Lecture 9

13.02.2019

Fermi-Dirac statistics

Maxwell-Boltzmann: indistinguishable particles

- System of identical, indistinguishable and free particles, such that there are n_1 particles in the energy state ϵ_1, n_2 particles in the energy state $\epsilon_2, \cdots$. For a specific partition of the number of particles in each energy state $\{n_i\}$ we have

$$W(\{n_i\}) = \prod_i \frac{g_i^{n_i}}{n_i!},$$ number of microstates where $g_i \gg 1$ corresponds to energy states at ϵ_i

- The total multiplicity of a macrostate would be a sum over all the partitions $\{n_i\}$ that correspond to the same macroscopic energy $U = \sum_i \epsilon_i n_i$ and $N = \sum_i n_i$

$$\Omega(U,N) = e^{S/k} = \sum_{\{n_i\}} W(\{n_i\}) \approx W\left(\left\{n_i^{(eq)}\right\}\right)$$

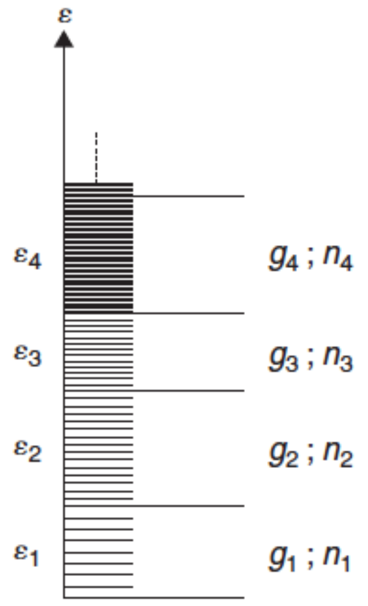
The sum is dominated by the partition with the largest number of microstates, which is the equilibrium distribution $\left\{n_i^{(eq)}\right\}$

- We determined the equilibrium distribution in the canonical ensemble

$$\boldsymbol{n_i = \frac{N}{Z_1} g_i e^{-\beta\epsilon_i}, \;\; Z_1 = \sum_i g_i\, e^{-\beta\epsilon_i}}$$

- Grand-canonical partition functions

$$\Xi(T,\mu) = \sum_{\boldsymbol{n}} \frac{\boldsymbol{1}}{\boldsymbol{n!}} \boldsymbol{e^{\beta n\mu} Z_1^n = e^{\lambda Z_1}}, \qquad \boldsymbol{\lambda = e^{\beta\mu}}$$



Bose-Einstein distribution: counting of microstates

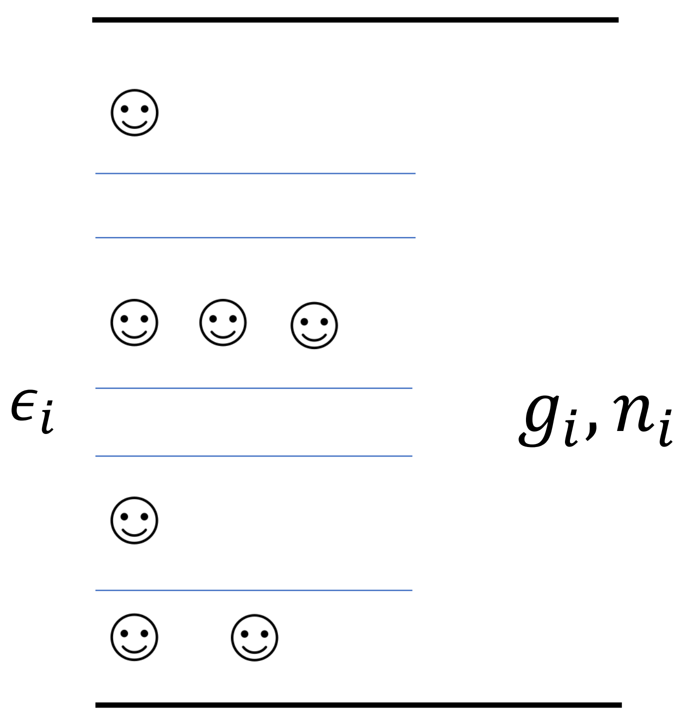
- Each energy levels ϵ_i has a degeneracy g_i

Number of ways of arranging n_i bosons in g_i quantum states with energy level ϵ_i:

g_i degenerate energy levels $\sim g_i$ identical boxes

n_i particles $\sim n_i$ identical balls

Number of ways of distributing n_i balls between g_i boxed equals the number of combinations with n_i balls and $(g_i - 1)$ –walls between the lined up boxes



$$\mathrm{W_i}(n_i, g_i) = \frac{(n_i + g_i - 1)!}{n_i!\,(g_i - 1)!}$$

Number of microstates for a partition $\{n_i\}$*:*

$$\mathrm{W_b}(\{\mathrm{n_i}\}) = \prod_i \mathrm{W}_i(n_i, g_i) = \prod_i \frac{(n_i+g_i-1)!}{n_i!(g_i-1)!}$$

- The total multiplicity of a macrostate would be a sum over all the partitions $\{n_i\}$ that correspond to the same macroscopic energy $U = \sum_i \epsilon_i n_i$ and $N = \sum_i n_i$

$$\Omega(U, N) = e^{S/k} = \sum_{\{n_i\}} W_b(\{n_i\}) \approx W_b\left(\left\{n_i^{(eq)}\right\}\right)$$

Bose-Einstein statistics (grand-canonical)

- Sponteneous fluctuations induce a change in the population number

$$n_i \rightarrow n_i + 1$$

- Change in entropy:

$$\Delta S = k\left[\ln\frac{(n_i + g_i)!}{(n_i + 1)!} - \ln\frac{(n_i + g_i - 1)!}{n_i!}\right] = k\ln\frac{g_i + n_i}{n_i}$$

- Change in energy: $\Delta U = \epsilon_i$
- Change in number of particles: $\Delta N = 1$

- These spontaneous fluctuations are in thermodynamic equilibrium: $T\Delta S = \Delta U - \mu\Delta N$

$$n_i = \frac{g_i}{e^{\beta(\epsilon_i - \mu)} - 1}$$

Bose-Einstein statistics

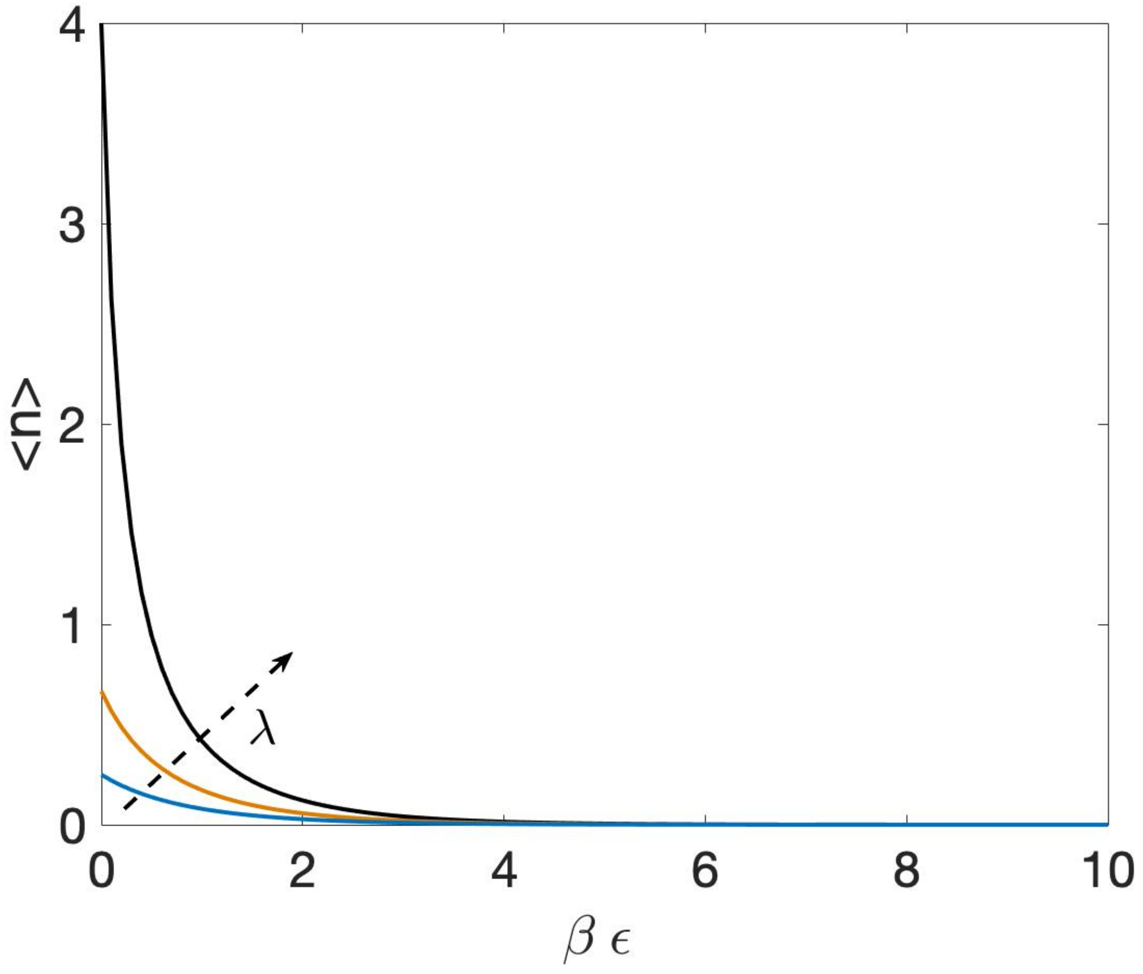
Equilibrium distribution of bosons over energy states

$$\boldsymbol{n_i = \frac{g_i}{e^{\beta(\epsilon_i - \mu)} - 1} = \frac{g_i}{e^{\beta\epsilon_i}\lambda^{-1} - 1}}$$

- Grand-canonical partition function

$$\Xi(T,\mu) = \prod_i \left(\sum_{n_i=0}^{\infty} e^{-\beta n_i (\epsilon_i - \mu)} \right)$$

$$\Xi(T,\mu) = \prod_i \frac{1}{1 - e^{-\beta(\epsilon_i - \mu)}}$$



Free fermions: Fermi-Dirac statistics

<u>Fermions:</u> ingistinguishable particles with $\frac{1}{2}$ spin obeying the Pauli exclusion principle

Number of ways of arranging n_i fermions in g_i quantum states at energy ϵ_i:

- *1st particle has* g_i *avalaible states, 2nd particle has* $(g_i{-}1)$ *possible states, 3rd particle has*

  $(g_i{-}2)$ *, …the* $n_i th$ *particle has* $(g_i - n_i + 1)$

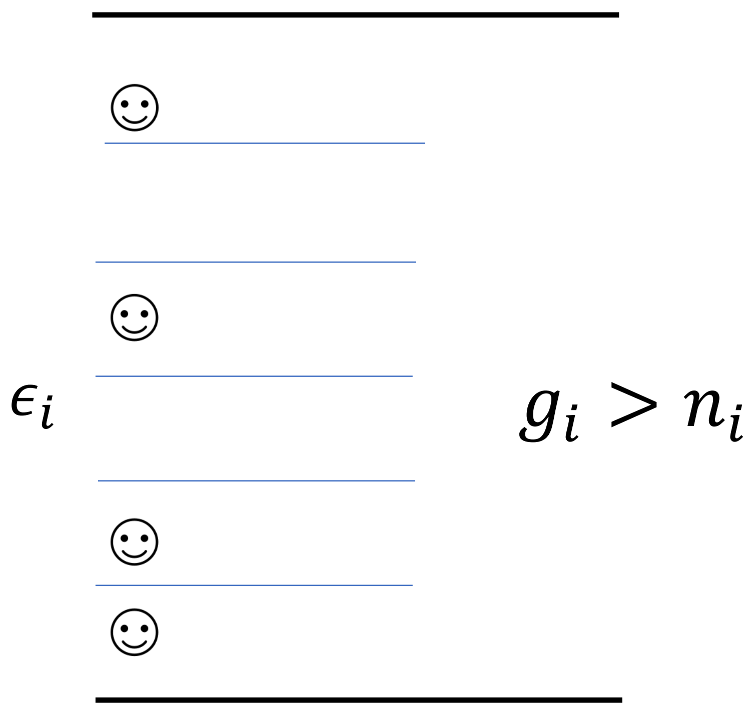
- $g_i(g_i-1)\cdots(g_i-n_i+1) = \frac{g_i!}{(g_i-n_i)!}$

Number of microstates for a partition $\{n_i\}$*:*

$$W_f(\{n_i\}) = \prod_i \frac{g_i!}{n_i!\,(g_i-n_i)!}$$

- The total multiplicity of a macrostate = sum over all the partitions $\{n_i\}$ that correspond to the same macroscopic energy $U = \sum_i \epsilon_i\, n_i$ and $N = \sum_i n_i$

$$\Omega(U,N) = e^{S/k} = \sum_{\{n_i\}} W_f(\{n_i\}) \approx W_f\left(\left\{n_i^{(eq)}\right\}\right)$$



Fermi-Dirac statistics: Grand-canonical ensemble

- Sponteneous fluctuations induce a change in the population number

$$n_i \rightarrow n_i + 1$$

- Change in entropy:

$$\Delta S = k\left[\ln\frac{g_i!}{(n_i+1)!\,(g_i-n_i-1)!} - \ln\frac{g_i!}{n_i!\,(g_i-n_i)!}\right] = k\ln\frac{g_i-n_i}{n_i}$$

- Change in energy:

$$\Delta U = \epsilon_i$$

- Change in number of particles: $\Delta N = 1$

Equilibrium fluctuations: $T\Delta S = \Delta U - \mu\Delta N \rightarrow kT\log\frac{g_i-n_i}{n_i} = \epsilon_i - \mu \rightarrow$

Fermi-Dirac statistics: Grand-canonical

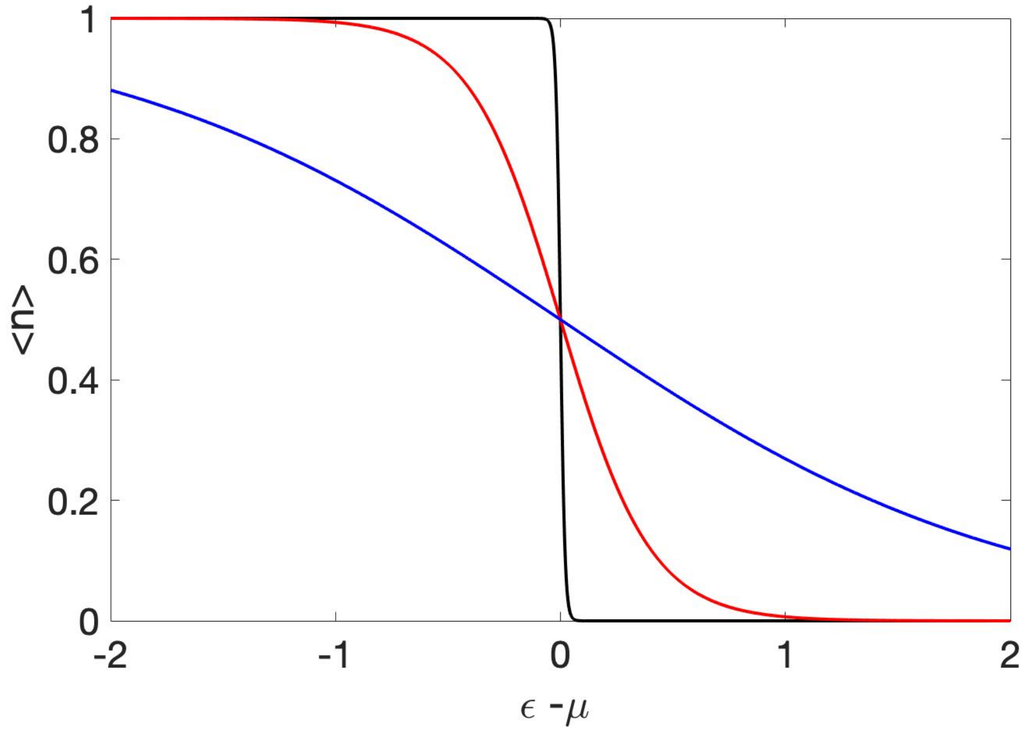
- Equilibrium distribution of the number of fermions in each energy state

$$\boldsymbol{n_i = \frac{g_i}{e^{\beta(\epsilon_i - \mu)} + 1}}$$

- Filling fraction $f_i = \frac{n_i}{g_i}$ of the energy state ϵ_i

$$\mathrm{f_i} = \frac{1}{e^{\beta(\epsilon_i - \mu)} + 1}$$

$$f_i = \frac{1}{e^{\beta\epsilon_i}\lambda^{-1} + 1}, \lambda = e^{\beta\mu}$$



Fermi-Dirac statistics

- Average occupation number

$$n_i = \langle n \rangle(\epsilon_i) = \frac{g_i}{e^{\beta(\epsilon_i - \mu)} + 1}$$

- Number of particles

$$N = \sum_i n_i = \sum_i \frac{g_i}{e^{\beta(\epsilon_i - \mu)} + 1}$$

- Energy

$$U = \sum_i \epsilon_i n_i = \sum_i \frac{\epsilon_i g_i}{e^{\beta(\epsilon_i - \mu)} + 1}$$

Classical limit: $f_i \ll 1 \;\; \leftrightarrow n_i \ll g_i$ (low density of particles per energy state)

- Fermi Dirac:

$$W_{FD}(n_1, n_2, \cdots) = \prod_i \frac{g_i!}{n_i!\,(g_i - n_i)!} = \prod_i \frac{1}{n_i!} g_i \cdot (g_i - 1) \cdots (g_i - n_i + 1) \approx \prod_i \frac{g_i^n}{n_i!}$$

- Bose Einstein:

$$W_{BE}(n_1, n_2, \cdots) = \prod_i \frac{(n_i + g_i - 1)!}{n_i!\,(g_i - 1)!} = \prod_i \frac{1}{n_i!} g_i \cdot (g_i + 1) \cdots (g_i + n_i - 1) \approx \prod_i \frac{g_i^n}{n_i!}$$

- Maxwell Boltzmann:

$$W_{MB}(n_1, n_2, \cdots) = \prod_i \frac{g_i^n}{n_i!}$$

Classical limit: $\epsilon_i \ll kT, \mu(T) \ll 0$ (high-T limit)

- Fermi Dirac/Bose-Einstein distribution:

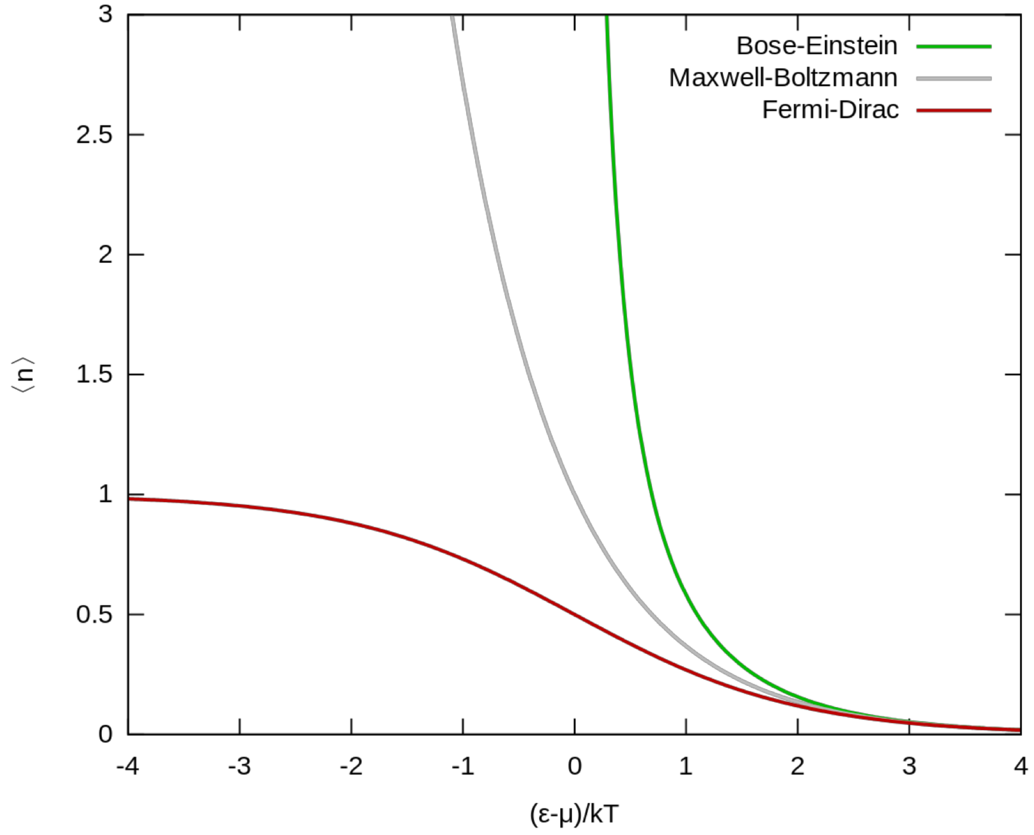
$$f_i = \frac{1}{e^{\beta(\epsilon_i - \mu)} \pm 1} = e^{\beta\mu} \frac{e^{-\beta\epsilon_i}}{1 \pm e^{-\beta\epsilon_i} e^{\beta\mu}} \approx e^{\beta\mu} e^{-\beta\epsilon_i}$$

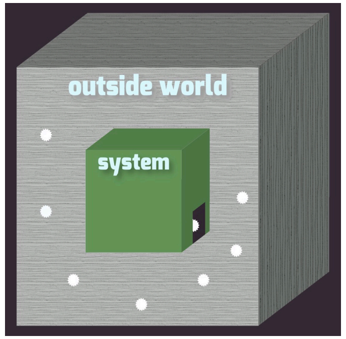
- Maxwell Boltzmann distribution:

$$f_i^{MB} = \frac{N}{Z_1} e^{-\beta\epsilon_i} = e^{\beta\mu} e^{-\beta\epsilon_i}$$

- Classical ideal gas limit: $\mu = -kT \ln \frac{V}{N\Lambda^3(T)} \ll 0 \rightarrow$

$$\boldsymbol{T \gg T^* = \left(\frac{h^2}{2\pi mk}\right)\rho^2, \qquad \rho = \frac{N}{V}}$$





Grand-canonical ensemble for free quantum particle

Each identical particle can occupy discrete energy states ϵ_j, $j = 1, 2, \cdots$ is the state number

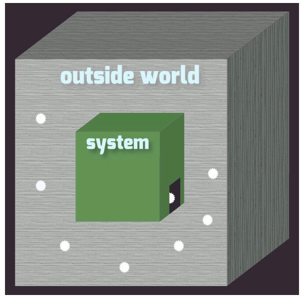
For N identical particles, there are n_j number of particles (occupation number) in the energy state ϵ_j

The energy of a specific microstate with $N_s = \sum_j n_j$ particles is $E_s = \sum_j n_j \epsilon_j$

$\sum_s \equiv$sum over all particles number N_s and over all the partitions of particles N_s in the quantum states with total energy E_s

$$\Xi(T,\mu) = \sum_{N_s} \sum_{\substack{\{n_j\} \\ \sum_j n_j = N_s}} e^{-\beta(E_s - \mu N_s)} = \sum_{\{n_j\}} e^{-\beta \sum_j n_j(\epsilon_j - \mu)}$$

$$\Xi(T,\mu) = \left(\sum_{n_1} e^{-\beta n_1(\epsilon_1 - \mu)}\right) \cdot \left(\sum_{n_2} e^{-\beta n_2(\epsilon_2 - \mu)}\right) \cdot\cdot \left(\sum_{n_3} e^{-\beta n_3(\epsilon_3 - \mu)}\right) \cdots$$



Occupation number of a microstate

Probability of the system in a specific microstate a fixed T and μ

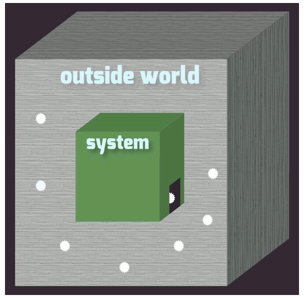
$$P(s) = \frac{1}{\Xi(T,\mu)} e^{-\beta(E_s-\mu N_s)} = \frac{e^{-\beta n_1(\epsilon_1-\mu)} \cdot e^{-\beta n_2(\epsilon_2-\mu)} \cdot e^{-\beta n_3(\epsilon_3-\mu)} \dots}{\left(\sum_{n_1} e^{-\beta n_1(\epsilon_1-\mu)}\right) \cdot \left(\sum_{n_2} e^{-\beta n_2(\epsilon_2-\mu)}\right) \cdot \left(\sum_{n_3} e^{-\beta n_3(\epsilon_3-\mu)}\right) \dots}$$

$$\boldsymbol{P(s) = \frac{e^{-\beta n_1(\epsilon_1-\mu)}}{\left(\sum_{n_1} e^{-\beta n_1(\epsilon_1-\mu)}\right)} \cdot \frac{e^{-\beta n_2(\epsilon_2-\mu)}}{\left(\sum_{N_2} e^{-\beta N_2(\epsilon_2-\mu)}\right)} \cdot \frac{e^{-\beta n_3(\epsilon_3-\mu)}}{\left(\sum_{n_3} e^{-\beta n_3(\epsilon_3-\mu)}\right)} \cdots}$$

$$\boldsymbol{P(s) = P(n_1) \cdot P(n_2) \cdot P(n_3) \cdots}$$

Probability for an occupation number n of the given energy level at fixed T and μ

$$\boldsymbol{P_\epsilon(n) = \frac{e^{-\beta n(\epsilon-\mu)}}{\left(\sum_n e^{-\beta n(\epsilon-\mu)}\right)}}$$



Free FERMIONS in grand canonical ensemble

The number of fermions in each energy states can be $n = 0, 1$

$$\sum_{n=0}^{1} e^{-\beta n(\epsilon-\mu)} = 1 + e^{-\beta(\epsilon-\mu)}$$

Grand-canonical partition function

$$\Xi(T,\mu) = \prod_i \left(\sum_{n_i} e^{-\beta n_i(\epsilon_1-\mu)} \right) = \prod_i \left(1 + e^{-\beta(\epsilon_i-\mu)}\right)$$

Probability for having n fermions in a given energy state a fixed T and μ

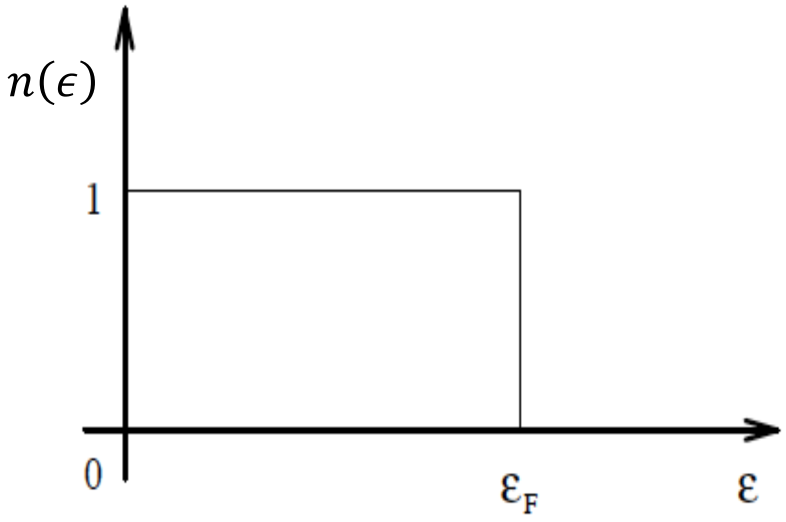
$$P_\epsilon(n) = \frac{e^{-\beta n(\epsilon-\mu)}}{1 + e^{-\beta(\epsilon-\mu)}}$$

Average number of fermions $\langle n \rangle$ with energy ϵ a fixed T and μ

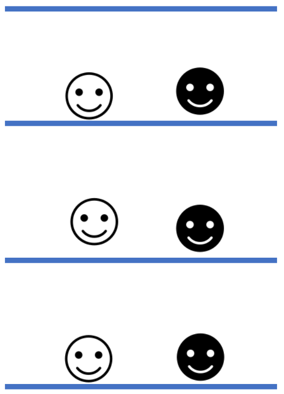
$$\langle n \rangle(\epsilon) = \sum_{n=0}^{1} n P_\epsilon(n) \rightarrow \langle n \rangle(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

Fermi Dirac distribution at T=0 K

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1} \to_{T\to 0} \begin{cases} 1, & \epsilon < \mu \\ 0, & \epsilon > \mu \end{cases}$$

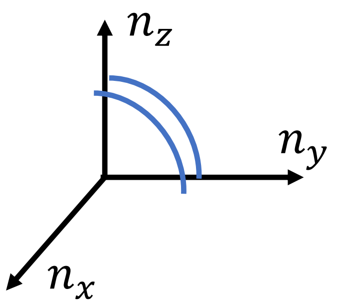


$\epsilon_F \equiv \mu$ Fermi energy level below which all states are occupied



Fermi energy is determined by the density of the Fermi gas $\epsilon_F = \epsilon_F(\rho)$

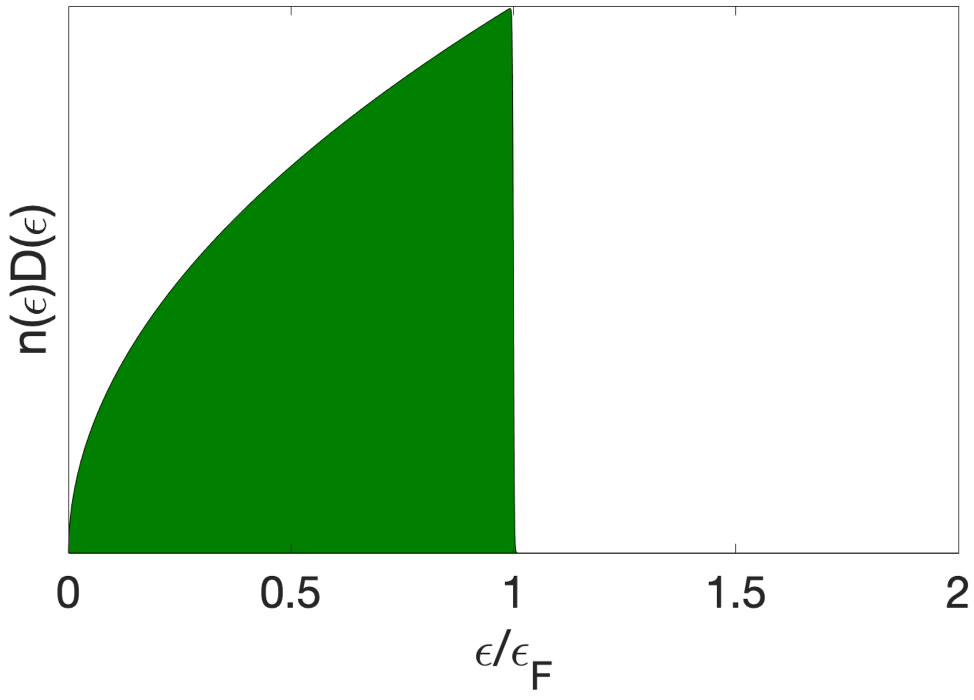
Fermi-Dirac statistics at T=0 K in 3D

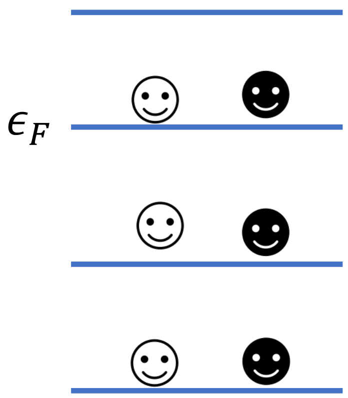


Ideal gas: $\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2$

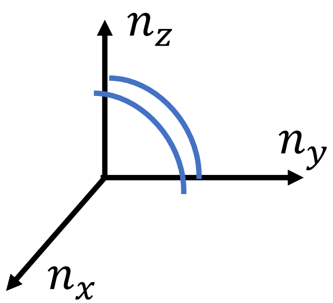
Density of states $D(\epsilon)d\epsilon = (4\pi n^2)dn \rightarrow$

$$D(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \epsilon^{1/2}, \qquad V = L^3$$





Fermi-Dirac statistics at T=0 K in 3D



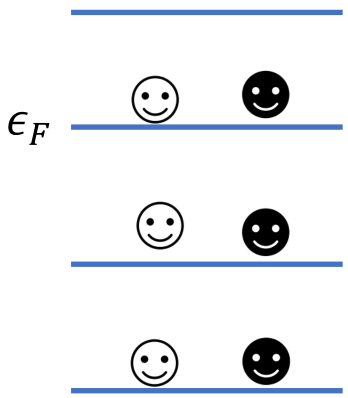
Ideal gas: $\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2$

Density of states $D(\epsilon)d\epsilon = (4\pi n^2)dn \rightarrow D(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \epsilon^{1/2}, \quad V = L^3$

Number of particles

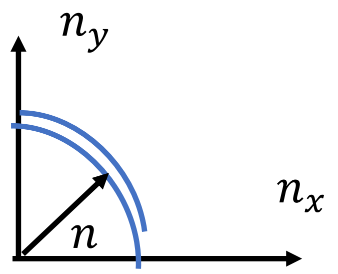
$$N = \sum_i \langle n\rangle(\epsilon_i) = 2\int_0^\infty d\epsilon\ D(\epsilon)H(\epsilon-\epsilon_F) = 2\int_0^{\epsilon_F} d\epsilon\ D(\epsilon)$$

$$N = 2\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^{\epsilon_F} d\epsilon\ \epsilon^{1/2} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}\ \epsilon_F^{3/2}$$



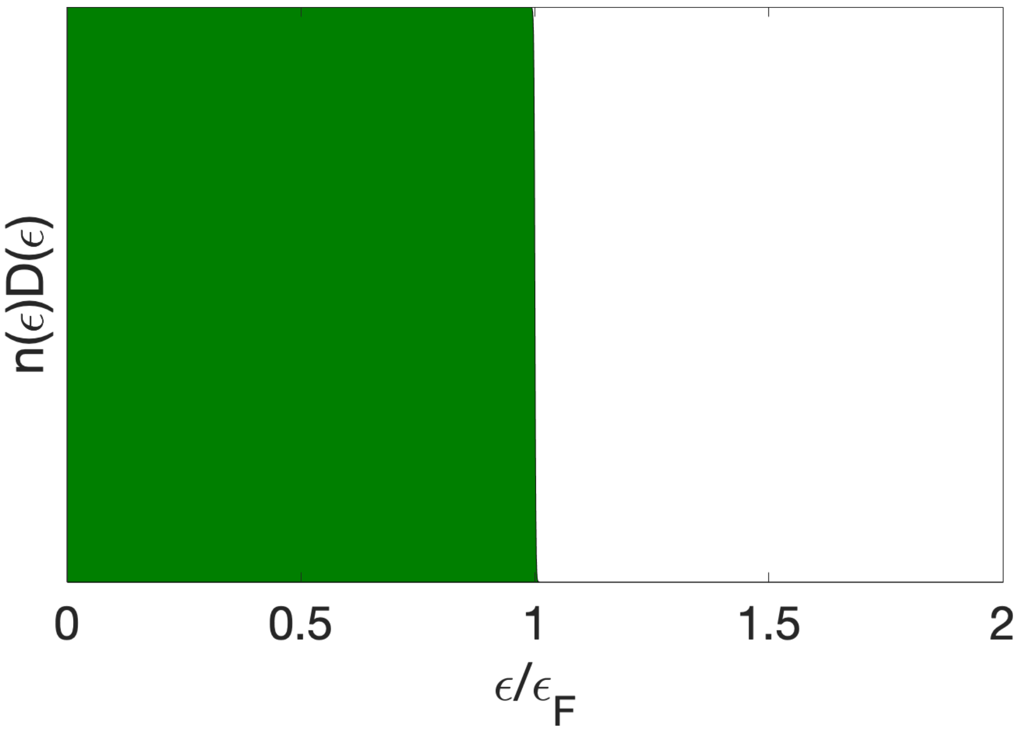
- Fermi energy $\boldsymbol{\epsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2\rho\right)^{\frac{2}{3}}}$
- Fermi temperature $\boldsymbol{T_F = \frac{\epsilon_F}{k} = \frac{\hbar^2}{2mk}\left(3\pi^2\rho\right)^{\frac{2}{3}} < \mathrm{T}^* = \left(\frac{h^2}{2\pi mk}\right)\rho^2}$
- Electron gas in metals $\boldsymbol{T_F \sim 10^4 - 10^5\ K \gg 3\times 10^2 K}$ (degenerate gas--- behaves as if it was $0K$ for a wide range of $T \ll T\_F$)

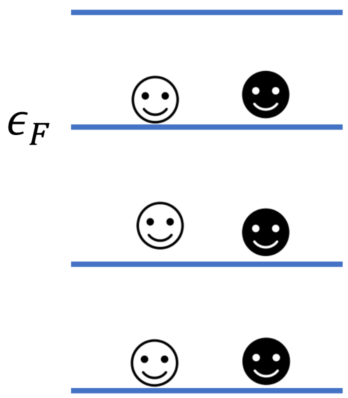
Fermi-Dirac statistics at T=0 K in 2D



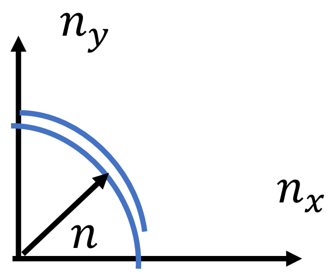
Ideal gas: $\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2$

Density of states $D(\epsilon)d\epsilon = (2\pi n)dn \rightarrow D(\epsilon) = \frac{L^2}{4\pi}\frac{2m}{\hbar^2}$





Fermi-Dirac statistics at T=0 K in 2D



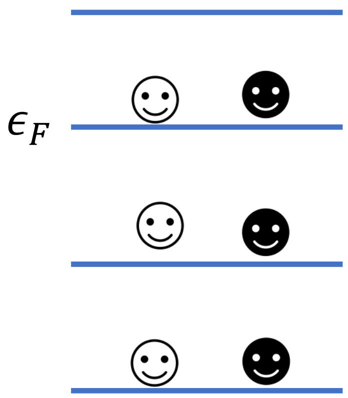
Ideal gas: $\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2$

Density of states $D(\epsilon)d\epsilon = (2\pi n)dn \rightarrow D(\epsilon) = \frac{L^2}{4\pi}\frac{2m}{\hbar^2}$

Number of particles

$$N = \sum_i \langle n \rangle(\epsilon_i) = 2\int_0^\infty d\epsilon\ D(\epsilon)H(\epsilon - \epsilon_F) = 2\int_0^{\epsilon_F} d\epsilon\ D(\epsilon)$$

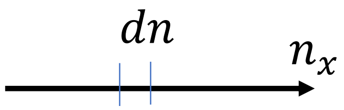
$$N = \frac{L^2}{\pi}\frac{m}{\hbar^2}\int_0^{\epsilon_F} d\epsilon = \frac{L^2}{\pi}\frac{m}{\hbar^2}\epsilon_F$$



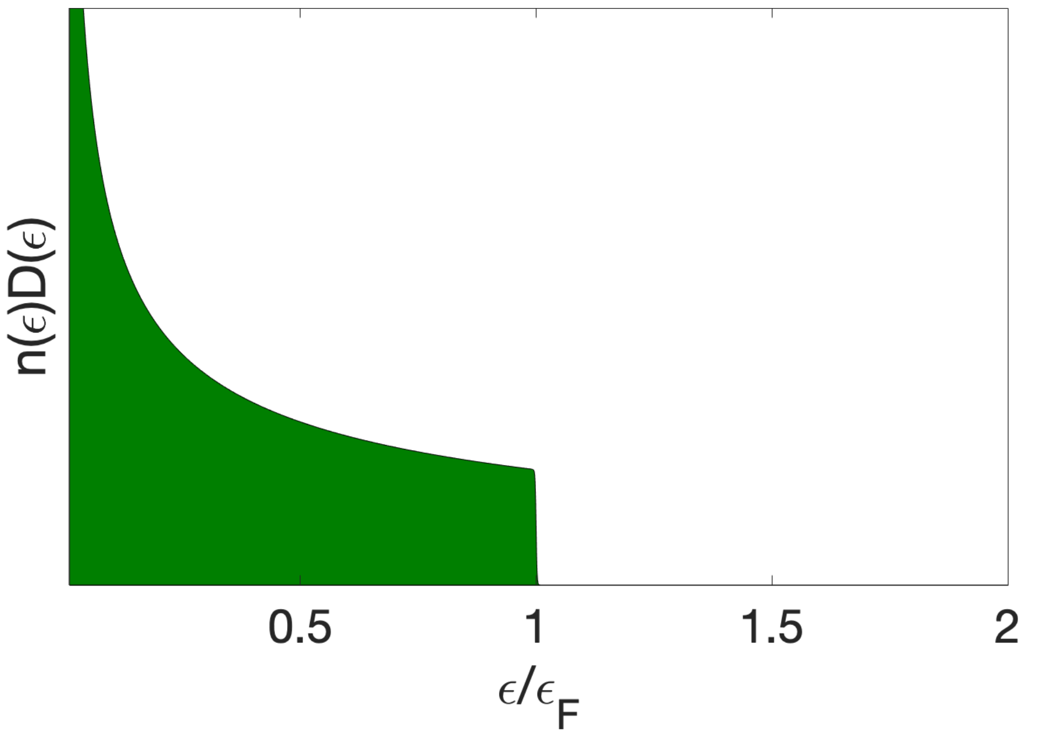
- Fermi energy $\boldsymbol{\epsilon_F = \frac{\hbar^2}{m}\pi\rho}$
- Fermi temperature $\boldsymbol{T_F = \frac{\epsilon_F}{k} = \frac{\hbar^2}{m}\pi\rho}$

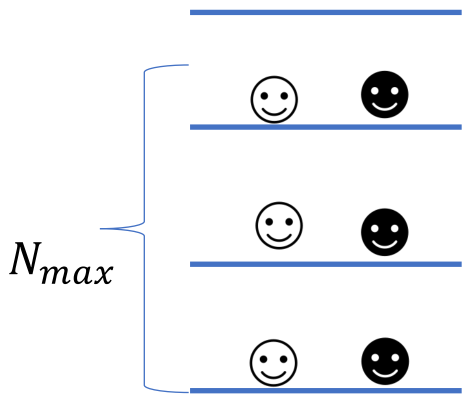
Fermi-Dirac statistics at T=0 K in 1D

Ideal gas: $\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2$

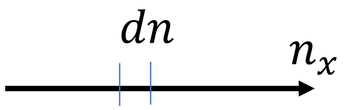


Density of states $D(\epsilon)d\epsilon = dn \rightarrow D(\epsilon) = \frac{L}{4\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \epsilon^{-1/2}$





Fermi-Dirac statistics at T=0 K in 1D

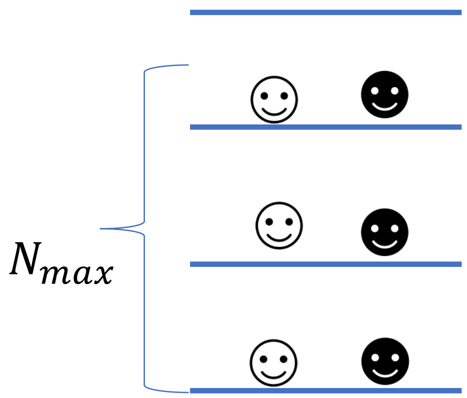


Ideal gas: $\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2$

Density of states $D(\epsilon)d\epsilon = dn \rightarrow D(\epsilon) = \frac{L}{4\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \epsilon^{-1/2}$

$$N = 2\int_0^{\epsilon_F} d\epsilon \; D(\epsilon) = \frac{L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \epsilon_F^{\frac{1}{2}} \rightarrow \epsilon_F = \frac{\hbar^2}{2m}(\pi\rho)^2$$

Number of particles $N = \sum_i \langle n \rangle(\epsilon_i) = 2N_{max}$

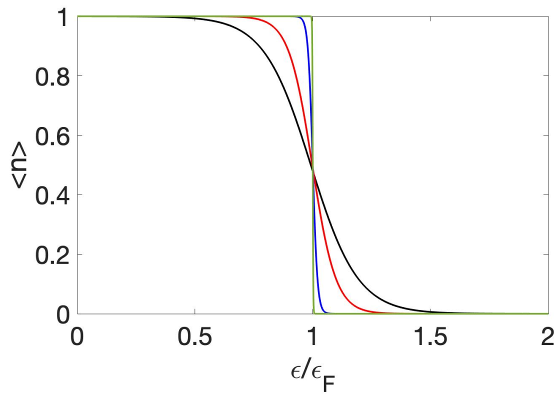


- Fermi energy $\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 N_{max}^2 \rightarrow$

$$\epsilon_F = \frac{\hbar^2}{2m}(\pi\rho)^2, \qquad \rho = \frac{N}{L}$$

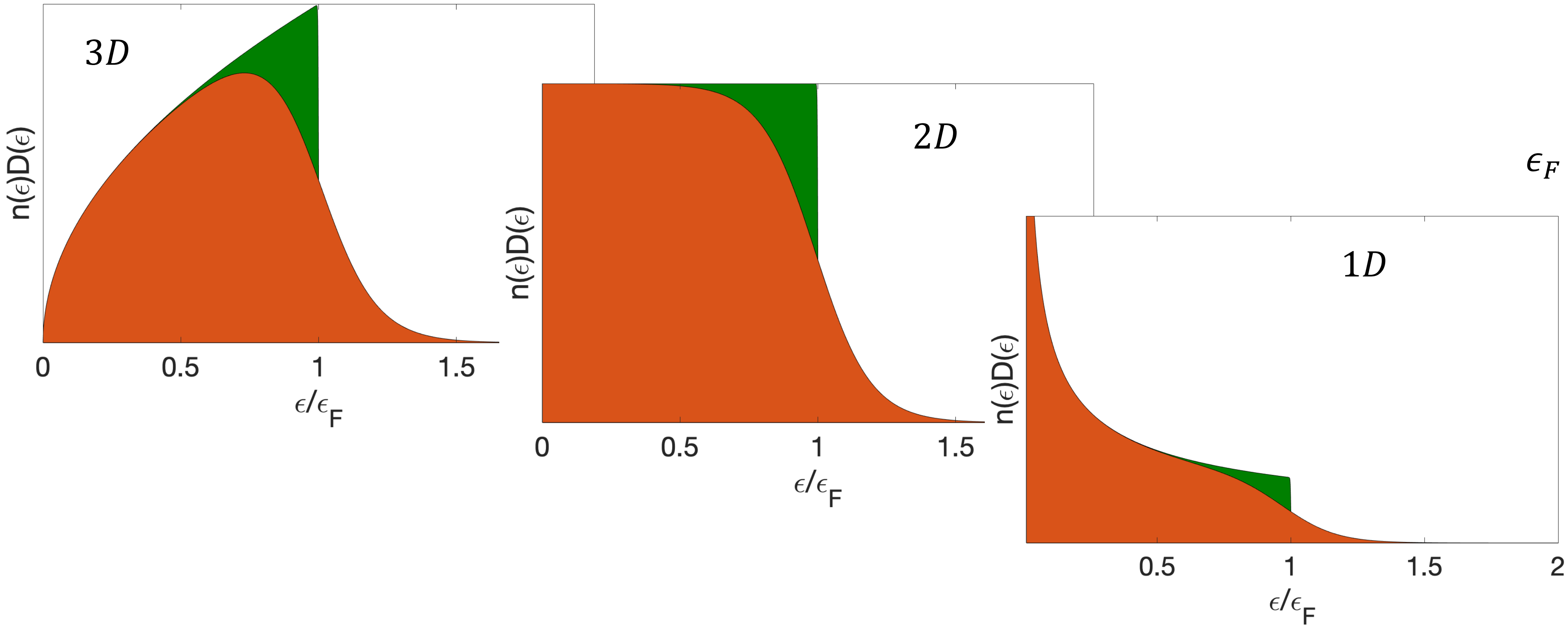
Fermi temperature $\mathrm{T_F} = \frac{\hbar^2}{2mk}(\pi\rho)^2$

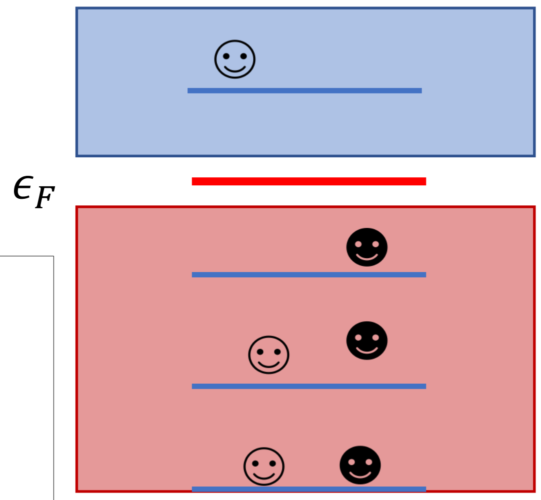
Fermi Dirac distribution at T>0 K

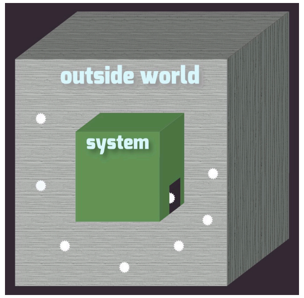


$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1}, \qquad \mu(\epsilon_F, T)$$

Energy states above the Fermi level are occupied by excited fermions







Particle number fluctuations

Probability for having $\boldsymbol{n}$ free fermions in a given energy state $\boldsymbol{\epsilon_i}$ at fixed T and $\boldsymbol{\mu}$

$$P_i(n) = \frac{\left(\lambda e^{-\beta\epsilon_i}\right)^n}{1+\lambda e^{-\beta\epsilon_i}} = \left(\frac{n_i}{1-n_i}\right)^n = \begin{cases} 1-n_i, & n=0 \\ n_i, & n=1 \end{cases}, \qquad n_i = \frac{1}{\lambda^{-1}e^{\beta\epsilon_i}+1}$$

$$\langle n\rangle_i = P_i(1) = n_i$$

$$\langle n^2\rangle_i = \sum_{i=0}^{1} n^2 P_i(n) = P_i(1) = n_i$$

Mean square fluctuations

$$\sigma_n^2 = \langle n^2\rangle_i - \langle n\rangle_i^2 = n_i - n_i^2$$

Relative mean square fluctuations

$$\frac{\sigma_n^2}{n_i^2} = \frac{1}{n_i} - 1 \rightarrow 0, as\ n_i \rightarrow 1$$

Negative statistical correlation– statistical repelling force