MAE212

Fermi Energy - Fermi Level

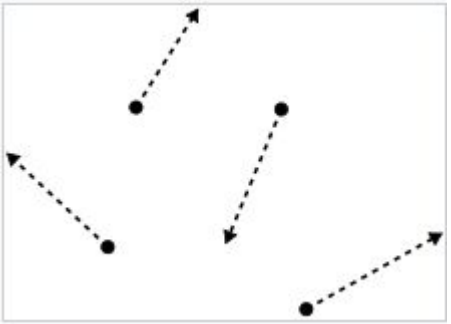
Joseph Sanchez, Dian Song, Pai Peng, and Eric Anthony Bonfadini

Fermi Systems

A Fermi System is concept in quantum mechanics where a system containing charged particles don't interact (collide.) The particles still have modes of energy(Vibrational, Translational and Rotational Energy.)

Fermi prefix

Examples = “Fermi Gas”, “Fermion”, “Fermi System”, “Fermi Energy”

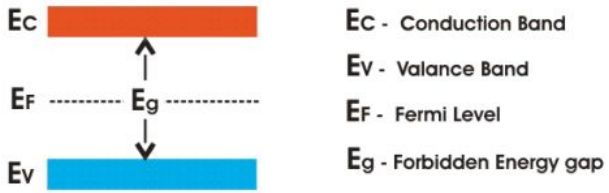


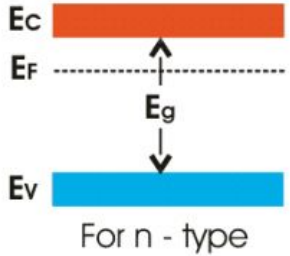
Fermi Level

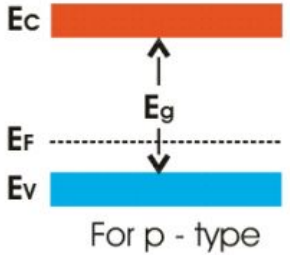
Fermi level is the term used to describe the top of the collection of electron energy levels. This concept comes from Fermi-Dirac statistics.

The Fermi level is the average electrons that are available (electrochemical potential for electrons) and is usually denoted by μ or E_F.The Fermi level of a body is a thermodynamic quantity, and the thermodynamic work required to add one electron to the body (not counting the work required to remove the electron from wherever it came from).

- Fermi level is defined for any temperature.
- Fermi level is a total energy level including kinetic energy and potential energy.
- Fermi level (the electrochemical potential of an electron) remains well defined even in complex interacting systems, at thermodynamic equilibrium.



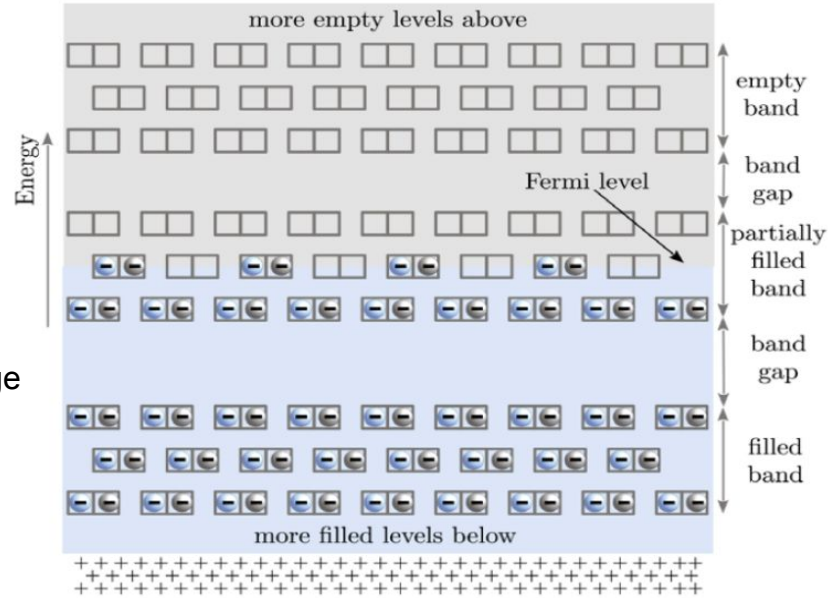




Fermi energy

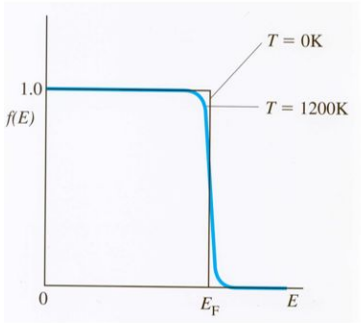
The **Fermi energy** is a concept in quantum mechanics usually referring to the energy difference between the highest and lowest occupied single-particle states in a quantum system of non-interacting electrons(Fermions) at absolute zero temperature.

- The Fermi energy is only defined at absolute zero
- The Fermi energy is an energy *difference* (usually corresponding to a kinetic energy)
- The Fermi energy can only be defined for non-interacting particles (Fermions where the potential energy or band edge is a static, well defined quantity)



Fermi-Dirac Distribution

- The probability of occupation
- It applies to fermions (½ spin quantum number). Other fermions include protons, neutrons, certain atoms, etc.
- T = 0 K, step function, step at Fermi level
- T > 0K, finite probability **near** Fermi level



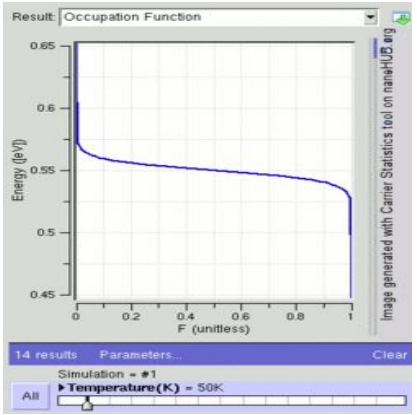
- At $T=0$ all states below E_F are occupied, above E_F are free

$$f(E) = \begin{cases} 1, E < E_F \\ 0, E > E_F \end{cases}$$

- When T increases some electrons get enough energy to get above E_F

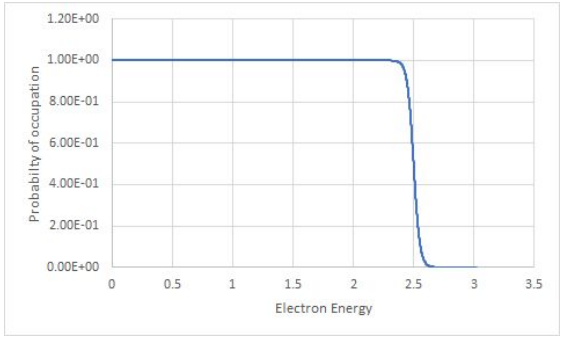
$$f(E) = \frac{1}{\exp((E - E_F)/kT) + 1}$$

- Fermi function – smoothened step

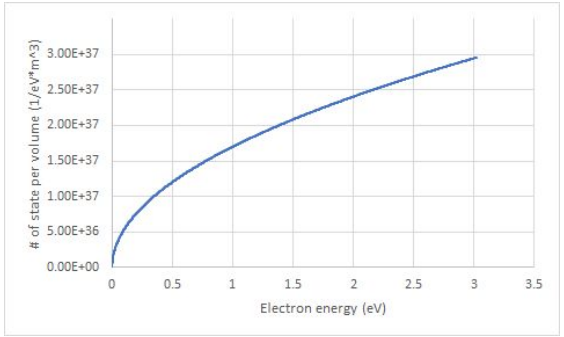


Density of occupied states

f(E) at 300K

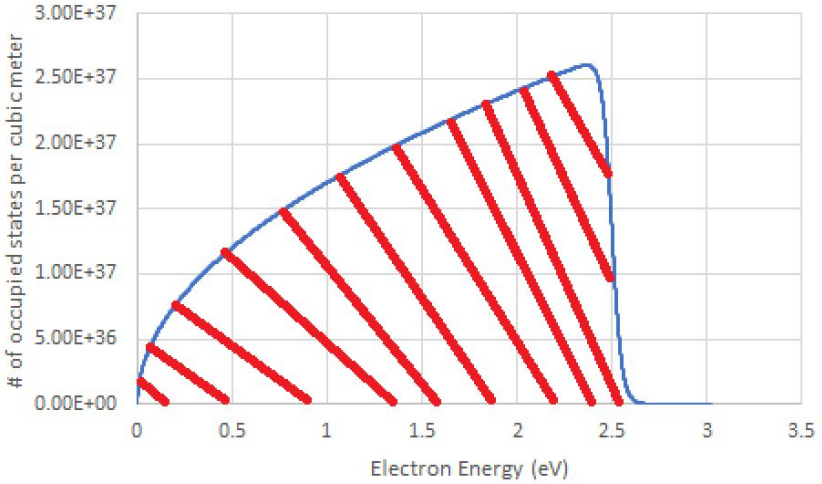


g(E)



g(E): density of available states
f(E): probability of a state occupied
g(E)f(E): density of occupied state
$\int g(E)f(E)dE$: total energy of electrons
$\int g(E)f(E)dE / \int g(E)f(E)$: avg. energy of electrons **(0.6EF)**

g(E)f(E)



What is electrochemical potential

Standard chemical potential μ_0 at certain T and P

For any substance: $\mu_i = \mu_0 + RT\ln a_i$

a_i is activity of chemical substance i

$$a_i = \gamma_{x,i} x_i = \gamma_{b,i} \frac{b_i}{b^\ominus} = \gamma_{w,i} w_i = \gamma_{c,i} \frac{c_i}{c^\ominus} = \gamma_{\rho,i} \frac{\rho_i}{\rho^\ominus}$$

For uncharged species : $\mu = \mu_i$ (Z=0)

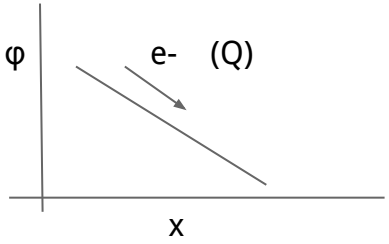
For charged species: $\mu = \mu_i + ZF\varphi_i = \mu_0 + RT\ln a_i + ZF\varphi_i$

Activity effects can be disregarded $\mu = \mu_i + ZF\varphi_i = \mu_0 + ZF\varphi_i$
(the electron concentration never changes appreciably $a_i = 1$)

What is electrochemical potential

$dw_{elec} = \varphi_i dQ$ φ_i is electrical potential Q is charge

dQ = ZFdn F Faraday constant Z charges n moles of ions



$dG = -SdT+VdP+ \Sigma\mu_i dn_i+dw_{elec}$

$= -SdT+ VdP+ \Sigma\mu_i dn_i+ \Sigma ZF\varphi_i dn_i$

$= -SdT+VdP+ \Sigma(\mu_i+ ZF\varphi_i)dn_i$

μ

At constant T and P $dG=\Sigma (\mu) dn_i$

For 1 mole electrons they have same energy $G=\mu N_A = \mu_t$ is the total electrochemical potential

xi

Relating Fermi Level to Gibbs

$$g_B(\epsilon) \equiv 2g(\epsilon) = \frac{3}{2}\frac{N}{\epsilon_F}\left(\frac{\epsilon}{\epsilon_F}\right)^{1/2}$$ ← Density of States in terms of E_f

$$U = \int_0^{\epsilon_F} d\epsilon g_B(\epsilon)\epsilon = \frac{3}{5}N\epsilon_F$$

Multiply density of states by E then integrate from 0 to Ef (@T=0K) to get total internal energy U

$G = U + PV$ ← Gibbs at T=0K

$U = (3/2)PV$ ←Derivation found online

$P = (2/3)(U/V)$

$G = U + (2/3)U$

$G = (3/5)NE_F + (2/5)NE_F$

$G = NE_F$

- In a metal, because valence electrons can move around, we can treat them as a quantum fluid (a fermion fluid).

$G = N_A E_F = \mu_t$

$E_F = \mu_t / N_A$

References

Online

1) https://en.wikipedia.org/wiki/Fermi_energy
2) https://en.wikipedia.org/wiki/Fermi_level
3) http://hyperphysics.phy-astr.gsu.edu/hbase/Solids/Fermi.html
4) http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/disfd.html#c1
5) http://ucibiomems.net/courses/ -PPT class 8
6) https://www.electrical4u.com/energy-brands-in-silicon/
7)

Textbooks

1. https://drive.google.com/open?id=1UwpzGHGkIZFl_wKns8inZlAEF17KZO2-QH5PtB0s9Qo
2. Henry R. Glyde-Intermediate Condensed Matter Physics, Chapter 8 notes(Solid State Physics N. Ashcroft and N. D. Mermin (Holt, Rinehart and Winston, New York, 1976)
3. Electrochemical Methods Fundamentals and Applications 2nd Allen J. Bard Larry Faulkner Dept of chemistry and biochemistry UTA