, n_2! \cdots n_k!}$$

- Total probability W of the distribution is the product GM.

$$W = \frac{N!}{n_1!\, n_2! \cdots n_k!} (g_1)^{n_1} (g_2)^{n_2} \ldots (g_k)^{n_k}$$

- By multinomial theorem,

$$\sum W = \sum \frac{N!}{n_1!\, n_2! \cdots n_k!} (g_1)^{n_1} (g_2)^{n_2} \ldots (g_k)^{n_k}$$

$$= (g_1 + g_2 + \cdots + g_k)^N = 1$$

Stirling's Formula

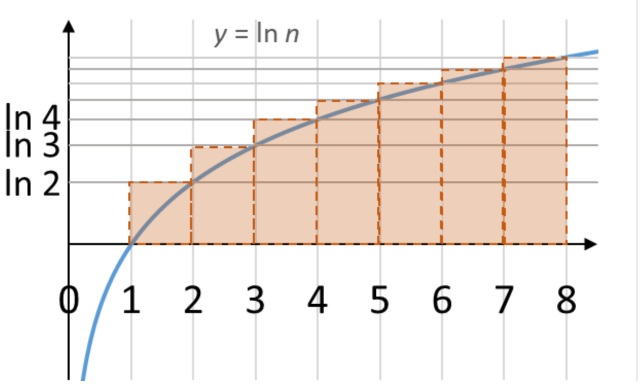
- What we are looking for is the most-probable distribution: the distribution that yields the largest W
- N! is usually very large number hard to handle.

$$\ln n! = \ln n + \ln(n-1) + \cdots + \ln 4 + \ln 3 + \ln 2$$

$$= \sum_{1}^{n} \ln n$$

$$= \int_{1}^{n} \ln n \, dn$$

$$= n \ln n - n + 1$$



$$\ln n! = n \ln n - n \qquad n \gg 1$$: Stirling's formula

Lagrange Multiplier Method

$$\ln W = \ln N! - \sum \ln n_i! + + \sum n_i \ln g_i$$

$$= N \ln N - N - \sum n_i \ln n_i + \sum n_i + \sum n_i \ln g_i$$

$$= N \ln N - \sum n_i \ln n_i + \sum n_i \ln g_i \qquad \text{(since } \sum n_i = N \text{)}$$

- Since ln(x) is monotonically increasing function, we can say

$$(\ln W)_{max} = \ln W_{max}$$

- By taking the derivative with respect to n_i,

$$\delta \ln W_{max} = -\sum n_i \delta \ln n_i - \sum \delta n_i \ln n_i + \sum \delta n_i \ln g_i = 0$$

Lagrange Multiplier Method(2)

$$\delta \ln W_{max} = -\cancel{\sum n_i \delta \ln n_i} - \sum \delta n_i \ln n_i + \sum \delta n_i \ln g_i = 0$$

- Since $\delta \ln n_i = \frac{1}{n_i} \delta n_i$ and $\sum \delta n_i = \delta n_1 + \delta n_2 + \cdots + \delta n_k = 0$,

$$\sum n_i \delta \ln n_i = \sum \delta n_i = 0 \,.$$

- Then, $\delta \ln W_{max} = -\sum \ln n_i \delta n_i + \sum \ln g_i \delta n_i = 0$
- Lagrange Multiplier Method is a way of finding local maxima and minima of a function subject to a constraint.

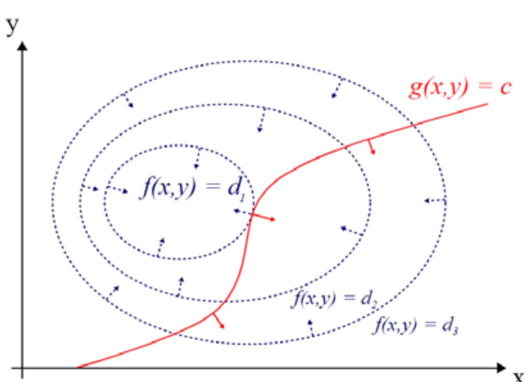
function : $f(x, y)$ (in our case $\ln W$)

constraint: g(x, y)= C (in our case $\sum n_i = N$)

$$L(x, y, \lambda) \stackrel{\text{def}}{=} f(x, y) - \lambda g(x, y)$$

$$\nabla_{x,y} L(x, y, \lambda) = \nabla_{x,y} f(x, y) - \lambda \nabla_{x,y} g(x, y) = 0$$

→ solution is maxima or minima



Lagrange Multiplier Method

- Add $\Sigma\alpha\delta n_i = 0$ to $\delta \ln W_{max}$, and here, α is the Lagrange multiplier.

$$-\sum \ln n_i \delta n_i + \sum \ln g_i \delta n_i + \sum \alpha\delta n_i = -\sum(-\ln n_i + \ln g_i + \alpha)\delta n_i = 0$$

- The solution for the above Eq. is

$$-\ln n_i + \ln g_i + \alpha = 0$$

$$n_i = g_i \mathrm{e}^{\alpha}$$

- Adding up all n_i yields

$$\Sigma n_i = \mathrm{e}^{\alpha}\Sigma g_i$$

- From $\sum g_i = 1$, $\sum n_i = \mathrm{e}^{\alpha} = N$

- Thus, $n_i = N g_i$, and since $g_i = \frac{a_i}{A}$, $n_i = \frac{N}{A} a_i$.

- The most probable number of balls in any cell is equal to the average density of balls (N/A) multiplied by the area of the cell. (Well, a long story for an easy answer)

Maxwell-Boltzmann Statistics - Classical

- Using the approach we studied so far, we will determine how a fixed total energy is distributed among the assembly (ensemble) of identical particles.
- The first type of particles are "identical particles of any spin (integer or half integer) that are sufficiently widely separated to be **distinguished**."

- For N particles whose energies are limited to the k values u_1, u_2, …, u_k, arranged in order of increasing energy, if there are n_i particles of energy u_i, and the total energy of the system is U, there are two conservation constraints;

$$\sum n_i = n_1 + n_2 \dots + n_k = N$$: conservation of particles

$$\sum n_i u_i = n_1 u_1 + n_2 u_2 \dots + n_k u_k = U$$: conservation of energy

- Then, we have to find the distribution of n_i that maximize W with these two constrains.

$$\delta \ln W_{max} = -\sum \ln n_i \delta n_i + \sum \ln g_i \delta n_i = 0$$

$$\sum \delta n_i = \delta n_1 + \delta n_2 \dots + \delta n_k = 0$$

$$\sum \delta n_i u_i = \delta n_1 u_1 + \delta n_2 u_2 \dots + \delta n_k u_k = 0$$

Maxwell-Boltzmann Statistics(2)

- Using two Lagrange multiplier α and β,

$$\sum(-\ln n_i + \ln g_i - \alpha - \beta u_i)\delta n_i = 0$$

$$-\ln n_i + \ln g_i - \alpha - \beta u_i = 0$$

$$\boxed{n_i = g_i \mathrm{e}^{-\alpha} \mathrm{e}^{-\beta u_i}}$$

Maxwell-Boltzmann distribution law

- Now, we will evaluate α and β. Let's consider a continuous energy level(u_i).

$$n(u)du = g(u)\ \mathrm{e}^{-\alpha} \mathrm{e}^{-\beta u_i} du$$

- Since $u = \dfrac{p^2}{2m}$ where p is the particle momentum,

$$n(p)dp = g(p)\mathrm{e}^{-\alpha} \mathrm{e}^{-\beta p^2/2m} dp$$

- g(p) is the probability that a molecule has a momentum between p and p+dp, so it is equal to the number of cells in phase space within which such a molecule may exist.

$$g(p)dp = \frac{\iiint \iint dxdydz\ dp_x dp_y dp_z}{h^3}$$

Phase-space volume occupied by particles with a specific momentum

Maxwell-Boltzmann Statistics(3)

- Since $\iiint dxdydz = V$ and $\iint dp_x dp_y dp_z = 4\pi p^2 dp$, $g(p)dp = \dfrac{4\pi V p^2 dp}{h^3}$.
- Thus, $n(p)dp = \dfrac{4\pi V p^2 \mathrm{e}^{-\alpha} \mathrm{e}^{-\beta p^2/2m}}{h^3} dp$.

$$\int_0^\infty n(p)\,\mathrm{dp} = N \longrightarrow N = \frac{4\pi \mathrm{e}^{-\alpha} V}{h^3} \int_0^\infty p^2 \mathrm{e}^{-\beta p^2/2m} dp$$

- Using the integral relation $\int_0^\infty x^2 \,\mathrm{e}^{-ax^2} dx = \dfrac{1}{4}\sqrt{\dfrac{\pi}{a^3}}$, $N = \dfrac{\mathrm{e}^{-\alpha} V}{h^3} \left(\dfrac{2\pi m}{\beta}\right)^{3/2}$.
- Hence, $\mathrm{e}^{-\alpha} = \dfrac{Nh^3}{V}\left(\dfrac{\beta}{2\pi m}\right)^{3/2}$ and $n(p)dp = 4\pi N \left(\dfrac{\beta}{2\pi m}\right)^{3/2} p^2 \mathrm{e}^{-\beta p^2/2m} dp$.

- To find β, we will calculate the total energy U.
- From $p^2 = 2mu$, $\mathrm{dp} = \dfrac{mdu}{\sqrt{2mu}}$.

Maxwell-Boltzmann Statistics(4)

$$n(p)dp = 4\pi N\left(\frac{\beta}{2\pi m}\right)^{3/2} p^2 \mathrm{e}^{-\beta p^2/2m} dp \longrightarrow n(u)du = \frac{2N\beta^{3/2}}{\sqrt{\pi}}\sqrt{u}\mathrm{e}^{-\beta u}du$$

- The total energy is then,

$$U = \int_0^\infty un(u)\,\mathrm{d}u$$
$$= \frac{2N\beta^{3/2}}{\sqrt{TL}}\int_0^\infty u^{3/2}\mathrm{e}^{-\beta u}\,\mathrm{d}u = \frac{3}{2}\frac{N}{\beta}$$

(We used this relation: $\int_0^\infty x^{3/2}e^{-ax}\,\mathrm{d}x = \frac{3}{4a^2}\sqrt{\frac{\pi}{a}}$)

- According to the kinetic theory of gases, the total energy U of N particles of an ideal gas at temperature T is $U = {}^3\!/_2\, Nk_BT$.

$$\boxed{\beta = \frac{1}{k_BT}}$$

Boltzmann Distribution of Energy

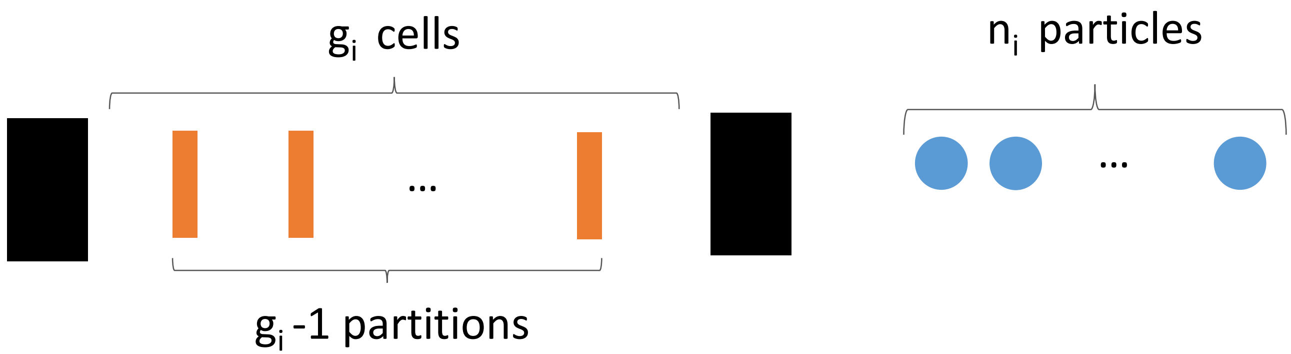
$$\boxed{n(u)\,\mathrm{d}u = \frac{2\pi N}{(\pi k_BT)^{3/2}}\sqrt{u}\mathrm{e}^{-u/k_BT}du}$$

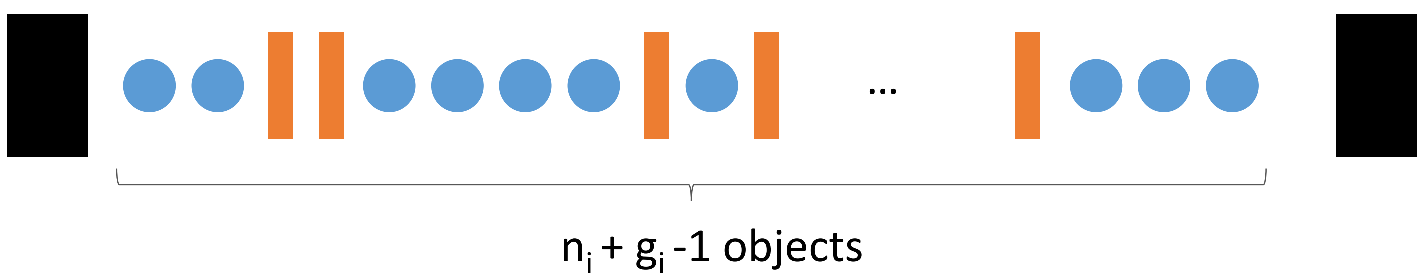
Bose-Einstein Statistics

- Bose-Einstein statistics governs identical and indistinguishable particles. (Maxwell-Boltzmann statistics governs identical but distinguishable particles.)
- Assumes all quantum state have equal probabilities - the cells that represent them in phase space have the same volumes.
- g_i represents the number of states that have the same energy level u_i (degeneracy of energy level i).
- The number of states g_i that are included in the level is equal to the probability that the energy level u_i be occupied.
- So, for each energy level u_i, we have to consider the number of possibilities that n_i particles are distributed in g_i cells.

Bose-Einstein Statistics(2)

- We can consider a series of $n_i + g_i - 1$ objects placed in a line.





- $(n_i + g_i - 1)!$ possible permutations.
- $n_i!$ permutations among particles and $(g_i - 1)!$ permutations among partitions are irrelevant.

$$\frac{(n_i + g_i - 1)!}{n_i!\,(g_i - 1)!}$$ possible distinguishable arrangement

Bose-Einstein Statistics(3)

- Probability W of entire N particle becomes

$$W = \prod \frac{(n_i + g_i - 1)!}{n_i!\,(g_i - 1)!}$$

and in case of $(n_i + g_i) \gg 1$

$$W = \prod \frac{(n_i + g_i)!}{n_i!\,(g_i - 1)!} \quad .$$

- Following a similar approach as in Maxwell-Boltzmann statistics,

$$\ln W = \sum [\ln(n_i + g_i)! - \ln n_i! - \ln(g_i - 1)!]$$

- By applying Stirling's formula ($\ln n! = n \ln n - n$)

$$\ln W = \sum [(n_i + g_i)\ln(n_i + g_i) - n_i \ln n_i - \ln(g_i - 1)! - g_i]$$

Bose-Einstein Statistics(4)

- As before, the condition for most probable distribution can be written, with respect to small changes δn_i, as $\delta \ln W_{max} = 0$. Thus,

$$\delta \ln W_{max} = \sum [\ln(n_i + g_i) - \ln n_i]\delta n_i = 0 \cdot$$

- There are two constraints; conservation of particles $\sum \delta n_i = 0$ and conservation of energy, $\sum u_i \delta n_i = 0$ ·
- Using the Lagrange multiplier method,

$$\sum [\ln(n_i + g_i) - \ln n_i - \alpha - \beta u_i]\delta n_i = 0 \quad .$$

- And the general solution for this is

$$\ln \frac{n_i + g_i}{n_i} - \alpha - \beta u_i = 0 \cdot$$

- This gives

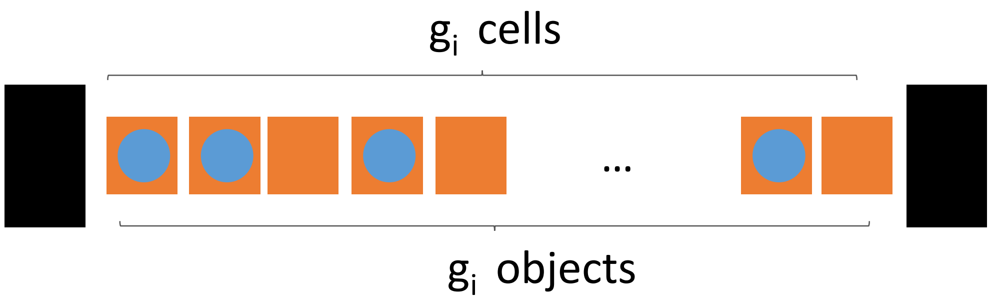
$$\boxed{n_i = \frac{g_i}{\mathrm{e}^{\alpha}\mathrm{e}^{\beta u_i} - 1} = \frac{g_i}{\mathrm{e}^{\alpha}\mathrm{e}^{u_i/k_B T} - 1}}$$

Bose-Einstein distribution law

$$\beta = \frac{1}{k_B T}$$

Fermi-Dirac Statistics

- Fermi-Dirac statistics governs identical and indistinguishable particles with exclusion principle.
- We assume each cell can be occupied by only one particle.
- Then, n_i cells are filled and $g_i - n_i$ cells are vacant.



- g_i cells can be rearranged in $g_i!$ different ways but $n_i!$ permutations and $(g_i - n_i)!$ permutations are irrelevant.
- Thus, the number of distinguishable arrangements among the cells is

$$\frac{g_i!}{n_i!\,(g_i - n_i)!}\ .$$

- The probability W of the entire distribution is then,

$$W = \prod \frac{g_i!}{n_i!\,(g_i - n_i)!}\ .$$

Fermi-Dirac Statistics(2)

- By taking the logarithms,

$$\ln W = \sum [\ln g_i! - \ln n_i! - \ln(g_i - n_i)!] \, .$$

- Applying Stirling's formula gives

$$\ln W = \sum [g_i \ln g_i - n_i \ln n_i - (g_i - n_i)\ln(g_i - n_i)] \, .$$

- The most probable distribution can be found by

$$\delta \ln W_{max} = \sum [-\ln n_i + \ln(g_i - n_i)]\delta n_i = 0 \, .$$

- The two constraints for the Lagrange multiplier method are

$$-\alpha \sum \delta n_i = 0 \quad \text{and} \quad -\beta \sum u_i \delta n_i = 0 \, .$$

- This gives

$$\sum [-\ln n_i + \ln(g_i - n_i) - \alpha - \beta u_i]\delta n_i = 0 \, .$$

Fermi-Dirac Statistics(2)

- The general solution is

$$\ln \frac{g_i - n_i}{n_i} - \alpha - \beta u_i = 0 \quad .$$

$$\frac{g_i}{n_i} - 1 = \mathrm{e}^{\alpha} \mathrm{e}^{\beta u_i}$$

$$\boxed{n_i = \frac{g_i}{\mathrm{e}^{\alpha} \mathrm{e}^{\beta u_i} + 1} = \frac{g_i}{\mathrm{e}^{\alpha} \mathrm{e}^{u_i / k_B T} + 1}}$$

Fermi-Dirac distribution law

Summary

- Maxwell Boltzmann: Classical Distinguishable Particles

$$\boxed{n_i = \frac{g_i}{\mathrm{e}^{\alpha}\mathrm{e}^{u_i/k_B T}}}$$

- Bose-Einstein: Indistinguishable Particles

$$\boxed{n_i = \frac{g_i}{\mathrm{e}^{\alpha}\mathrm{e}^{u_i/k_B T} - 1}}$$

- Fermi-Dirac: Indistinguishable Particles with Exclusion Principle

$$\boxed{n_i = \frac{g_i}{\mathrm{e}^{\alpha}\mathrm{e}^{u_i/k_B T} + 1}}$$