# Semiconductors

Effective Mass
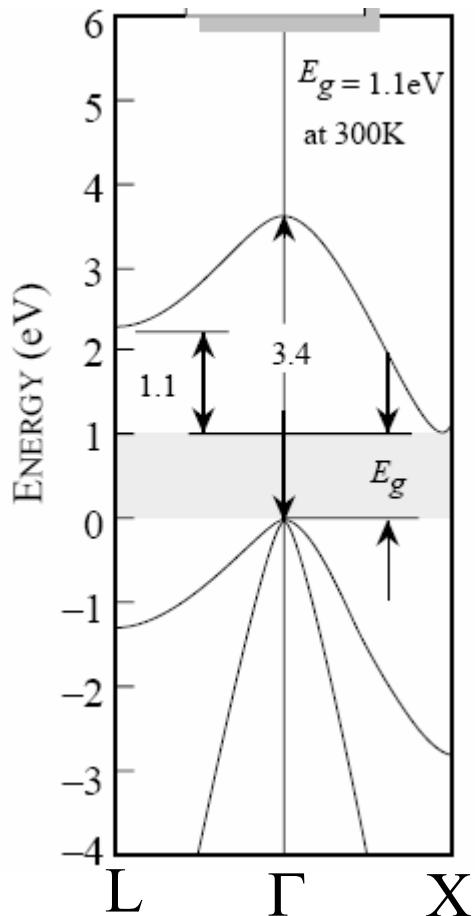
$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0 \right)^2}{2m^*} + E_c$$

$$m_e^* = \frac{\hbar^2}{\dfrac{d^2 E}{dk_x^2}}$$

$$E = \frac{-\hbar^2 \left(\vec{k} - \vec{k}_0 \right)^2}{2m^*} + E_v$$

$$m_h^* = \frac{-\hbar^2}{\dfrac{d^2 E}{dk_x^2}}$$

Holes
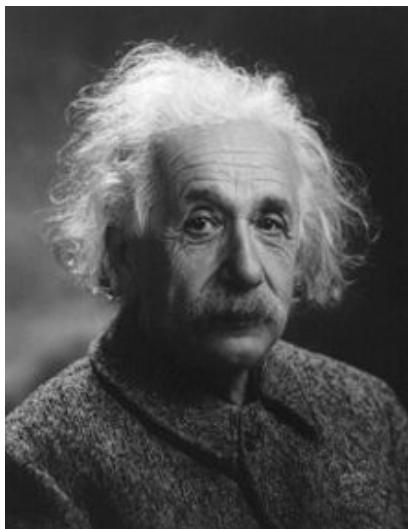
Albert Einstein
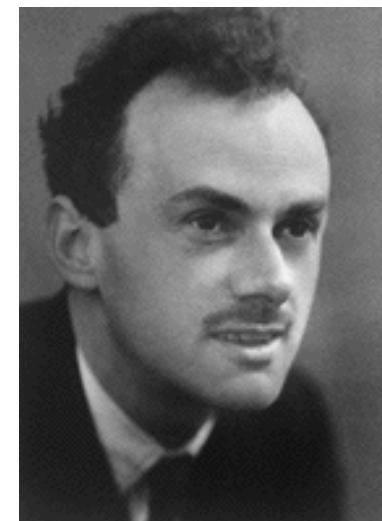
Erwin Schrödinger

Paul Adrien Maurice Dirac

Holes
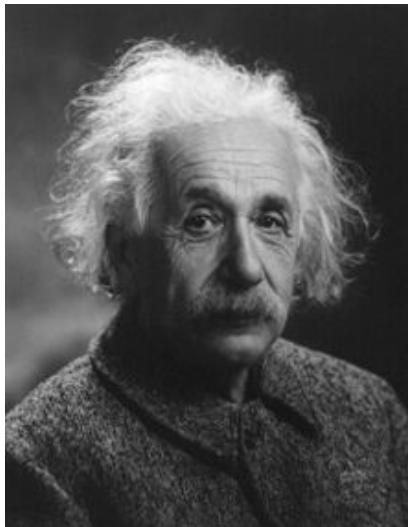
Albert Einstein   Erwin Schrödinger   Paul Adrien Maurice Dirac

$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2}$$ Wave equation

$$\frac{du}{dt} = k \frac{d^2u}{dx^2}$$ Heat equation

Holes
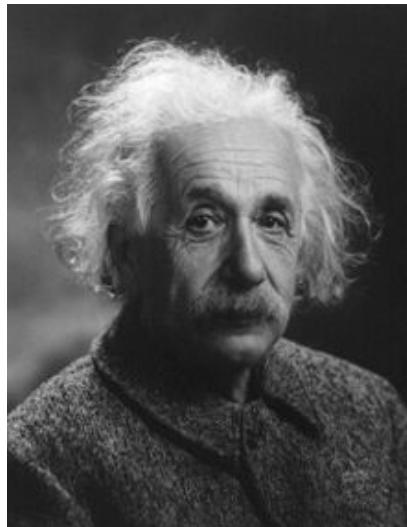
Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

$$\left(\beta mc^2 + \sum_{j=1}^{3} \alpha_j p_j c \right) \psi = i\hbar \frac{\partial \psi}{\partial t}$$

Dirac equation

$E = mc^2$
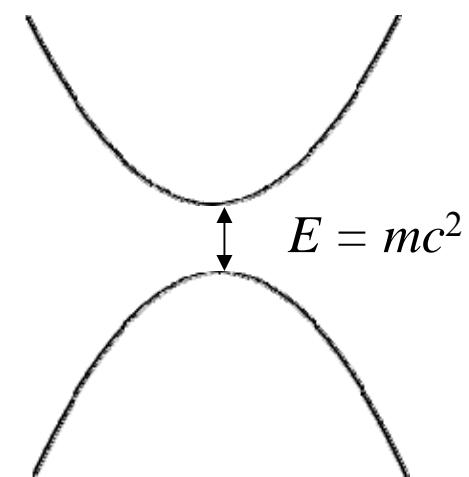
Free electron Fermi gas

1 - d
$$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1}\text{m}^{-1}$$

2 - d
$$D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1}\text{m}^{-2}$$

3 - d
$$D(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2 \pi^2}\right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}}\sqrt{E} \quad \text{J}^{-1}\text{m}^{-3}$$
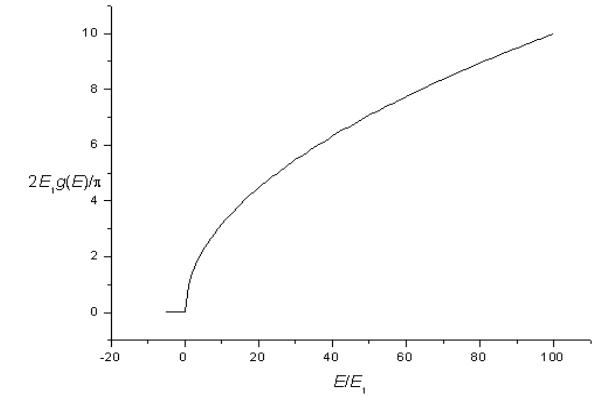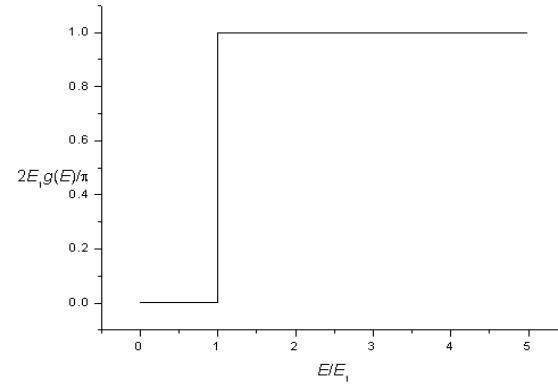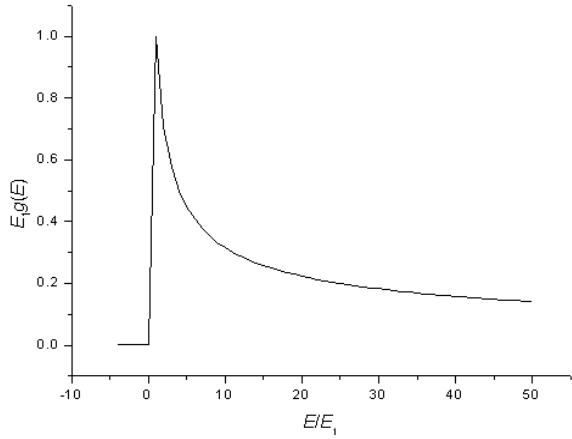
$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$

$$D(E) = \begin{cases} \dfrac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\[3mm] 0 & E_v < E < E_c \\[3mm] \dfrac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

E_g

E_v

E_c
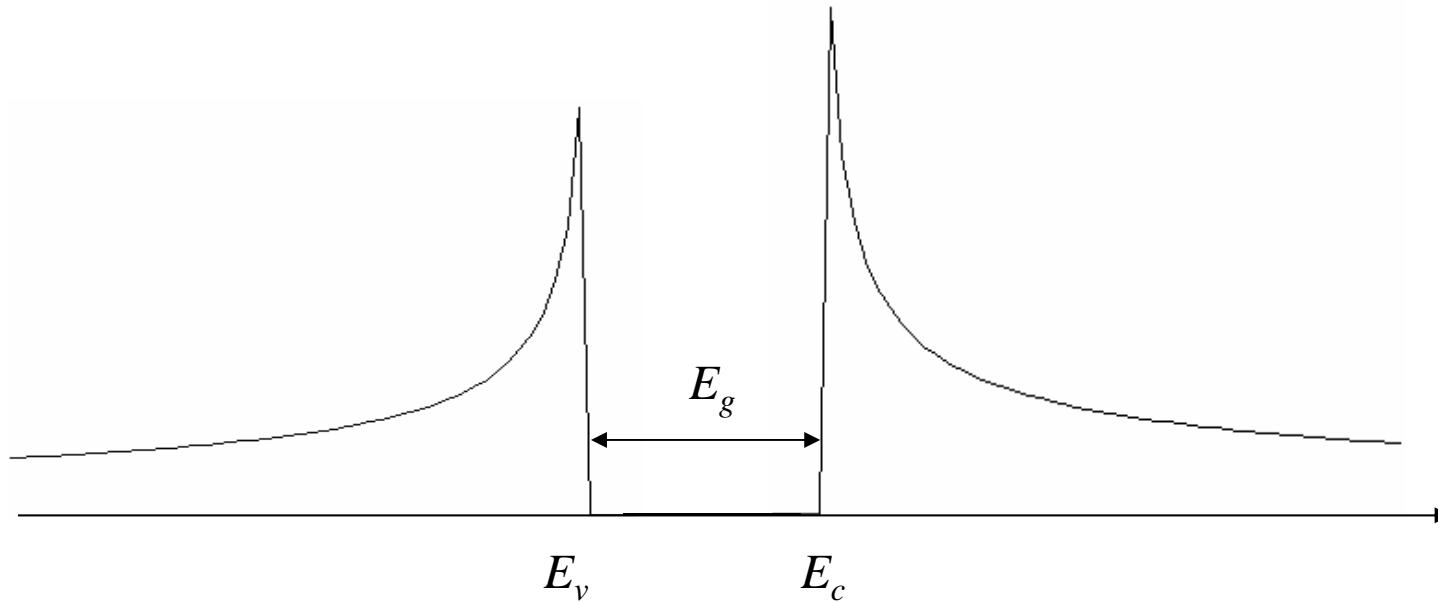
$$D(E) = \begin{cases} D_c & E < E_v \\ 0 & E_v < E < E_c \\ D_v & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$
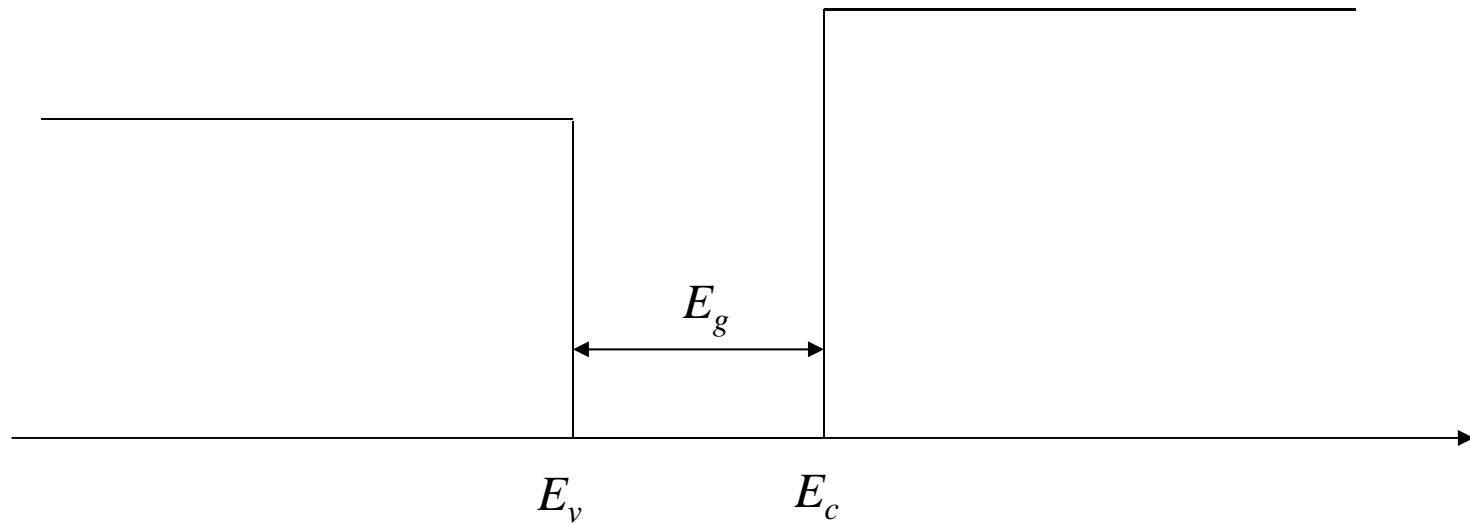
$$D(E) = \begin{cases} D_c \sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \quad \mathrm{J^{-1}m^{-3}} \\ D_v \sqrt{E - E_c} & E_c < E \end{cases}$$

E_g

E_v E_c
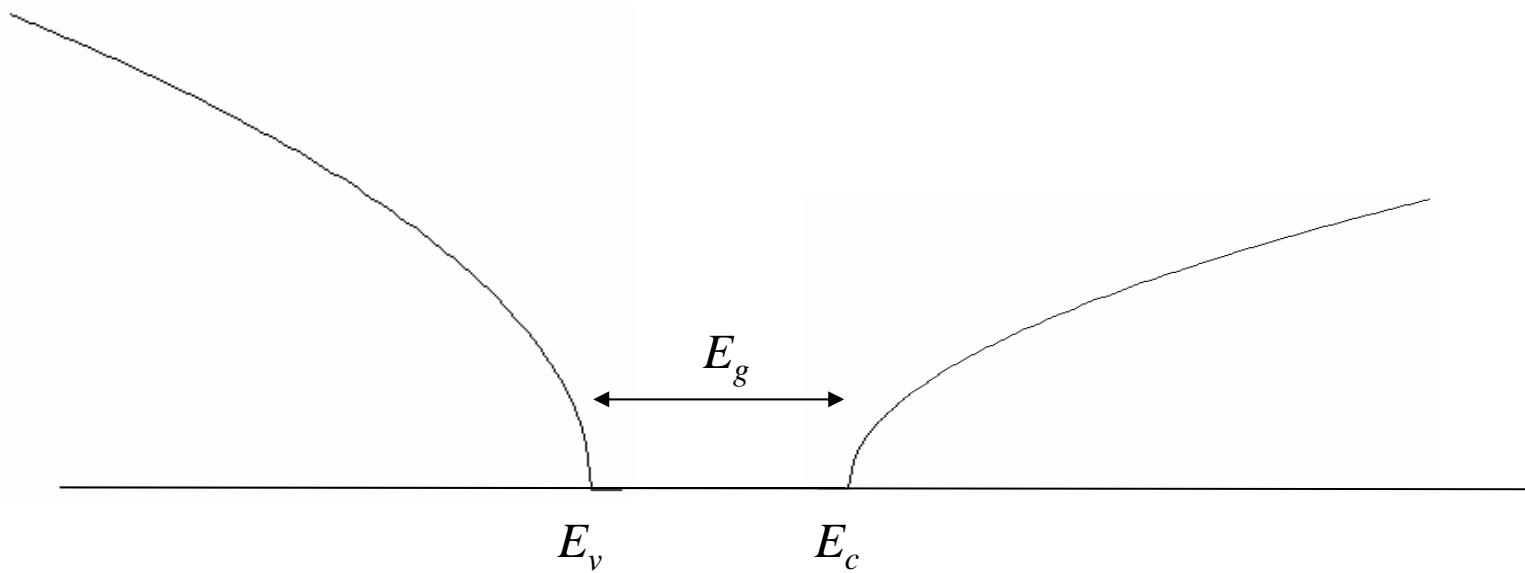
Silicon density of states
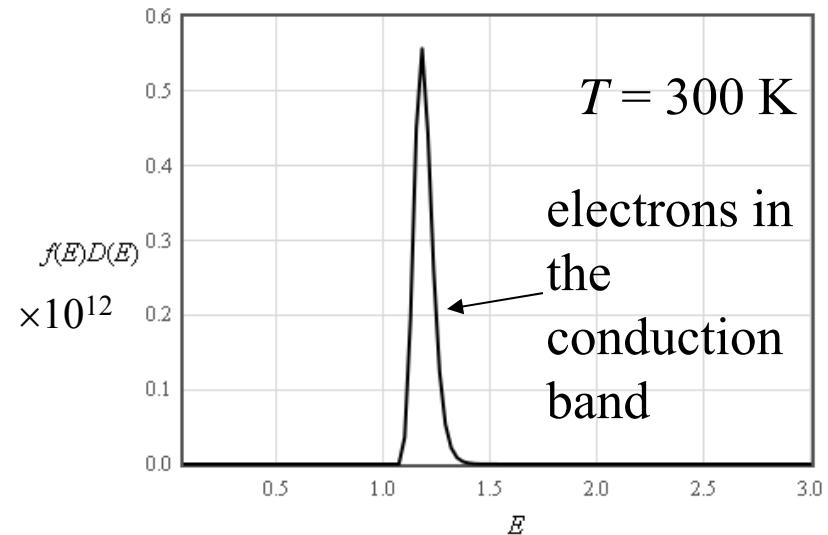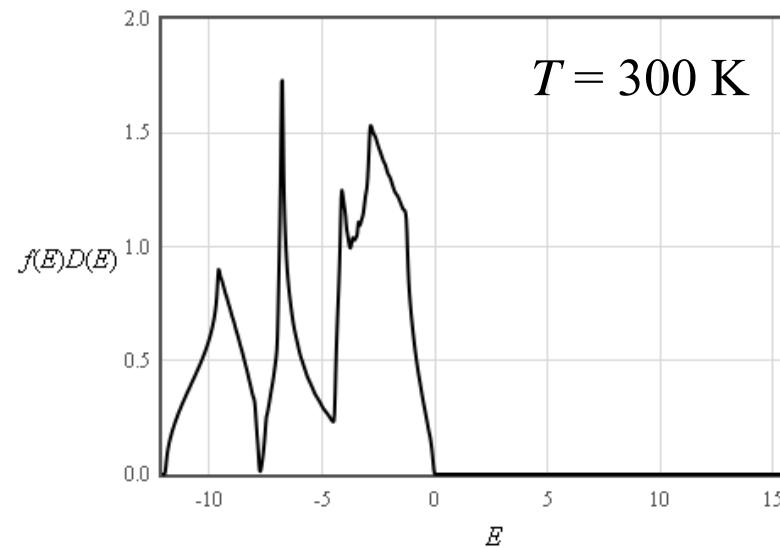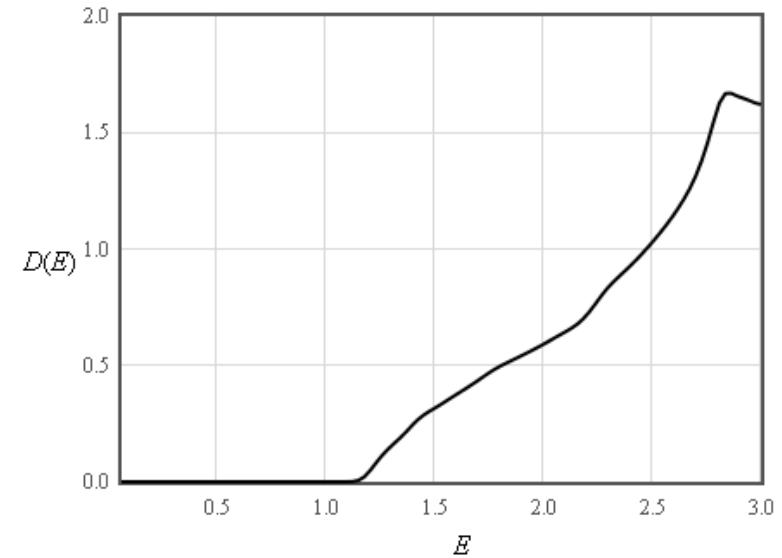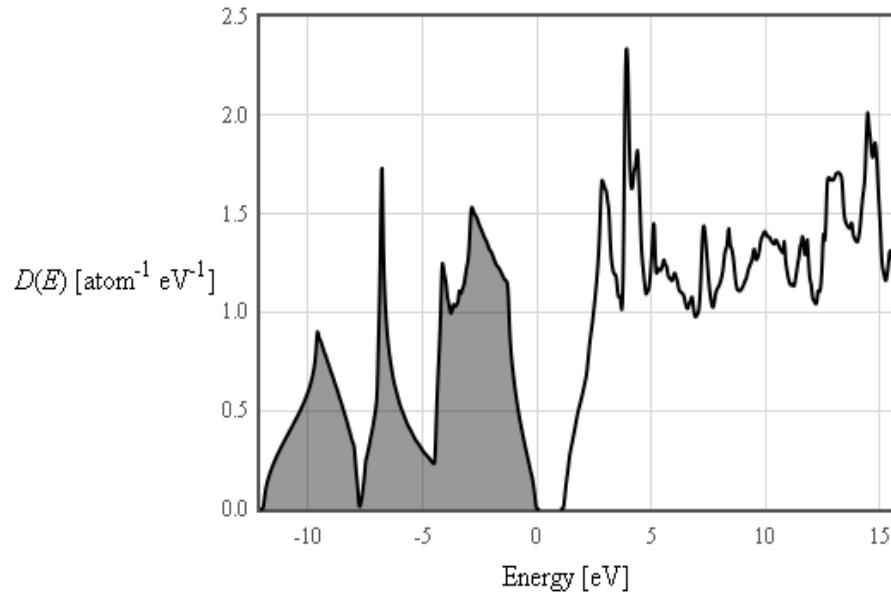
Density of electrons in the conduction band

The free electron density of states is modified by the effective mass.

$$D(E) = D_c \sqrt{E - E_c}$$

$$f(E) = \frac{1}{1 + \exp\left(\dfrac{E - \mu}{k_B T}\right)} \approx \exp\left(\dfrac{\mu - E}{k_B T}\right)$$

f(E)

Boltzmann
approximation
$E_c - \mu > 3 k_B T$

E_v　　　　　E_c
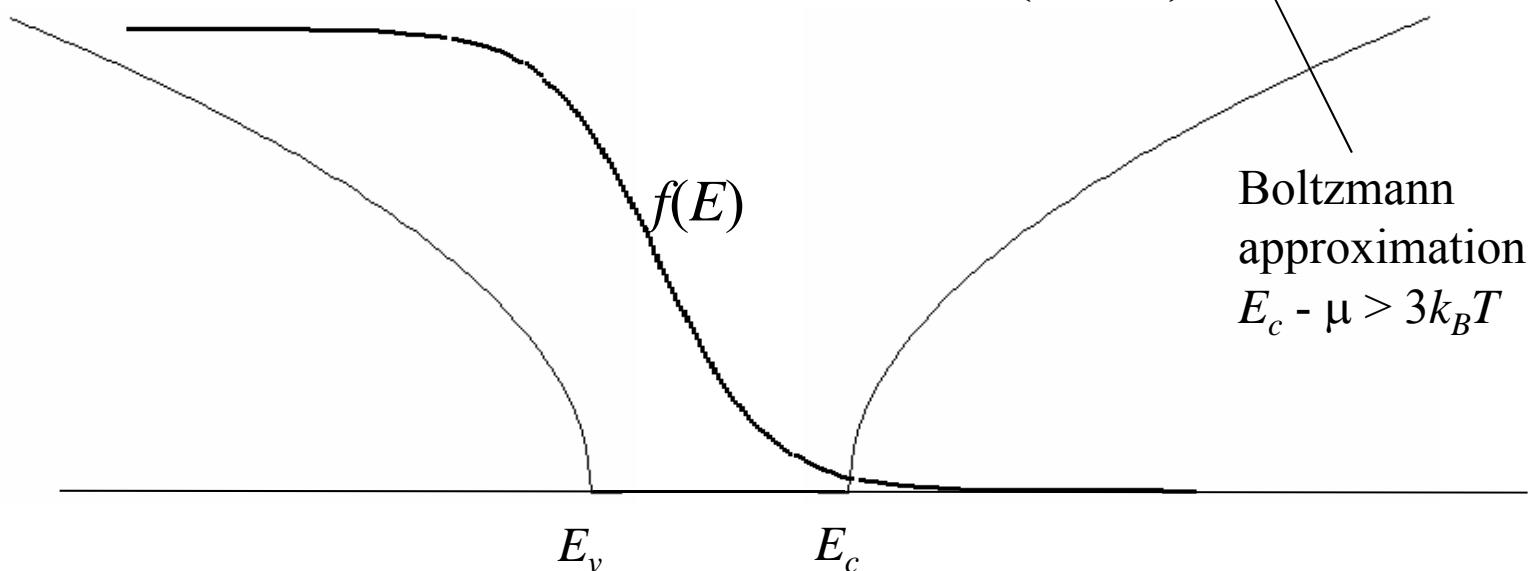
$$n = \int_{E_c}^{\infty} D(E) f(E) \, dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} \, dE$$

Density of electrons in the conduction band

$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c}\, dE$$

$$x = E - E_c \qquad \int_0^{\infty} \sqrt{x} \exp\left(\frac{-x}{k_B T}\right) dx = \frac{2}{\sqrt{\pi}} \left(k_B T\right)^{3/2}$$

$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right) = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)}$$

$$N_c = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} = 2\left(\frac{m^* k_B T}{2\pi \hbar^2}\right)^{3/2} = \text{effective density of states}$$

Density of holes in the valence band

$$D(E) = D_v \sqrt{E_v - E}$$

$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\dfrac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{E - \mu}{k_B T}\right)$$

$1 - f(E)$

Boltzmann
approximation
$\mu - E_v > 3 k_B T$

E_v

E_c
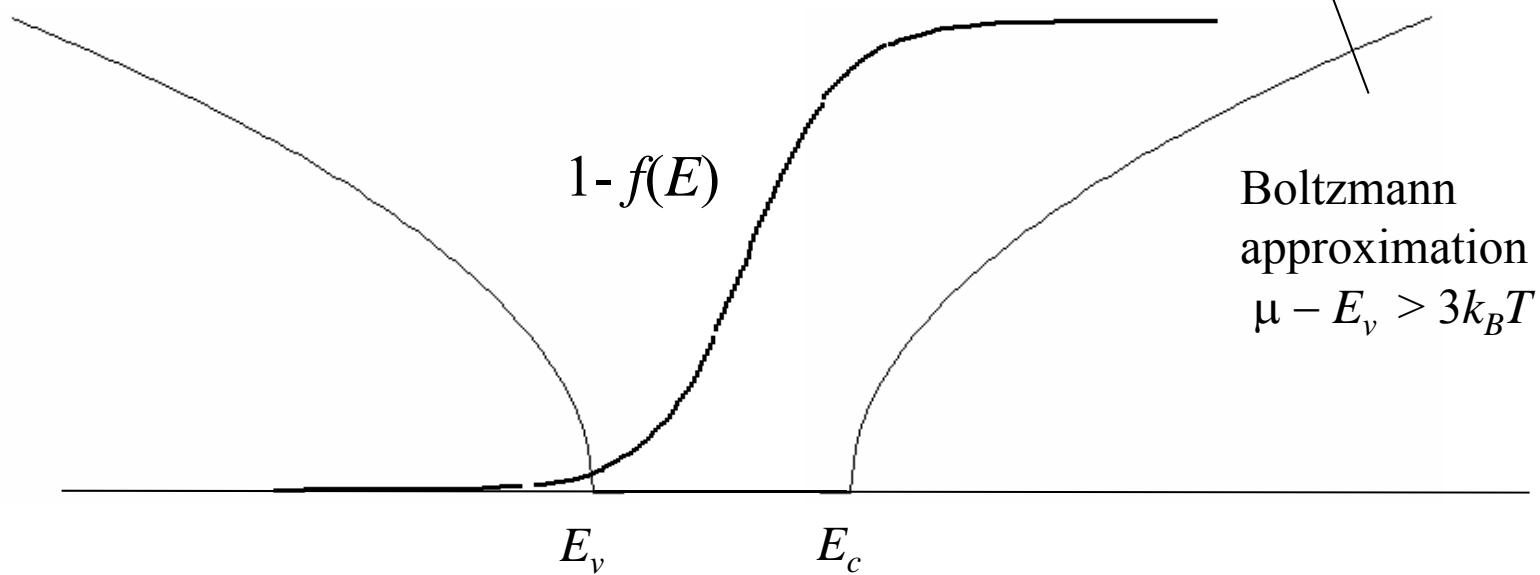
$$p = \int_{-\infty}^{E_v} D(E)\left(1 - f(E)\right) dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E - \mu}{k_B T}\right) \sqrt{E_v - E}\, dE$$

Density of holes in the valence band
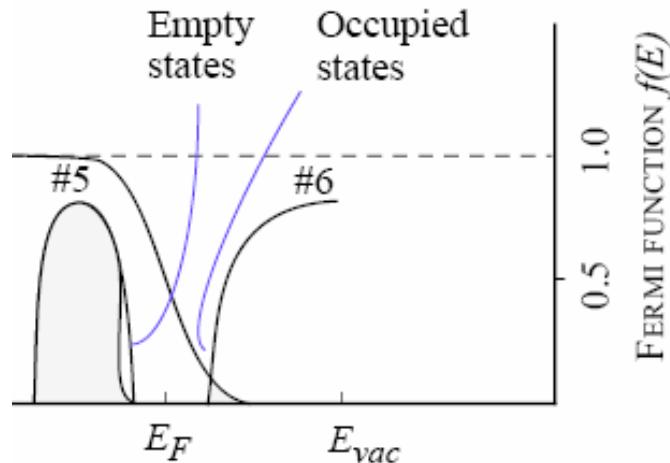
$$p = \int_{-\infty}^{E_v} D(E)\big(1 - f(E)\big)\,dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E - \mu}{k_B T}\right) \sqrt{E_v - E}\,dE$$

$$\boxed{p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)} = \frac{2D_v}{\sqrt{\pi}}\left(k_B T\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$N_v = 2\left(\frac{m_h^* k_B T}{2\pi \hbar^2}\right)^{3/2} \qquad \text{= Effective density of states in the valence band}$$

Law of mass action

$$np = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

E_c ⎯⎯⎯⎯

E_g

E_v ⎯⎯⎯⎯
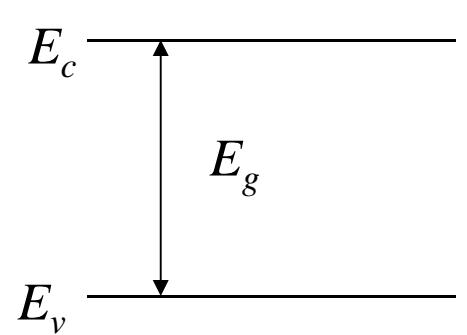
For intrinsic semiconductors (no impurities)

$$n = p = n_i = \sqrt{N_c N_v} \exp\left(\frac{-E_g}{2k_B T}\right)$$

intrinsic carrier density

Intrinsic carrier concentration
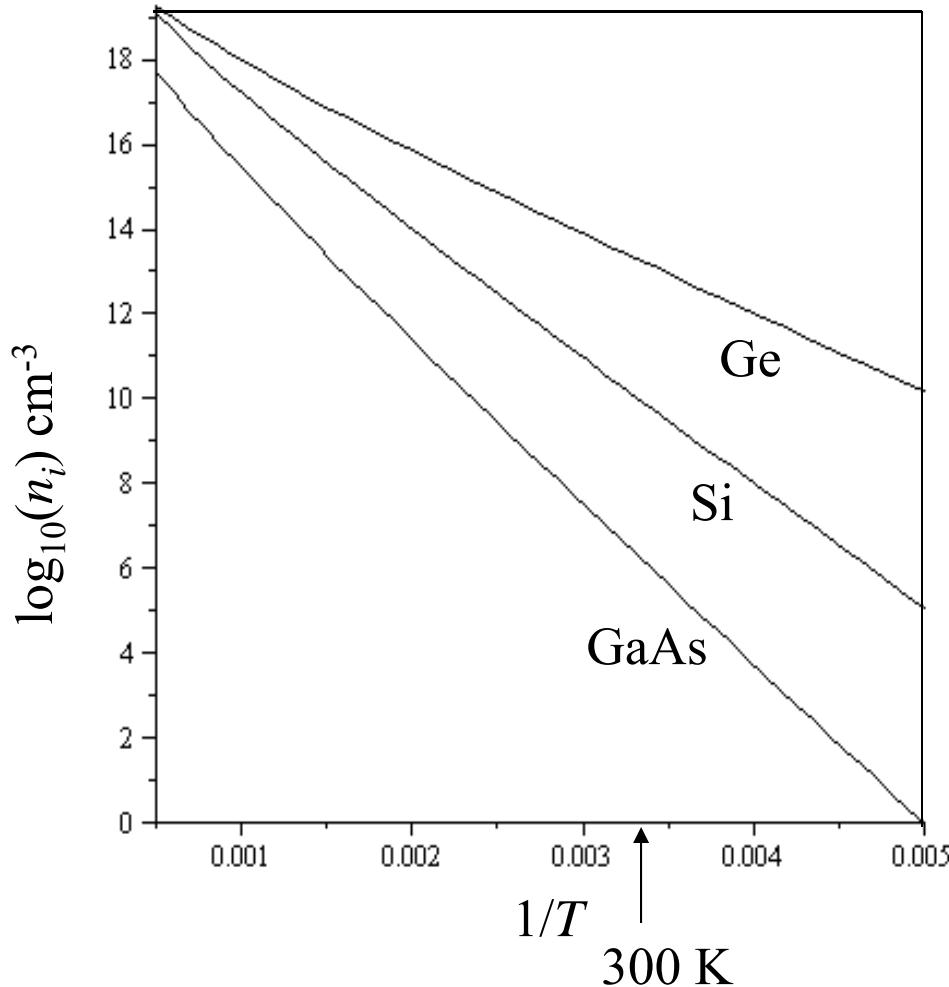
$$n_i = \sqrt{N_v N_c \left(\frac{T}{300}\right)^3 \exp\left(-\frac{E_g}{2k_B T}\right)}$$

~ 5 x 10^{22} atoms/cm^3

Chemical potential of an intrinsic semiconductor

$$n = p = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$\exp\left(\frac{\mu - E_c - E_v + \mu}{k_B T}\right) = \frac{N_v}{N_c}$$

$$\frac{2\mu}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

$$\boxed{\mu = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)}$$

Empty states   Occupied states

#5   #6

μ E_{vac}

FERMI FUNCTION $f(E)$

0.5   1.0

E_c

μ
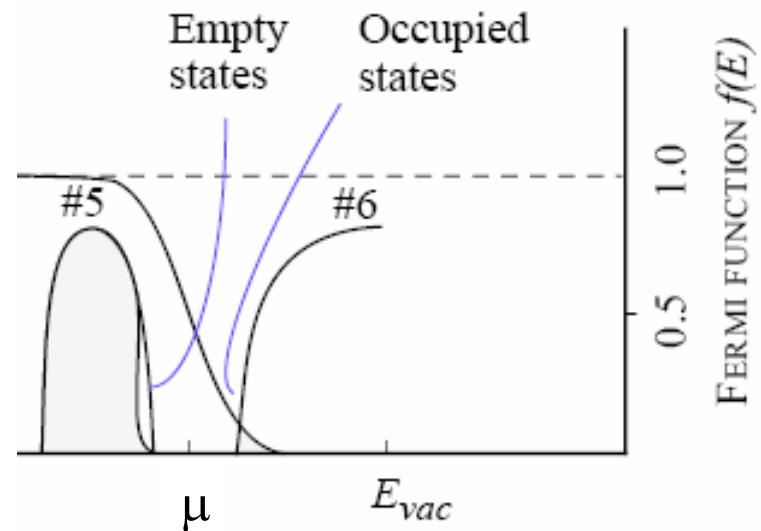
E_v

Density of electrons in the conduction band
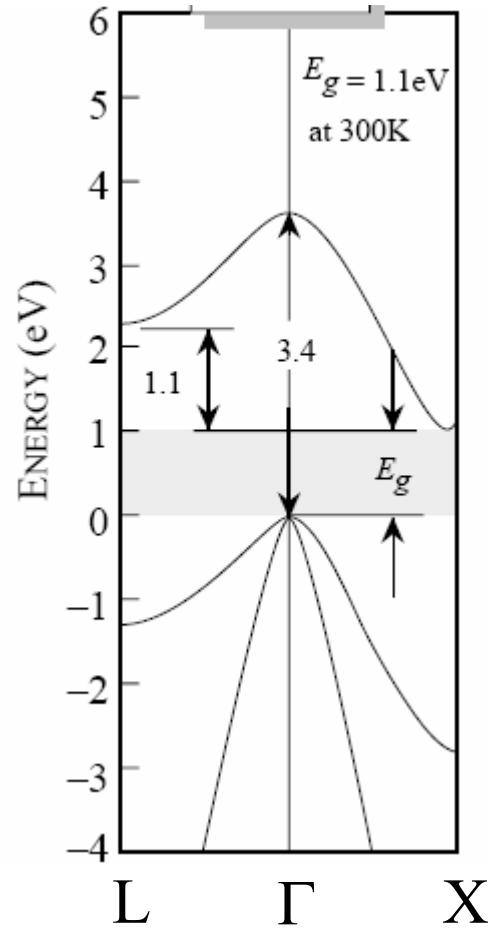
$$n = N_c(T)\exp\left(\frac{\mu - E_c}{k_B T}\right) = \frac{2D_v}{\sqrt{\pi}}(k_B T)^{3/2}\exp\left(\frac{\mu - E_c}{k_B T}\right)$$

$E_g = 1.1\,\text{eV}$

at 300K

E_g

1.1

3.4

ENERGY (eV)

6 5 4 3 2 1 0 -1 -2 -3 -4

L   Γ   X

k_z

(001)

$(0\bar{1}0)$ $(\bar{1}00)$

k_x (100)   (010) k_y

$(00\bar{1})$
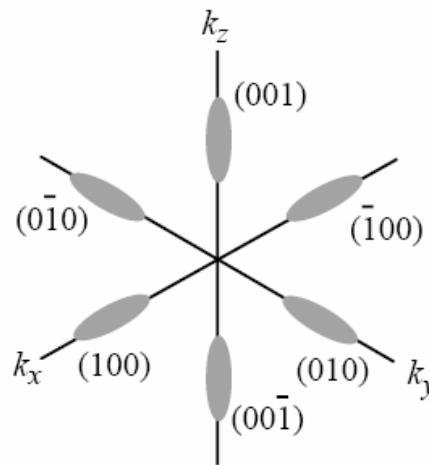
$$n = N_c\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_F - E_c}{k_B T}\right)$$

Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}

Density of electrons in the conduction band
Density of holes in the valence band

I   Heavy Hole Band

II   Light Hole Band

III   Split-Off Band

Δ = Split-Off Energy
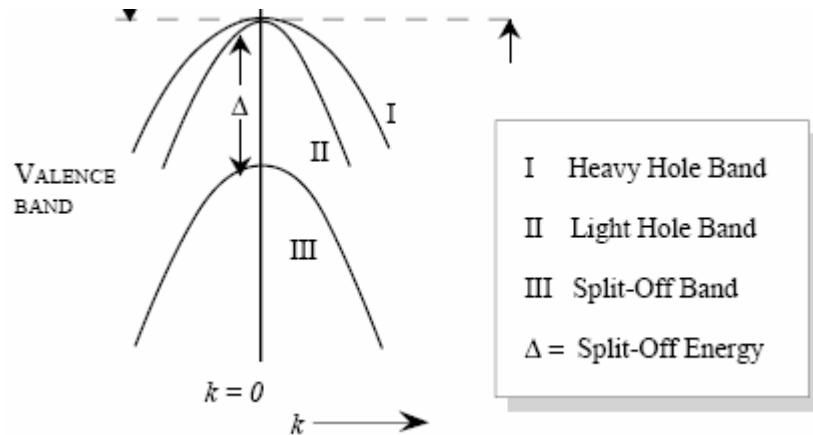
$$n = N_c \left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

$$p = N_v \left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}
Effective density of states in valence band (300 K) N_v	9.84×10^{24} m^{-3}	6.0×10^{24} m^{-3}	7.72×10^{24} m^{-3}
Effective mass electrons m^*/m_0	$m_l^* = 0.98$ $m_t^* = 0.19$	$m_l^* = 1.64$ $m_t^* = 0.082$	$m^* = 0.067$
Effective mass holes m^*/m_0	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$	$m_{lh}^* = 0.044$ $m_{hh}^* = 0.28$	$m_{lh}^* = 0.082$ $m_{hh}^* = 0.45$
Crystal structure	diamond	diamond	zincblende
Density	2.328 g/cm³	5.3267 g/cm³	5.32 g/cm³
Atoms/m³	5.0×10^{28}	4.42×10^{28}	4.42×10^{28}

The electrical contribution to the thermodynamic properties of insulators depend on band edges

Boltzmann approximation

The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results where calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_BT$ from the band edge. The electronic contribution to the thermodynamic quantities are usually much smaller than the contribution of the phonons and thus the electronic components are often simply ignored.

	1-d	2-d
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E) = \begin{cases} \dfrac{1}{\hbar\pi}\sqrt{\dfrac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{1}{\hbar\pi}\sqrt{\dfrac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases}$ $\mathrm{J^{-1}\,m^{-1}}$	$D(E) = \begin{cases} \dfrac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases}$ $\mathrm{J^{-1}\,m^{-2}}$ $H(x) = 0$ for $x < 0$ and $H(x) = 1$ for $x > 0$
Density of states N_v and N_c are the effective densities of states	$D(E) = \begin{cases} N_v(300)\sqrt{\dfrac{2}{300\pi k_B (E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ N_c(300)\sqrt{\dfrac{2}{300\pi k_B (E - E_c)}} & E > E_c \end{cases}$ $\mathrm{J^{-1}\,m^{-1}}$	$D(E) = \begin{cases} \dfrac{N_v(300)}{300 k_B} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{N_c(300)}{300 k_B} H(E - E_c) & E > E_c \end{cases}$ $\mathrm{J^{-1}\,m^{-2}}$
Density of electrons in the conduction band $n = \int_{E_c}^{\infty} D(E) f(E)\,dE$	$n = \sqrt{\dfrac{m_e^* k_B T}{\hbar^2 \pi}} \exp\left(\dfrac{\mu - E_c}{k_B T}\right)$ $\mathrm{m^{-1}}$ $= N_c \exp\left(\dfrac{\mu - E_c}{k_B T}\right)$	$n = \dfrac{m_e^* k_B T}{\hbar^2 \pi} \exp\left(\dfrac{\mu - E_c}{k_B T}\right)$ $\mathrm{m^{-2}}$ $= N_c \exp\left(\dfrac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E)(1 - f(E))\,dE$	$p = \sqrt{\dfrac{m_h^* k_B T}{\hbar^2 \pi}} \exp\left(\dfrac{E_v - \mu}{k_B T}\right)$ $\mathrm{m^{-1}}$ $= N_v \exp\left(\dfrac{\mu - E_c}{k_B T}\right)$	$p = \dfrac{m_h^* k_B T}{\hbar^2 \pi} \exp\left(\dfrac{E_v - \mu}{k_B T}\right)$ $\mathrm{m^{-2}}$ $= N_v \exp\left(\dfrac{\mu - E_c}{k_B T}\right)$