PHY 530
STEEM Refresher course 3
Occupation factor

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STEEM Refresher 3

1. Occupation factor

2. (Tutorial) Thermal ensemble of classical particles

3. (Tutorial) Thermal ensemble of Bosons

4. (Tutorial) Thermal ensemble of Fermions

5. Take home message

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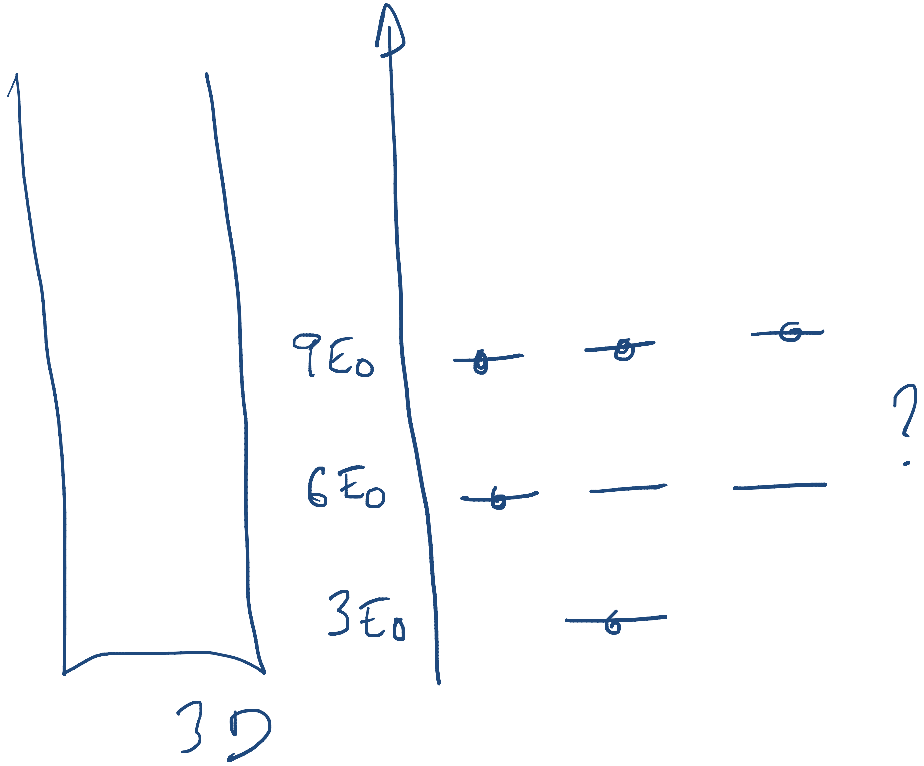
Towards the occupation factor

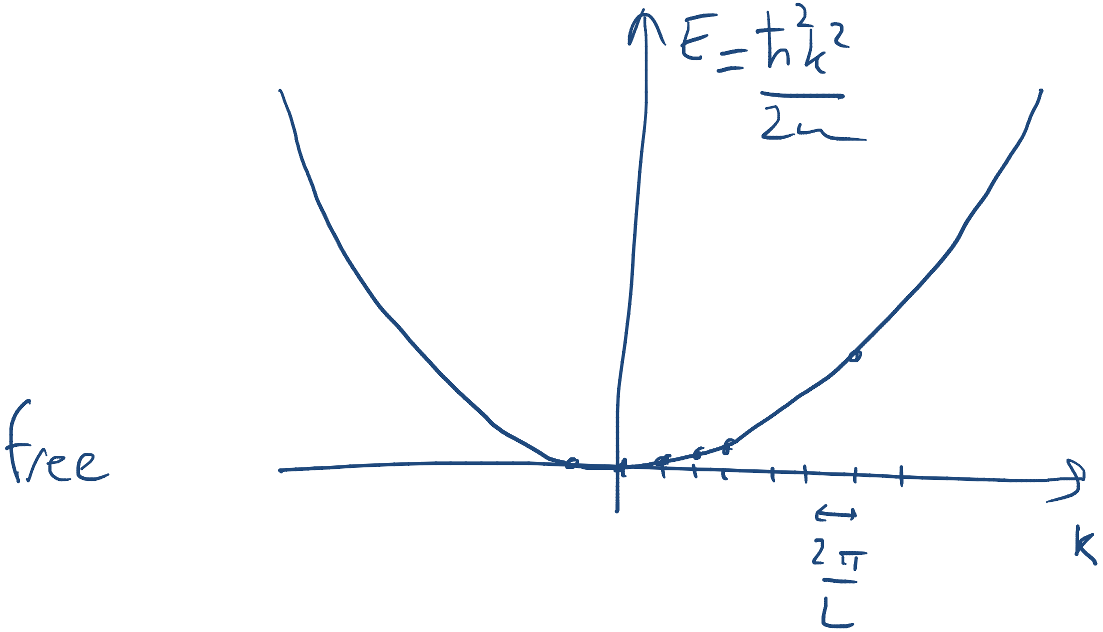
Lecture 2

Consider a given Hamiltonian.
How many states are there
with a given energy ?



Lecture 3

Introduce N>>1 particles to populate these states.
What is the probability for finding a particle
in any given state?



Occupation factor

The probability for finding a particle in any given state depends only on :

- the *energy* of the **state**
- the *statistics* of the **particles**
- the *temperature* and *chemical potential* of the **ensemble**

occupation factor

$$f(\epsilon) = \frac{1}{\exp\left(\frac{\epsilon-\mu}{k_B T}\right) + \alpha}$$

with $\alpha = \begin{cases} +1 & \text{Fermions} \to \text{Fermi Dirac distribution} \\ 0 & \text{Classical} \to \text{Maxwell Boltzmann distribution} \\ -1 & \text{Bosons} \to \text{Bose Einstein distribution} \end{cases}$

ADMITTED

Fermions, bosons and classical particles

$$f(\epsilon) = \frac{1}{\exp\left(\frac{\epsilon-\mu}{k_B T}\right) + \alpha} \quad \text{with } \alpha = \begin{cases} +1 & \text{Fermions} \rightarrow \text{Fermi Dirac distribution} \\ 0 & \text{Classical} \rightarrow \text{Maxwell Boltzmann distribution} \\ -1 & \text{Bosons} \rightarrow \text{Bose Einstein distribution} \end{cases}$$

1/2 3/2

Fermions ↔ half-integer spin

Electrons, quarks…

0, 1

Bosons ↔ integer spin

Photons, phonons…

For $\epsilon - \mu \gg k_B T$

Fermions ~ bosons ~ classical particles

$$f(\varepsilon) \sim \exp\left(\frac{\mu - \varepsilon}{k_T}\right)$$

Dealing with N>>1 (non-interacting) particles

Which particles are we talking about ?

Fermions ?
Bosons ?
Classical ?

Fermi-Dirac
Bose-Einstein
Maxwell-Boltzmann

What are the ensemble properties ?

Temperature ?
Chemical potential ?

Occupation factor

What is the "landscape" in which these particles live ?

1D, 2D, 3D ?
Hamiltonian ?

Density of State

Number of particles, total energy, density, pressure…

$$N = \int_0^\infty \underbrace{d\epsilon\, \overset{\text{DoS}}{D(\epsilon)}}_{\mathcal{E},\ \mathcal{E}+d\mathcal{E}}\, f(\epsilon) \qquad E = \int_0^\infty d\epsilon\, \epsilon\, D(\epsilon)\, f(\epsilon)$$

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Classical free particles – chemical potential

Consider N classical massive free particles in 3D, at a temperature T .

M.B

$$f(\varepsilon) = e^{\frac{\mu-\varepsilon}{kT}}$$

$$\hat{H} = \frac{p^2}{2m} + 3D \longrightarrow D(\varepsilon) = L^3 \gamma \sqrt{\varepsilon}$$

$$N = \int d\varepsilon \, D(\varepsilon) f(\varepsilon) = L^3 \gamma \int d\varepsilon \sqrt{\varepsilon}\, e^{\mu/kT} e^{-\varepsilon/kT} = L^3 \gamma \sqrt{(kT)^3} \left(\int du \sqrt{u}\, e^{-u} \right) e^{+\mu/kT}$$

$$u = \varepsilon/kT$$

$$= L^3 \gamma (kT)^{3/2} e^{+\mu/kT} \frac{\sqrt{\pi}}{2}$$

$$\boxed{\exp\left[\frac{\mu}{kT}\right] = \frac{2}{\sqrt{\pi}\,\gamma} \frac{1}{(kT)^{3/2}} \frac{N}{L^3}}$$

$\frac{N}{L^3} \rightarrow n$

$$\int_{>0} dx \sqrt{x}\, e^{-x} = \frac{\sqrt{\pi}}{2}$$

Classical free particles – energy per particle

Consider N classical massive free particles in 3D, at a temperature T .

$$\exp\left(\frac{\mu}{k_B T}\right) = \frac{N}{L^3 (k_B T)^{3/2}} \frac{2}{\gamma\sqrt{\pi}}$$

$\langle E \rangle = \dfrac{E \rightarrow ?}{N \rightarrow \text{ok!}}$

$$E = \int d\varepsilon\, D(\varepsilon) f(\varepsilon)\, \varepsilon = L^3 \gamma e^{\mu/kT} \int d\varepsilon\, \varepsilon \sqrt{\varepsilon}\, e^{-\varepsilon/kT}$$

$u = \dfrac{\varepsilon}{kT}$

$$= \underline{L^3 \gamma e^{\mu/kT}} (kT)^{5/2} \underbrace{\int du\, u\sqrt{u}\, e^{-u}}_{\frac{3\sqrt{\pi}}{4}}$$

$$= \frac{2N}{(kT)^{3/2}\sqrt{\pi}} (kT)^{5/2} \times \frac{3\sqrt{\pi}}{2\cdot 4} = \frac{3}{2} N kT$$

$$\boxed{\langle E \rangle = \frac{3}{2} kT}$$

in 2D? $D_{2D}(\varepsilon) = D_0 \rightarrow \langle E \rangle = kT$

1D $\quad D_{1D}(\varepsilon) = \dfrac{D_0}{\sqrt{\varepsilon}} \rightarrow \langle E \rangle = \dfrac{1}{2} kT$

$$\int_{>0} dx\, x\sqrt{x}\, e^{-x} = \frac{3\sqrt{\pi}}{4}$$

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Free bosons

Consider N free massless bosons in 3D, at a temperature T .

→ Bose Einstein $f(\varepsilon) = \dfrac{1}{e^{\frac{\varepsilon-\mu}{kT}} - 1}$

Free bosons density of states

$E = pc = \hbar c k$ with $\mathbf{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$

$L \to \infty$

How many states with energy between E and E+dE?

$$= \rho(E)dE = D(\varepsilon)dE$$

How many states with wave-vector between k and k+dk?

$E = \hbar c \times k \qquad dE = \hbar c \, dk \longrightarrow dk = dE/\hbar c$

Which "volume" does this represent ? $dV = V(k+dk) - V(k) = \frac{4}{3}\pi(k+dk)^3 - \frac{4}{3}\pi k^3 = 4\pi k^2 dk$

How many states are located in this "volume" ? $dV/\left(\frac{2\pi}{L}\right)^3$

$$\rho(E)dE = dV/\left(\frac{2\pi}{L}\right)^3 = \frac{L^3}{(2\pi)^3} 4\pi k^2 dk = \underbrace{\frac{L^3}{(2\pi)^3} \frac{4\pi E^2}{(\hbar c)^3}}_{D_{3D,\text{massless}}(\varepsilon)} dE$$

Free bosons

Consider N free massless bosons in 3D, at a temperature T .

Number of photons with an energy between ϵ and $\epsilon + d\epsilon$?

$$dN(\varepsilon) = D(\varepsilon)\, d\varepsilon\, f_{BE}(\varepsilon) = \frac{L^3}{(2\pi\hbar c)^3} \frac{4\pi\varepsilon^2}{e^{\varepsilon/kT}-1}\, d\varepsilon$$

$$D(\varepsilon)\, d\varepsilon \rightarrow \frac{L^3}{(2\pi)^3} \frac{4\pi E^2}{(\hbar c)^3} \qquad f_{BE}(\varepsilon) \rightarrow \frac{1}{e^{\varepsilon/kT}-1}$$

$\mu = 0$

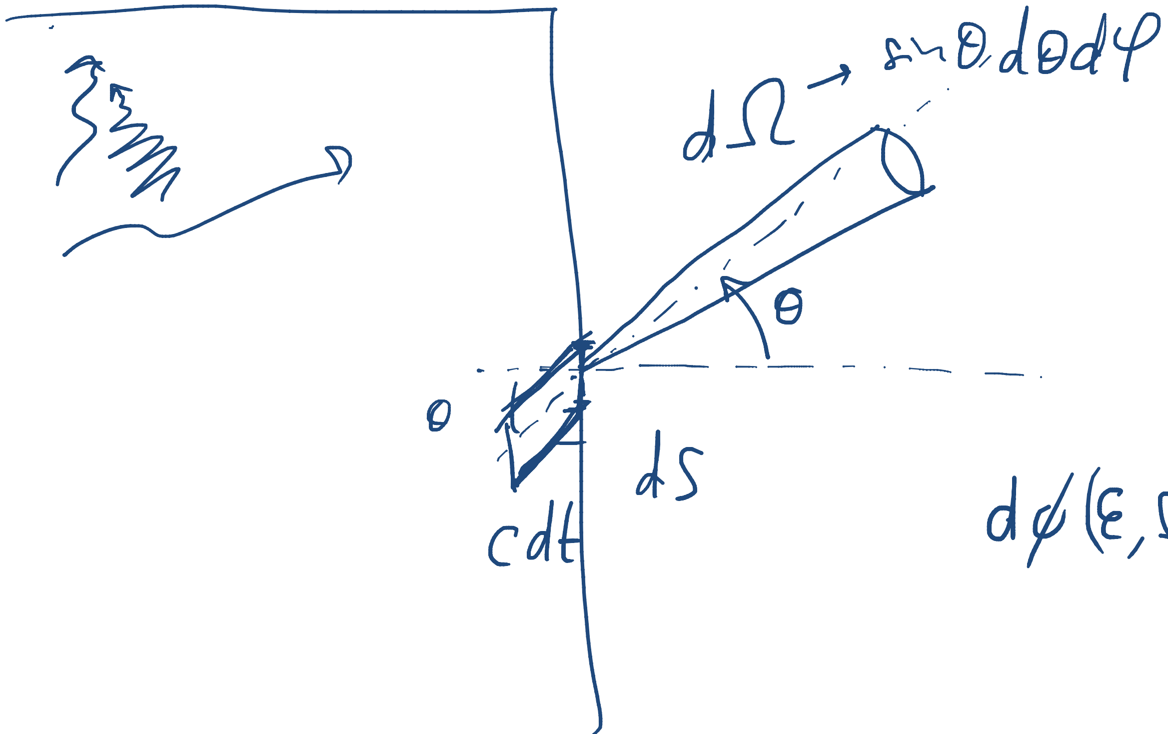
$$\boxed{dn(\varepsilon) = \frac{dN(\varepsilon)}{L^3} = \frac{4\pi}{(2\pi\hbar c)^3} \frac{\varepsilon^2}{e^{\varepsilon/kT}-1}\, d\varepsilon}$$

Free bosons

Consider N free massless bosons in 3D, at a temperature T .

$$dn(E) = \frac{E^2}{\pi^2 \hbar^3 c^3} \frac{1}{\exp\left(\frac{E}{k_B T}\right) - 1} dE$$

Number of photons with an energy between ϵ and $\epsilon + d\epsilon$
going out through dS, in direction Ω during time dt ?



$dV = dS\, c\, dt \cos\theta$ | direction $\frac{d\Omega}{4\pi}$

photons in volume dV with $\epsilon \leq E \leq \epsilon + d\epsilon$

$$dn(\epsilon) \times dV \times \frac{d\Omega}{4\pi}$$

$$d\phi(\epsilon, \Omega) = \frac{\epsilon^2}{\pi^2 \hbar^3 c^3} \frac{1}{4\pi} c \cos\theta \sin\theta \, d\theta \, d\varphi \, dS \, dt$$

Free bosons

Number of photons with an
energy between ϵ and $\epsilon + d\epsilon$
going out through dS,
in direction Ω up to dΩ
during time dt

$$dN_{\mathrm{out}}(E,\,\Omega) = \frac{\epsilon^2}{\pi^2\hbar^3 c^2}\frac{1}{\exp\left(\frac{\epsilon}{k_B T}\right) - 1}\frac{\cos\theta\sin\theta d\theta d\varphi}{4\pi} dS dt d\epsilon$$

Spectral intensity of the emitted radiation ?

$\phi_E \, dS \, dt \, d\mathcal{E} =$ amount of energy emitted through dS over duration dt carried by photons with $\mathcal{E} \leq E \leq \mathcal{E} + d\mathcal{E}$

$$= \int_{\substack{\Omega \\ \theta,\varphi}} \mathcal{E} \times dN_{out}(\mathcal{E}, \Omega)$$

$$= \frac{\mathcal{E}^3}{\pi^2\hbar^3 c^2}\frac{1}{e^{\mathcal{E}/kT} - 1} \underbrace{2\pi\int_0^{\pi/2}\frac{\cos\theta\sin\theta d\theta}{4\pi}}_{1/4} dS dt d\mathcal{E}$$

$$\boxed{\phi_E(\mathcal{E}) = \frac{1}{4\pi^2\hbar^3 c^2}\frac{\mathcal{E}^3}{e^{\mathcal{E}/kT} - 1}}$$

Planck law

total output power ? $\int \phi_E(\mathcal{E})\, d\mathcal{E} = \sigma T^4$

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Free Fermions

Consider N free massive fermions in 3D, at “low” T.

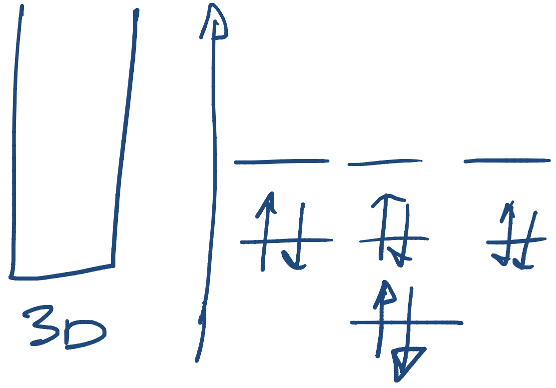
$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

+ 3D

$$\Rightarrow D(\varepsilon) = \gamma\sqrt{\varepsilon}$$

$$= \underbrace{\left(\frac{L}{2\pi\hbar}\right)^3 4\pi\sqrt{2m^3}}_{\gamma}\sqrt{\varepsilon}$$

$$f_{FD}(\varepsilon) = \frac{1}{e^{\frac{\varepsilon-\mu}{kT}}+1} \leq 1$$

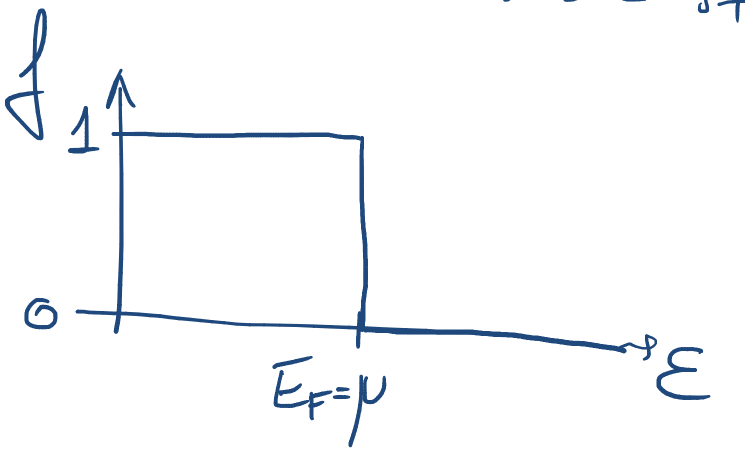


Pauli exclusion principle: never 2 fermions in the exact same state.

▷ $T \to 0K$

$\varepsilon < \mu \quad f(\varepsilon) = 1$

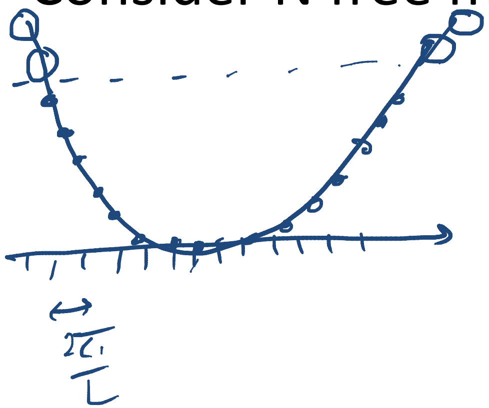
$\varepsilon > \mu \quad f(\varepsilon) = 0$



Fermi Energy

Consider N free massive fermions in 3D, at “low” T.

Fermi Energy $= \mu(T=0)$



$$f(\varepsilon) \underset{T\to 0}{=} \theta(\varepsilon - \mu)$$

$$N = \int_0^{E_F} D(\varepsilon)\,d\varepsilon = \gamma \int_0^{E_F} \sqrt{\varepsilon}\,d\varepsilon = 8\pi \left[\frac{L}{2\pi\hbar}\right]^3 \sqrt{2m^3} \left[\varepsilon^{3/2}\,\frac{2}{3}\right]_0^{E_F}$$

$$\boxed{E_F = \frac{h^2}{8m}\left[\frac{3n}{\pi}\right]^{2/3}} \qquad n = \frac{N}{L^3}$$

How cold is a "low" temperature ?

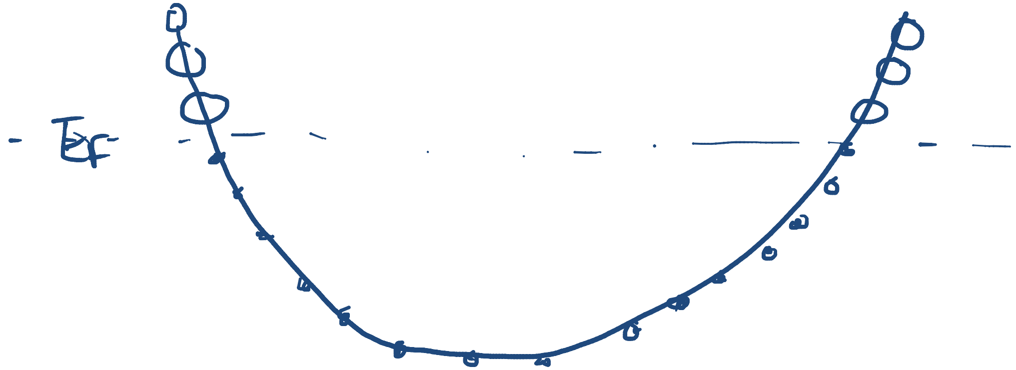
Consider N free massive fermions in 3D, at "low" T.

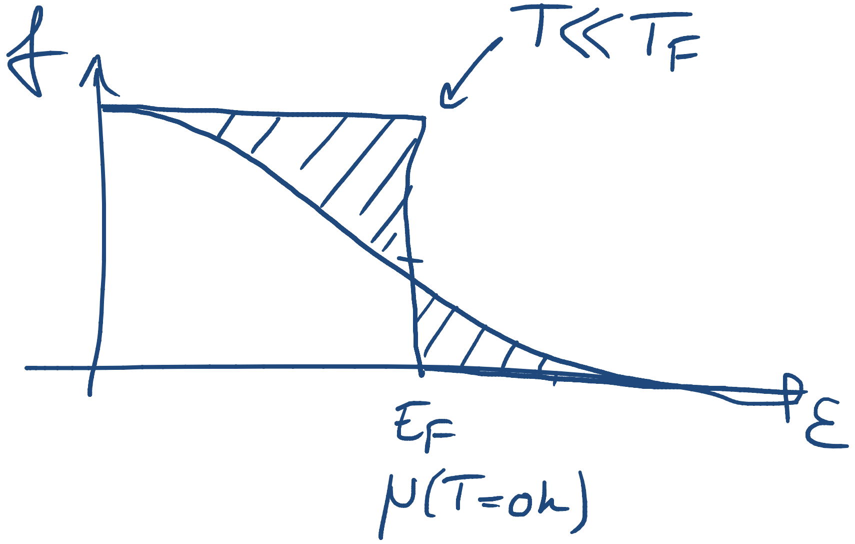
$$N = L^3 \frac{4}{3}\pi \left(\frac{\sqrt{2m}}{2\pi\hbar} \right)^3 E_F^{3/2}$$

m	n	T_F	
10^{-27} kg	10^{45} m^{-3}	$\sim 10^{9}$ K	nuclear
10^{-30} kg	10^{30} m^{-3}	$\sim 10^{6}$ K	~~atom~~ metal

$$E_F = \frac{h^2}{8m}\left[\frac{3n}{\pi}\right]^{2/3} \qquad \hbar = \frac{h}{2\pi}$$

$$= k_B T_F$$





Fermi Energy and energy per particle

Consider N free massive fermions in 3D, at "low" T.

$$\underline{N} = L^3 \frac{4}{3}\pi \left(\frac{\sqrt{2m}}{2\pi\hbar}\right)^3 \underline{E_F^{3/2}}$$

$$E_{tot} = \int_0^{E_F} D(\varepsilon)\times\varepsilon\, d\varepsilon = \underbrace{8\pi\left[\frac{L}{2\pi\hbar}\right]^3\sqrt{2m^3}}_{\gamma}\underbrace{\int_0^{E_F}\varepsilon^{3/2}\,d\varepsilon}_{\frac{2}{5}E_F^{5/2}}$$

$$N = \gamma\,\frac{2}{3}E_F^{3/2}$$

$$= \frac{3}{5}NE_F$$

$$\boxed{\langle E\rangle = \frac{E_{tot}}{N} = \frac{3}{5}E_F}$$

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Take home message

Hamiltonian + dimension → Density Of State

Statistics (or spin) of the particles → Occupation factor

$$f(\epsilon) = \frac{1}{\exp\left(\frac{\epsilon-\mu}{k_B T}\right) + \alpha}$$

with $\alpha = \begin{cases} +1 & \text{Fermions} \rightarrow \text{Fermi Dirac distribution} \\ 0 & \text{Classical} \rightarrow \text{Maxwell Boltzmann distribution} \\ -1 & \text{Bosons} \rightarrow \text{Bose Einstein distribution} \end{cases}$

Density of state + occupation factor →

$$N = \int d\epsilon \, D(\epsilon) \, f(\epsilon) \qquad E = \int d\epsilon \, \epsilon \, D(\epsilon) \, f(\epsilon)$$

Classical particles
Equi-partition theorem

Bosons
Black body radiation

Fermions
Fermi energy