

Introduction to Semiconductor Physics

Andrei Novitskii, Academic Research Center for Energy Efficiency, NUST MISIS
Email: novitskiy@misis.ru
@anovitzkij

- **Electrical conduction**
 - Ohm's law
 - Classification of materials
 - Model of semiconductors conductivity, the concept of a hole
- **Fundamentals of the band theory of semiconductors**
 - Brillouin zones
 - Band structure of some semiconductors
 - Effective mass
- **Electron and hole statistics in semiconductors**
 - Density of states
 - Fermi-Dirac distribution function
 - Fermi integral

Ohm's law. Classical Drude-Lorentz model

Ohm's law defines the conductivity σ of a material as proportionality constant between the current density \vec{j} and the applied electric field \vec{E} resulting in a simple relation $\vec{j} = \sigma \vec{E}$. Considering that every electron feels an electric force $\vec{F} = m\vec{a}$ equal to $-e\vec{E}$ (e being the absolute value of the electron charge, \vec{a} is the electron's acceleration and m^* is the electron effective mass) the drift velocity $\vec{v}_d = \vec{a}\tau = -e\vec{E}\tau/m^*$. Here, τ is the mean free time which is the average time between scattering events. τ is also known as the conductivity relaxation time because it represents the time scale for the momentum gained from an external field to relax. Equivalently, $1/\tau$ is the average probability per unit time that an electron is scattered.^[1-3] The distance an electron travels between scattering events is called the free path. The average or mean free path for an electron is simply $\vec{l} = \vec{v}_t\tau$ (Fig. 1). Here, \vec{v}_t is thermal velocity $\vec{v}_t = \sqrt{3k_B T/m^*}$, where k_B is the Boltzmann constant and T is the temperature. Thus, the mean speed of electron $\vec{u} = \vec{v}_d + \vec{v}_t$. Ohm's law is valid only when τ is independent from \vec{E} and $\vec{v}_t \gg \vec{v}_d$.

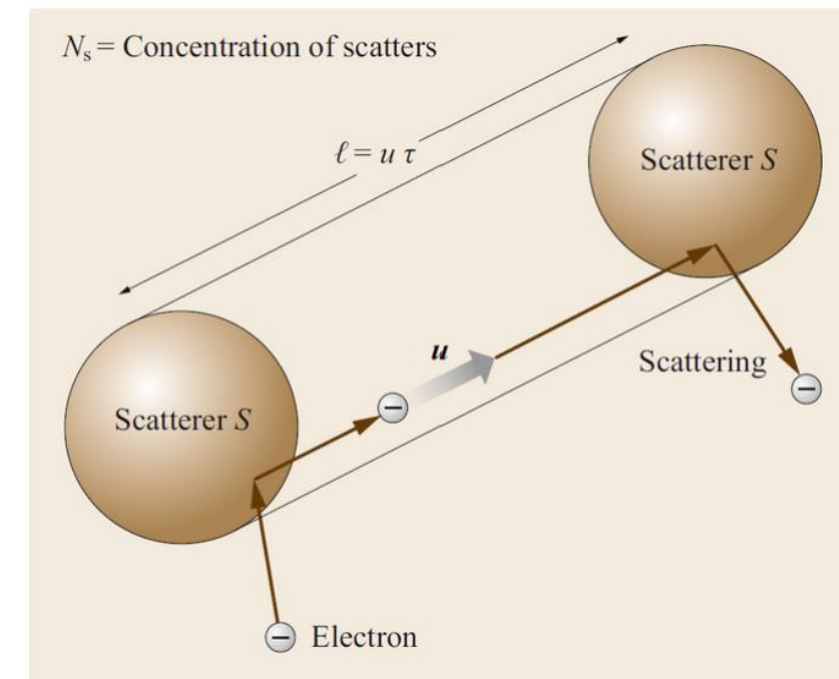


Figure 1. Scattering of an electron from a scattering center. The electron travels a mean distance $\vec{l} = \vec{u}\tau$ between collisions.^[2] Here, $\vec{u} = \vec{v}_t$.

In order to determine the main quantities of semiconductor physics one should consider that the drift velocity gives rise to an electric current. If the density of electrons is n then the current density $\vec{j} = -en\vec{v}_d$. Considering the Ohm's law, the conductivity and drift velocity can now be related to the scattering time.^[1,4] However, one should consider that electrons have different relaxation time and thus $\langle\tau\rangle = \omega^{-1}$, where ω is the probability of scattering. In this case, drift velocity should be calculated as integral: $\vec{v}_d = \int_0^\infty \vec{v}(t)\omega(t)dt = \frac{e\tau}{m^*}\vec{E} = \mu_d\vec{E}$, here $\vec{v}(t) = \frac{et}{m^*}\vec{E}$ and $\omega(t) = \frac{1}{\tau}e^{-t/\tau}$. Thus, we can define one of the main parameter of semiconductors – drift mobility, $\mu_d = \frac{e\tau}{m^*}$, as the proportionality coefficient between drift velocity and the applied electric field \vec{E} ; and the electrical conductivity of a material as $\sigma = en\mu_d$.



Initially, solids were divided into several groups according to the absolute value of their electrical resistivity, ρ , at room temperature as shown in Table 1. However, it is not accurate enough. It is more important to consider the temperature dependence of the electrical resistivity as well as features of the electronic structure. In metals, the resistivity increases when the temperature is raised (see Fig. 2a) as $\rho(t) = \rho_0(1 + \alpha t)$, where ρ_0 is the resistivity at $t = 0^\circ\text{C}$, α is thermal resistivity coefficient $\sim \frac{1}{273}$. For metals $\alpha = \frac{d\rho}{dt} > 0$. Such behaviour is attributed to an increase in the amplitude of the vibrations of the network, and this has the effect of slowing down the electronic motion. In other words, the electron-phonon coupling is more pronounced when the temperature increases.^[1,3,5] (A phonon is a quantum of vibrational energy of the periodic elastic arrangements of atoms or molecules.^[1-3]) For semiconductors $\rho = \rho_0 e^{\beta/T}$, $\beta < 0$ (Fig. 2b).

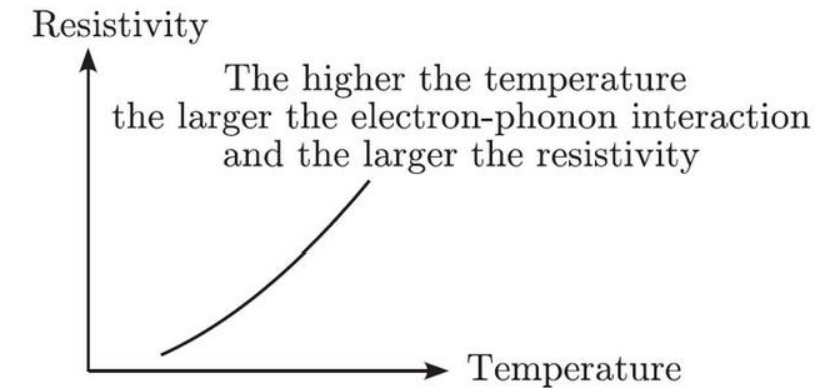


Figure 2a. Temperature dependence of the electrical resistivity for a metallic system.^[2]

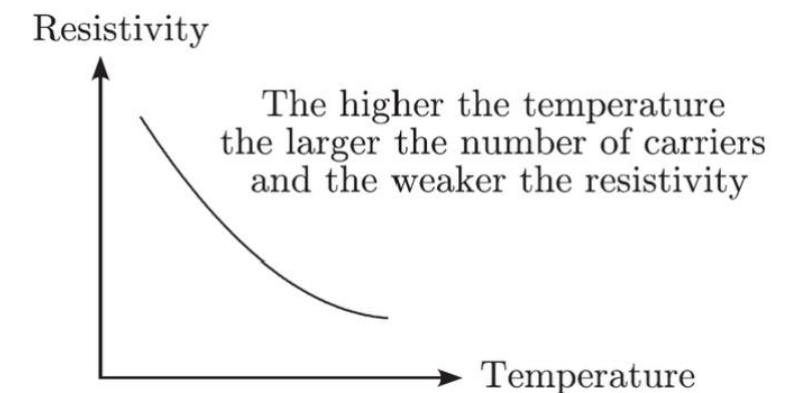


Figure 2b. Temperature dependence of the electrical resistivity for a semiconducting system.^[2]

Classification of materials

Table 1. Number of carriers, electrical resistivity at room temperature and main features of the band structure for different bulk materials

Material	Number of carriers	Electrical resistivity	Feature of the electronic structure
Metals	$> 10^{22} \text{ cm}^{-3}$	$10^{-6} - 10^{-4} \Omega \cdot \text{cm}$	Conduction and valence bands are overlapped; Fermi level inside the highest occupied band
Semimetals	$10^{17} - 10^{22} \text{ cm}^{-3}$	$10^{-4} - 10^3 \Omega \cdot \text{cm}$	Small overlap between the conduction band and the valence band (no bandgap); Fermi level occurs where two bands merge or slightly overlap
Semiconductors	$10^{13} - 10^{17} \text{ cm}^{-3}$	$10^{-4} - 10^{10} \Omega \cdot \text{cm}$	Bandgap $< 3 \text{ eV}$; Fermi level is inside a bandgap
Insulators	$< 10^{13} \text{ cm}^{-3}$	$> 10^{10} \Omega \cdot \text{cm}$	Bandgap $> 3 \text{ eV}$; Fermi level is inside a bandgap

To summarize, the main differences between metal and semiconductor are (1) absolute value of the electrical conductivity (resistivity); (2) different temperature dependences of the conductivity: linear for metals and exponential for semiconductors (activation character); (3) the electrical conductivity of metals is virtually independent of the number of impurities or defects, while the semiconductor conductivity strongly depends on the chemical purity and crystal perfection; (4) external influences such as lighting or radiation do not affect significantly the conductivity of metals, but strongly affect the conductivity of semiconductors.



The electrical conductivity of a semiconductor in particular essentially depends on four parameters:

- the density of states near the Fermi level;
- the electron-phonon coupling;
- the temperature (or other external conditions);
- the defects.

The concept of a hole was introduced to describe transport in semiconductors. In simple words, a hole can be considered as the lack of an electron at a position where one could exist in an atom or atomic lattice. It was found very useful for the description of the electrical transport in semiconductors since the movement of holes to some extent is similar to those of valent electrons meaning that all the transport equations appropriate for electrons would be also appropriate for holes. In that case the conductivity of intrinsic semiconductor can be written as $\sigma = e_n n \mu_n + e_p p \mu_p$, where e_n is the absolute value of the electron charge, $e_p = -e_n$, n , p and μ_n , μ_p are the concentration and mobility of electrons and holes, respectively; in some books all parameters related to the electrons are subscripted with e , like n_e , μ_e , while parameters for holes subscripted with h , like n_h (not p) and μ_h . See more in Refs. [4–6].



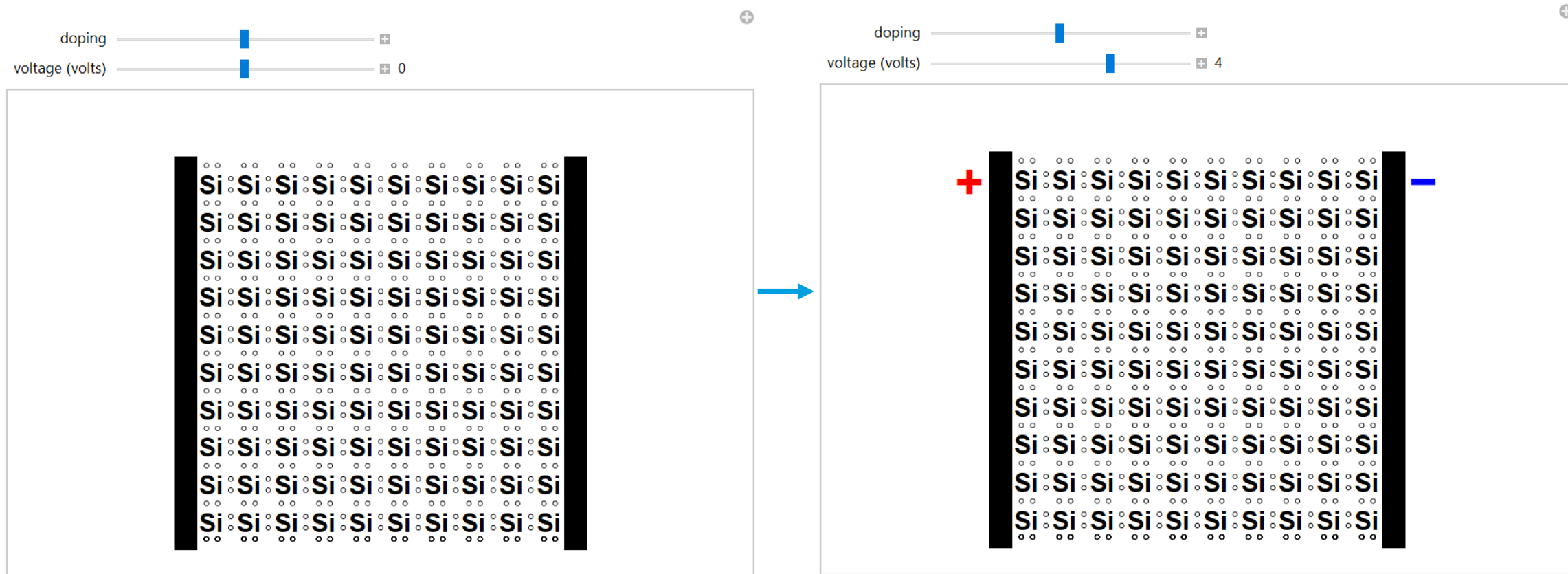
Concept of a hole

The concept of a hole was introduced to describe transport in semiconductors. In simple words, a hole can be considered as the lack of an electron at a position where one could exist in an atom or atomic lattice. It was found very useful for the description of the electrical transport in semiconductors since the movement of holes to some extent is similar to those of valent electrons meaning that all the transport equations appropriate for electrons would be also appropriate for holes. In that case the conductivity of intrinsic semiconductor can be written as $\sigma = e_n n \mu_n + e_p p \mu_p$, where e_n is the absolute value of the electron charge, $e_p = -e_n$, n , p and μ_n , μ_p are the concentration and mobility of electrons and holes, respectively; in some books all parameters related to the electrons are subscripted with e , like n_e , μ_e , while parameters for holes subscripted with h , like n_h (not p) and μ_h . See more in Refs. [4–6].



Intrinsic semiconductor

$n = p$ and thus $\sigma = \sigma_p + \sigma_n = e_n \mu_n n + e_p \mu_p p = e_p \mu_p p (1 + b)$, where $b = |\mu_n|/|\mu_p|$



n -type semiconductor

$n \gg p$ and thus $\sigma = \sigma_n = e_n \mu_n n$

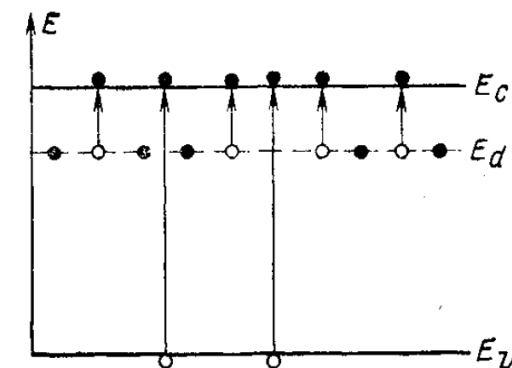
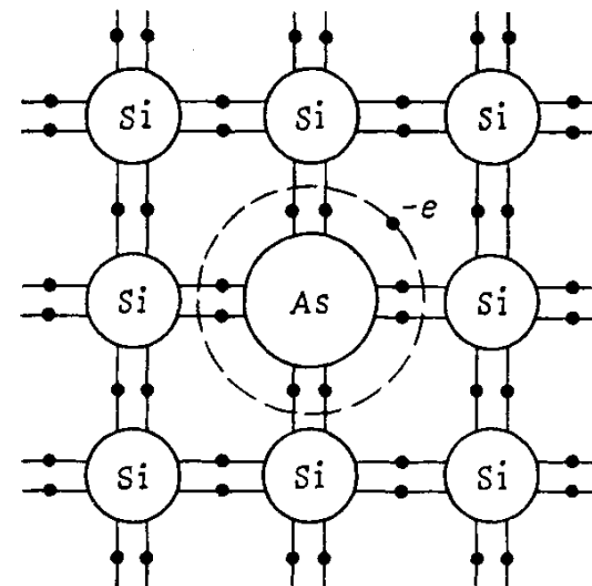
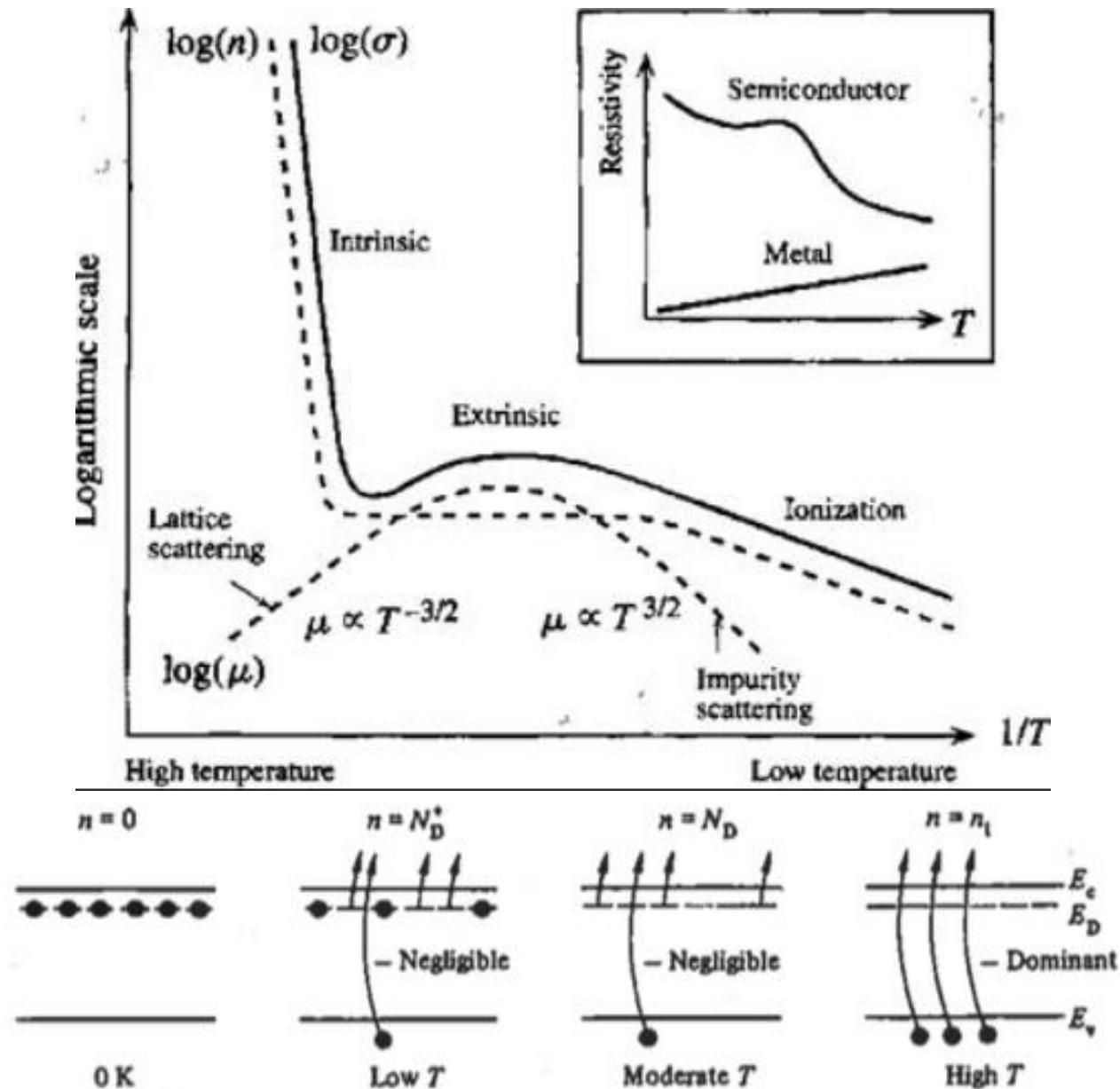
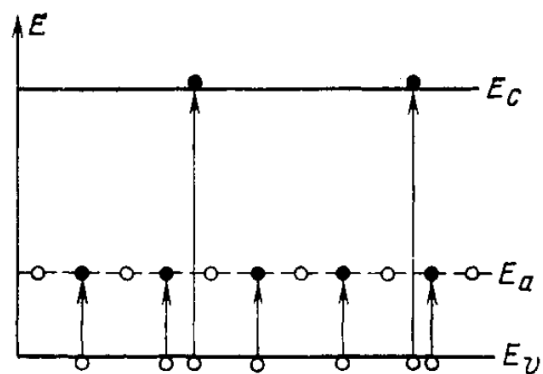
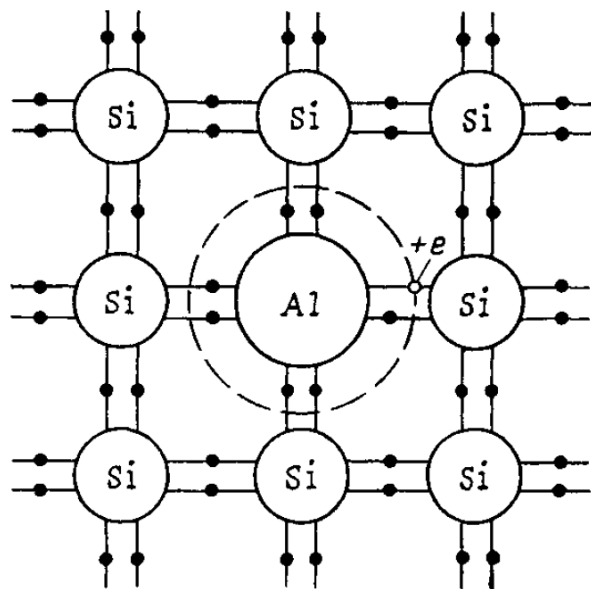


p-type semiconductor

$n \ll p$ and thus $\sigma = \sigma_p = e_p \mu_p p$

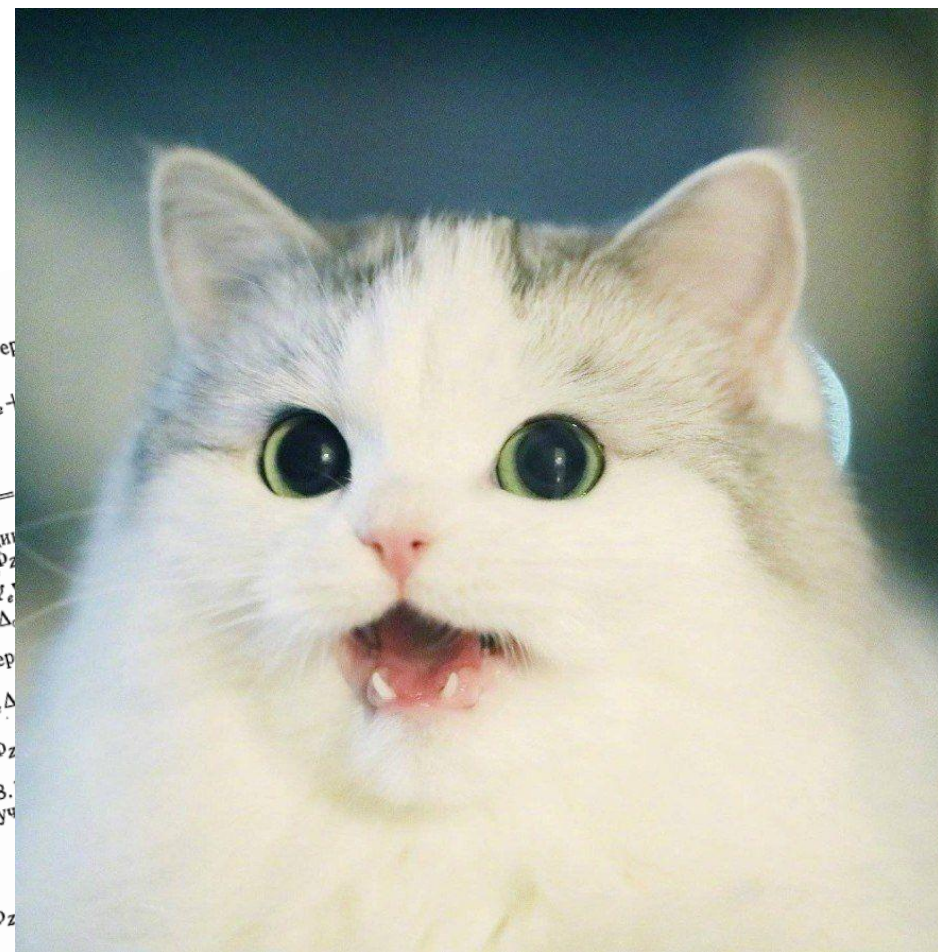


Temperature dependencies of σ , n , and μ



- Schrödinger equation for a crystal

- ## Stochastic approximation



Глава II ТЕОРИИ ПОЛУПРОВОДНИКОВ

УРАВНЕНИЕ ШРЕДИНГЕРА ДЛЯ КРИСТАЛЛА

$$\hat{H}\Psi = E\Psi, \quad (7.1)$$

$$\Psi(r_i; R_a), \quad (7.2)$$

$$\left(-\frac{\hbar^2}{2m} \Delta_l\right), \quad (7.3)$$

$$+ \frac{\partial^2}{\partial x_l^2}; \quad (7.4)$$

$$(7.5)$$

где E_k

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жестокости
щениях
Ниж

4) энергию

$$U_z = \frac{1}{2} \sum_{\alpha \neq \beta} \frac{Z_\alpha Z_\beta e^2}{4\pi\epsilon_0 |R_\alpha - R_\beta|} = 1$$

$$U_{ez} = - \sum_{i, \alpha} \frac{Z_{\alpha} e^2}{4\pi\epsilon_0 |r_i - R_{\alpha}|} = \sum_{i, \alpha} U_{i\alpha}$$

$$\hat{H} = \hat{T}_e + \hat{T}_i$$

$$\hat{H}\Psi = E\Psi, \quad (7.11)$$
 содержит 3 ($Z=1$)

трудности, но и с трудностями принципиально решить уравнение системы по частям, необходимо для механики частиц, особенно в квантовой механике.

отношением

$$\Psi_k(r_k), \quad (7.16)$$

действующих частиц к системе
и только в результате прибли-
е или менее очевидных упро-
шение поля отсутствуют:

подставим его в уравнение Шредингера
уравнение для $\Phi_Z(R_1, \dots)$:

или, учитывая (8.3), запишем

Так как Ψ_e зависит от Φ , найдем, например, $\Delta_\alpha \Psi_e \Phi$

$$\Delta_\alpha \Phi Z \Psi_e = \nabla_\alpha (\Psi_e \Phi) = \Psi_e \Delta_\alpha \Phi + \Phi \Delta_\alpha \Psi_e$$

$$\hat{H}_Z \Psi_e \Phi_Z = \sum_{\alpha} \left(-\frac{\hbar^2}{2M_{\alpha}} \right) [\Psi_e \Delta_{\alpha} + U_Z \Psi_e \Phi_Z]$$

(7. Умножим уравнение (8. по координатам электронов; у

$$\sum_{\alpha} \left(-\frac{\hbar^2}{2M_{\alpha}} \right) \left[\Delta_{\alpha} \Phi_Z + \Phi_Z \Delta_{\alpha} \right]$$

ние для гамильтониана, кото-
рого гамильтонианом электро-

Волновую функцию электрона Ψ_e можно считать зависящей от координат электрона \mathbf{r}_e и координат ядра \mathbf{R}_α , причем $\Psi_e(\mathbf{r}_e; \mathbf{R}_\alpha)$ должна удовлетворять уравнению Шредингера для любых значений координат ядра \mathbf{R}_α .

$$\int \Psi_e^* (r_1, \dots; R_1^0$$

ние для гамильтониана, который обозначим теперь через \hat{H}_e и назовем его гамильтонианом электронов:

$$\hat{H}_e = \hat{T}_e + \hat{U}_e + \hat{U}_{ez}. \quad (8.1)$$

Волновую функцию электронов обозначим через Ψ_e . Она должна зависеть от координат электронов \mathbf{r}_i и координат покоящихся ядер \mathbf{R}_a^0 , причем $\Psi_e(\mathbf{r}_i; \mathbf{R}_a^0)$ должна быть нормирована к единице при любых значениях координат ядер при интегрировании по координатам электронов:

$$\int \Psi^*(\mathbf{r}_1, \dots, \mathbf{r}_N; \mathbf{R}^0, \dots) \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N; \mathbf{R}^0, \dots) d\tau_1 \dots d\tau_N \quad (8.2)$$

Уравнение Шредингера может быть записано в следующем виде:

оложения о характере зависи
преоблечь в H_c взаимодейст
ся в гамильтоновой системы не
вая функция такой системы бу
томных волновых функций,
том случае

реписать в следующем виде:

$$\frac{1}{m} \Delta_1 \Psi_e d\tau_e = - \sum_{i, \alpha} \frac{m}{M_\alpha} \langle T_i \rangle, \quad (8.17)$$

$$\alpha \Psi_e d\tau_e = -ZN \cdot \frac{m}{M} \langle T_1 \rangle.$$

... $\langle \mathbf{p}_a \rangle \cdot \langle \mathbf{p}_i \rangle$.

$$\left\langle \frac{p_i^2}{2M_\alpha} \right\rangle = \left\langle \frac{p_\alpha^2}{2M_\alpha} \right\rangle$$

$$\langle p_e \rangle^2 = \frac{8}{3\pi} \langle p_e^2 \rangle,$$

$$\langle p_z \rangle \approx \sqrt{\frac{m}{M}} \langle p_z \rangle,$$

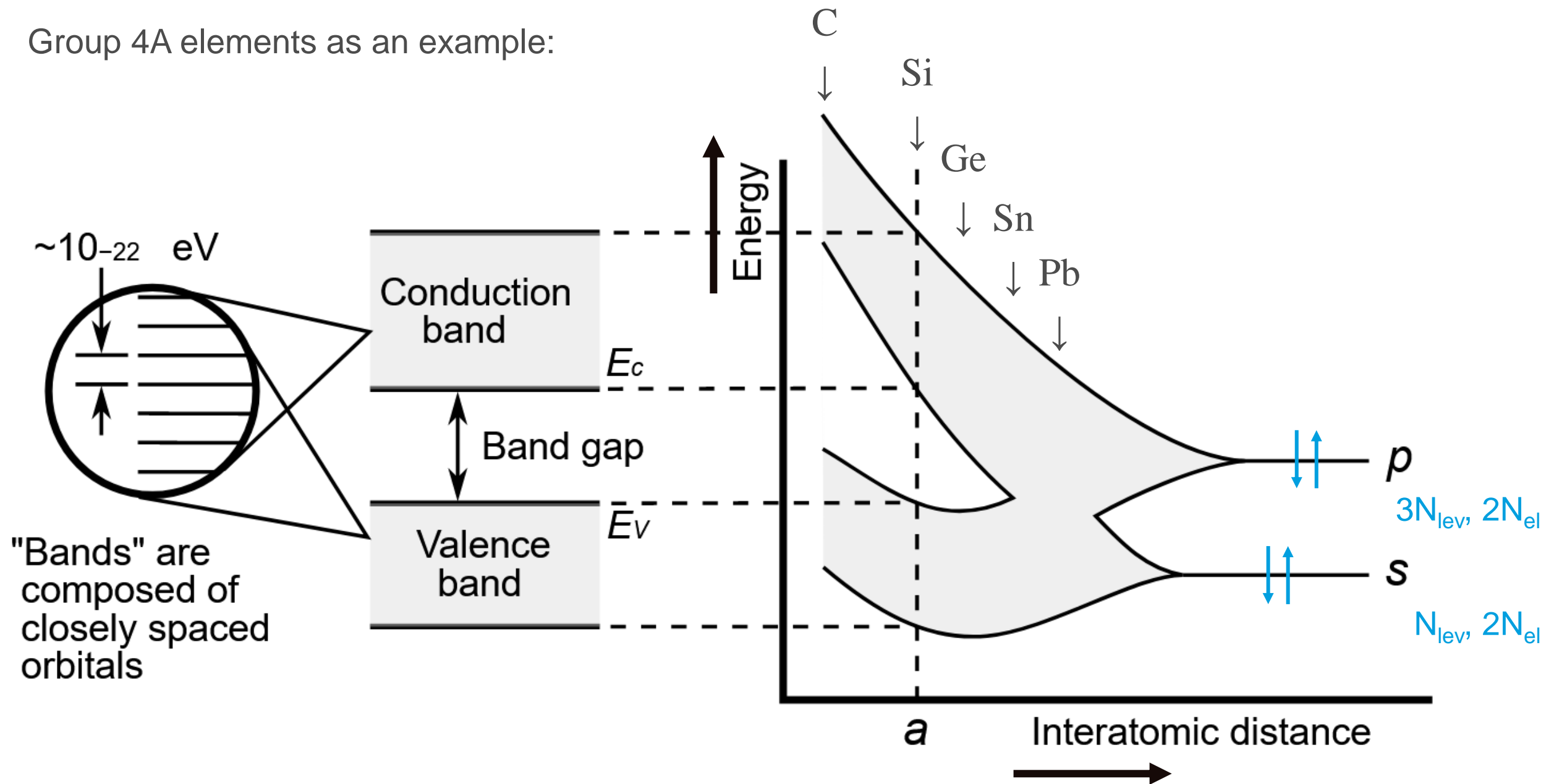
поэтому второй член в (8.15) составляет величину, от полной энергии кристалла.

Мы ввели функцию электр-
новых функций (так называемую функцию электр-
электронов). Если бы волновая функция свободных
координат ядер (приближение свободных
поправки в (8.15) были бы равны нулю.

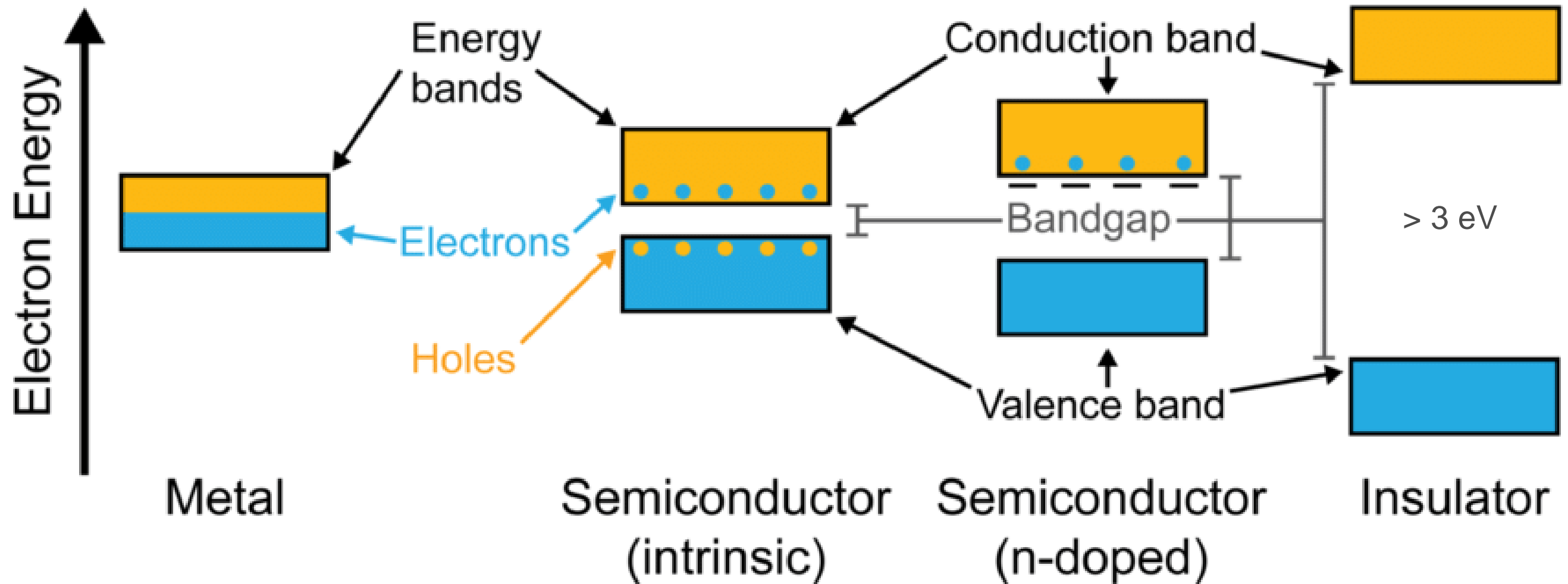
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Formation of bands

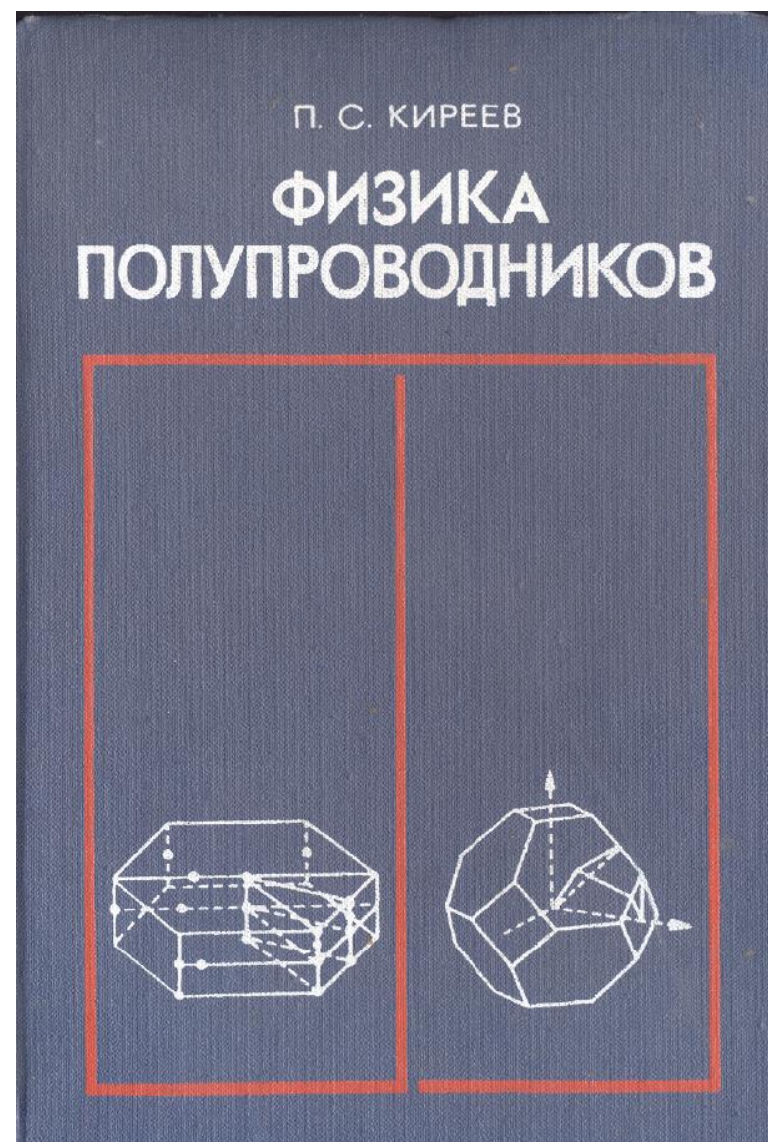
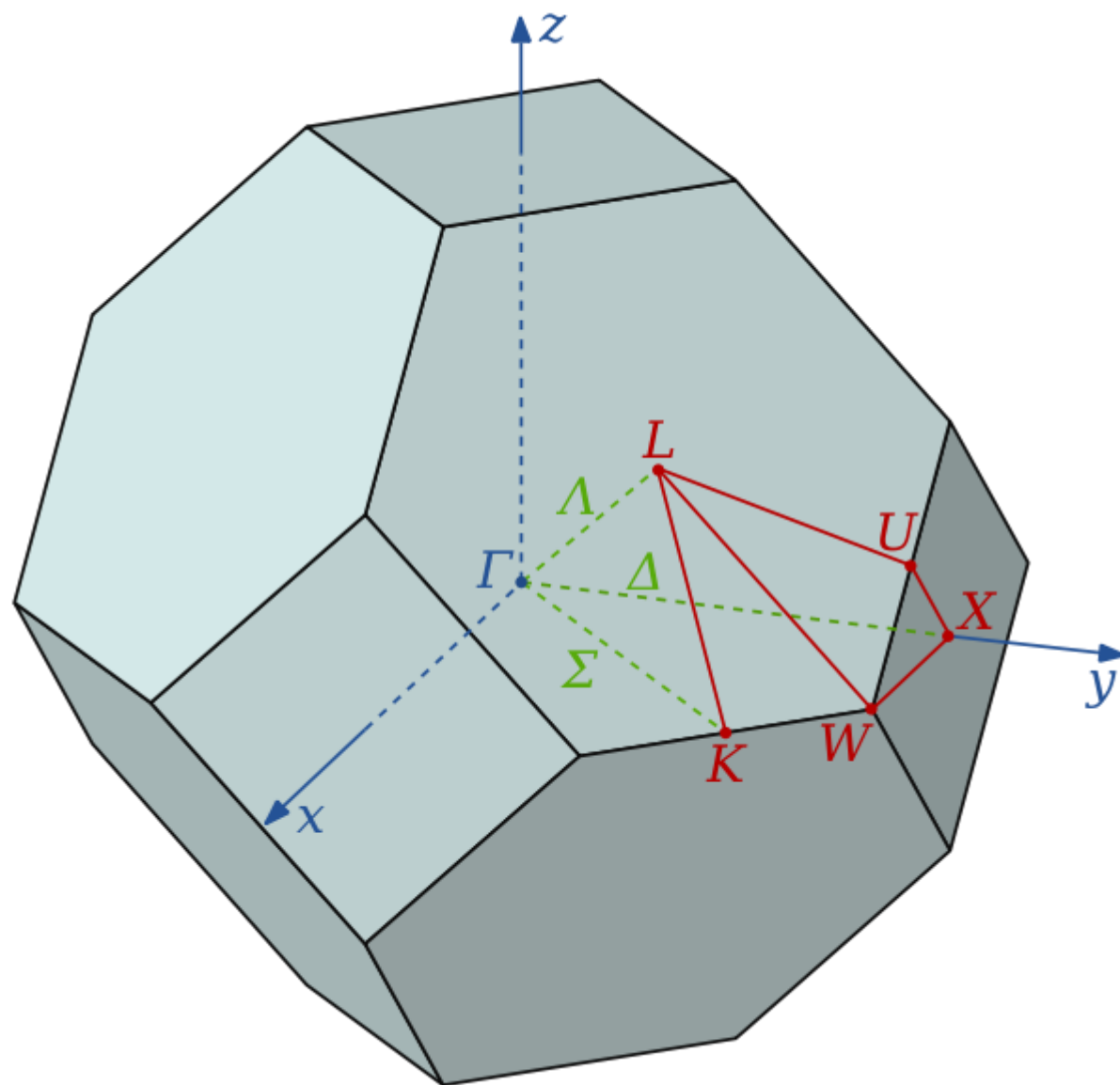
Group 4A elements as an example:



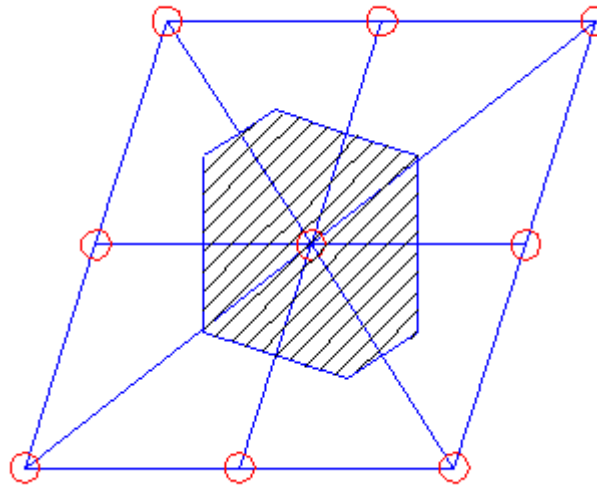
Schematic band structures of solids



Brillouin zone



The first Brillouin zone is a uniquely defined primitive cell in reciprocal space. In fact, the Brillouin zone can be considered as Wigner–Seitz cell of the reciprocal space. For example, Wigner–Seitz cell for a 2D lattice looks as follows



and exhibits the following properties:

- there is only one Wigner–Seitz cell for any given lattice and it contains only one lattice point
- it is a primitive cell with the smallest volume for particular symmetry
- it has the same point symmetry group as the entire Bravais lattice of the crystal, which implies that the Wigner–Seitz cell spans the entire direct space without leaving any gaps or holes

In the real space (direct lattice) the position of the lattice points is indicated by vector $R_n = n_1 a_1 + n_2 a_2 + n_3 a_3$, here $n_1, n_2, n_3 \in \mathbb{Z}$, where \mathbb{Z} is the set of integers and a_i is a primitive translation vector. In the same manner a vector G_m for the reciprocal space can be represented considering that the reciprocal space is based on its own primitive translation vectors (b_1, b_2, b_3) where:

$$b_1 = \frac{[a_2 a_3]}{(a_1 [a_2 a_3])} \quad b_2 = \frac{[a_3 a_1]}{(a_1 [a_2 a_3])} \quad b_3 = \frac{[a_1 a_2]}{(a_1 [a_2 a_3])}$$

and thus, $G_m = m_1 b_1 + m_2 b_2 + m_3 b_3$, here $m_1, m_2, m_3 \in \mathbb{Z}$.



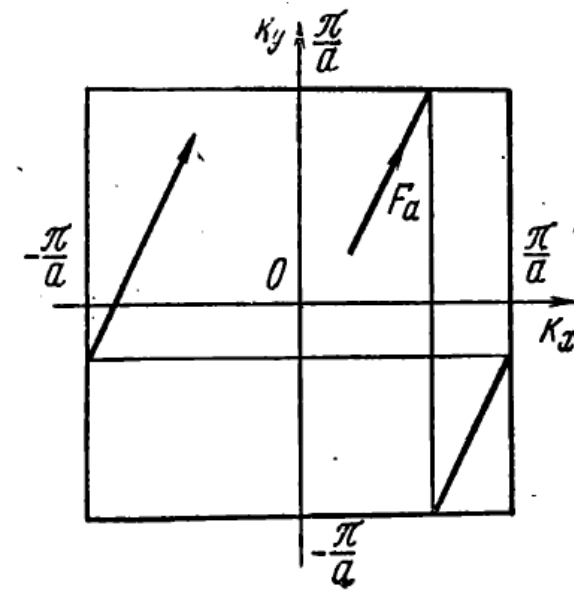
Considering that the crystal lattice is periodic, then, according to the Bloch theorem, the wave function for the periodic potential of the solid body lattice is completely described by its behavior in the first Brillouin zone.

Once again, since the Coulomb field in the crystal is periodic, then the energy has a periodic dependence on the wave vector $E(k + 2\pi G_m) = E(k)$, where k is the wave vector $k = 2\pi/\lambda$. In other words, the states characterized by the vector k and $k + 2\pi G_m$ are physically equivalent, and the energy of the electrons in these two states is the same.

Thus

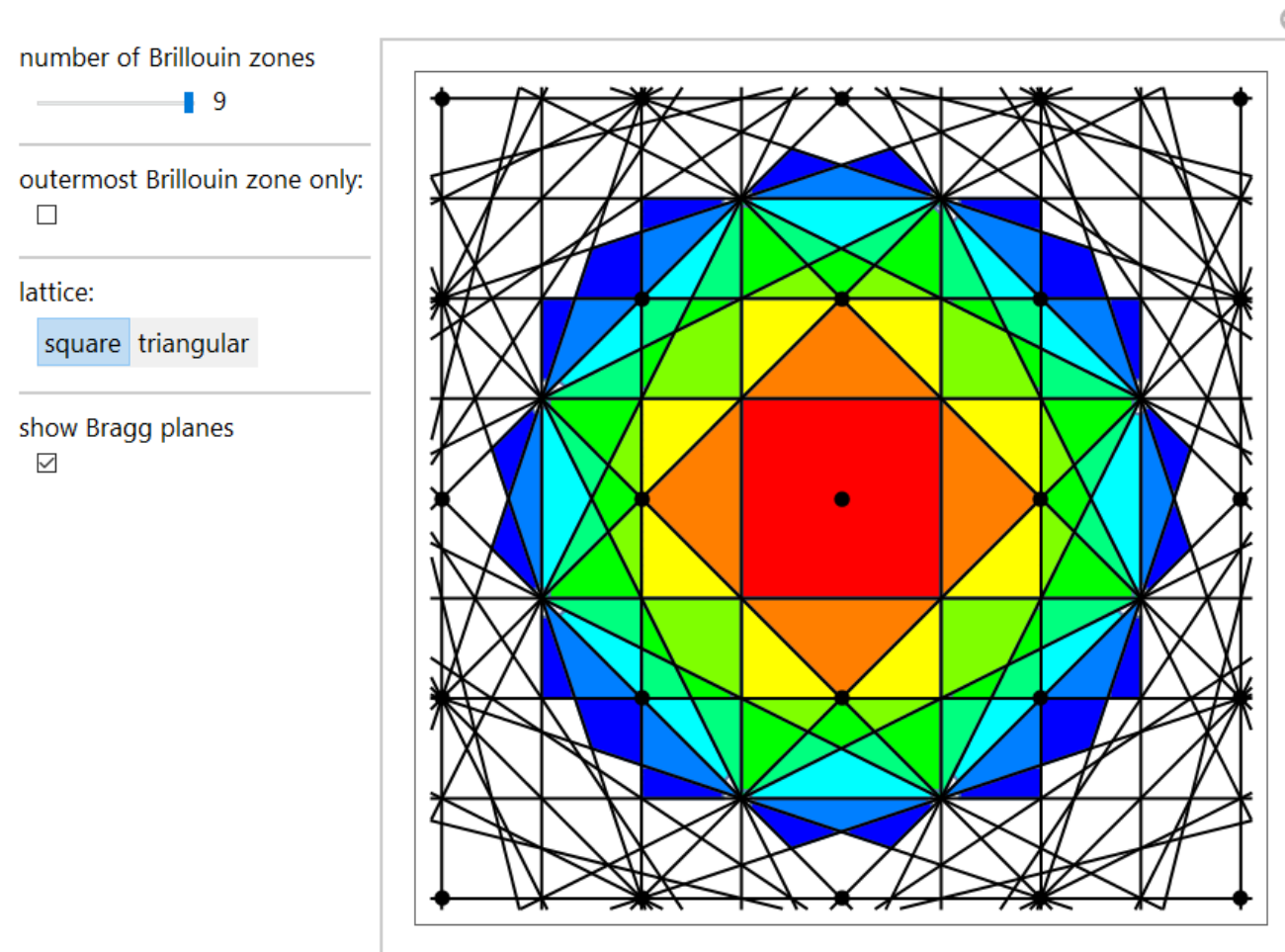


- all the allowed quantum mechanical states are in the first Brillouin zone
- the particle trajectory in k -space can be considered only within the first Brillouin zone (see Figure)
- for any lattice, the intervals of the 1st Brillouin zone can be given as $-\pi/a_i \leq k_i \leq \pi/a_i$, where a is the lattice parameter



Brillouin zone construction

For 2D cubic lattice:

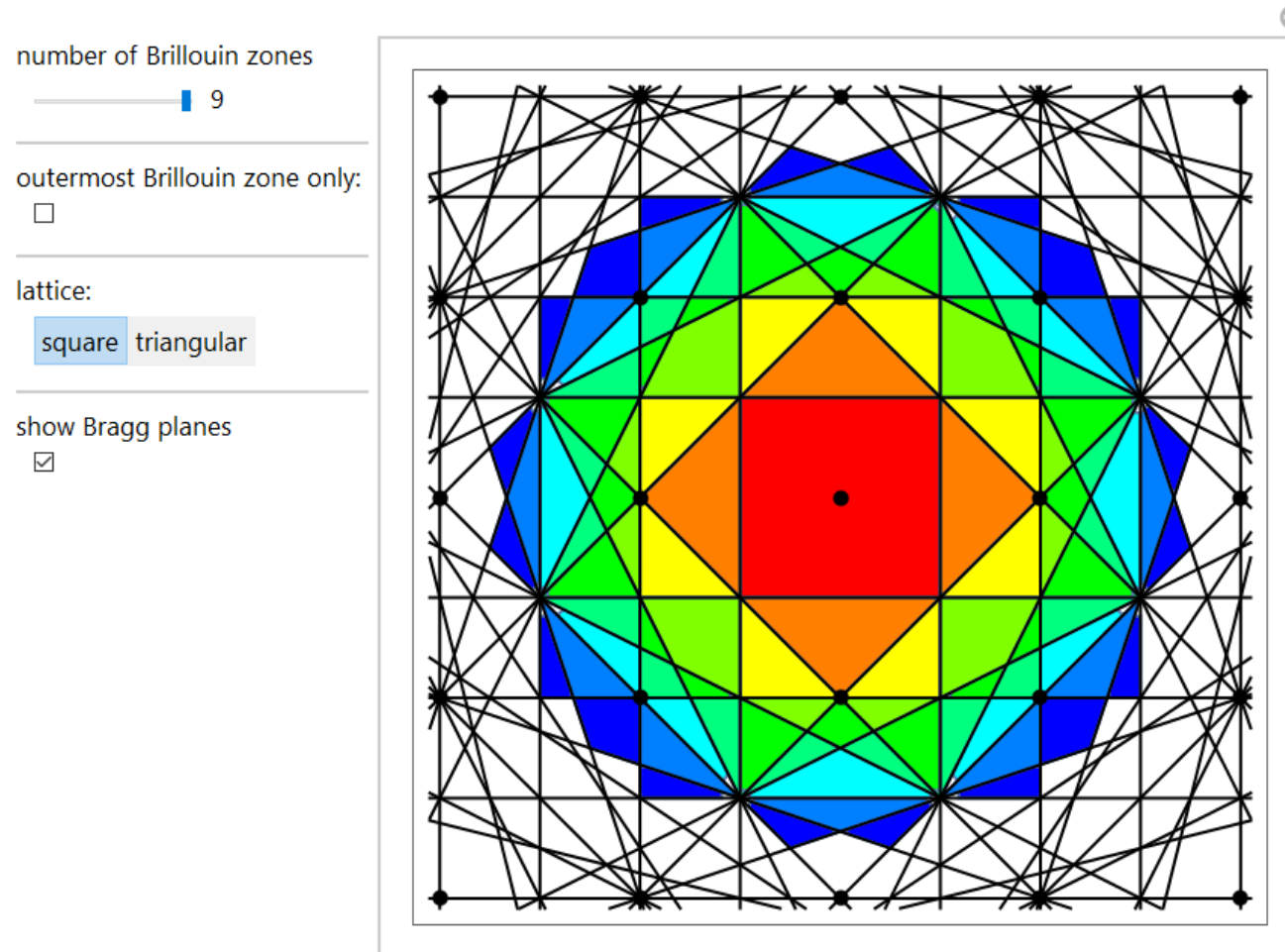


<https://demonstrations.wolfram.com/2DBrillouinZones/>

also see <https://github.com/hedhyw/BrillouinZones>

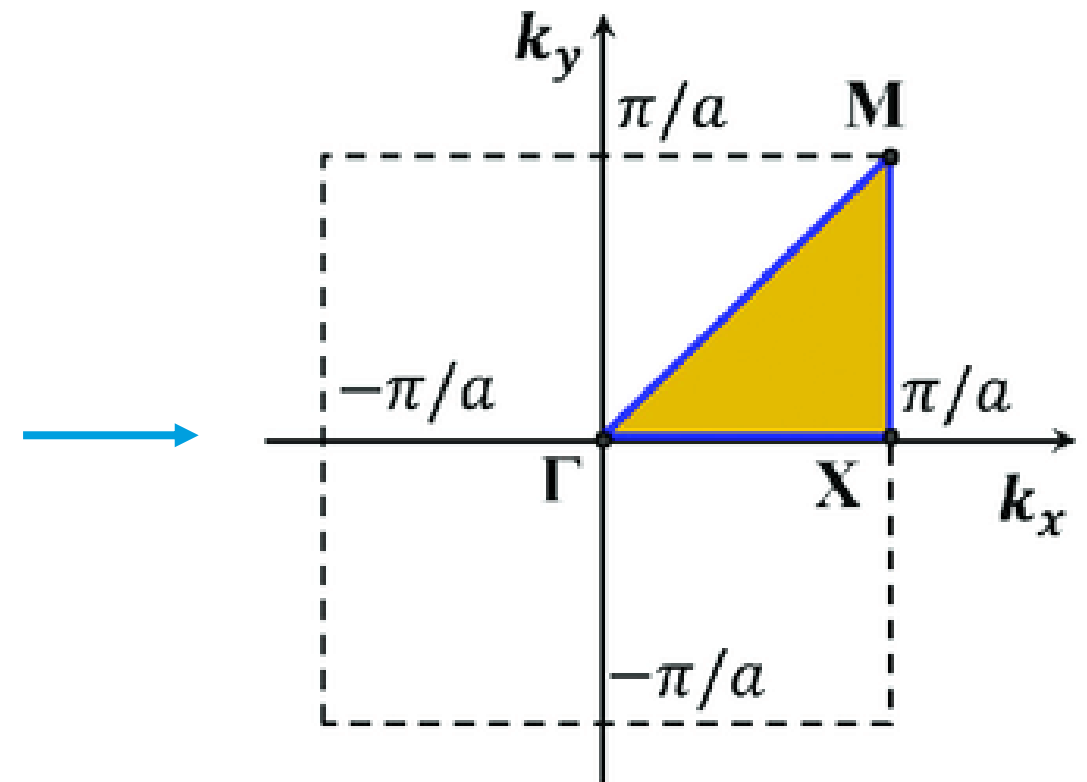
Irreducible Brillouin zone

For 2D cubic lattice:



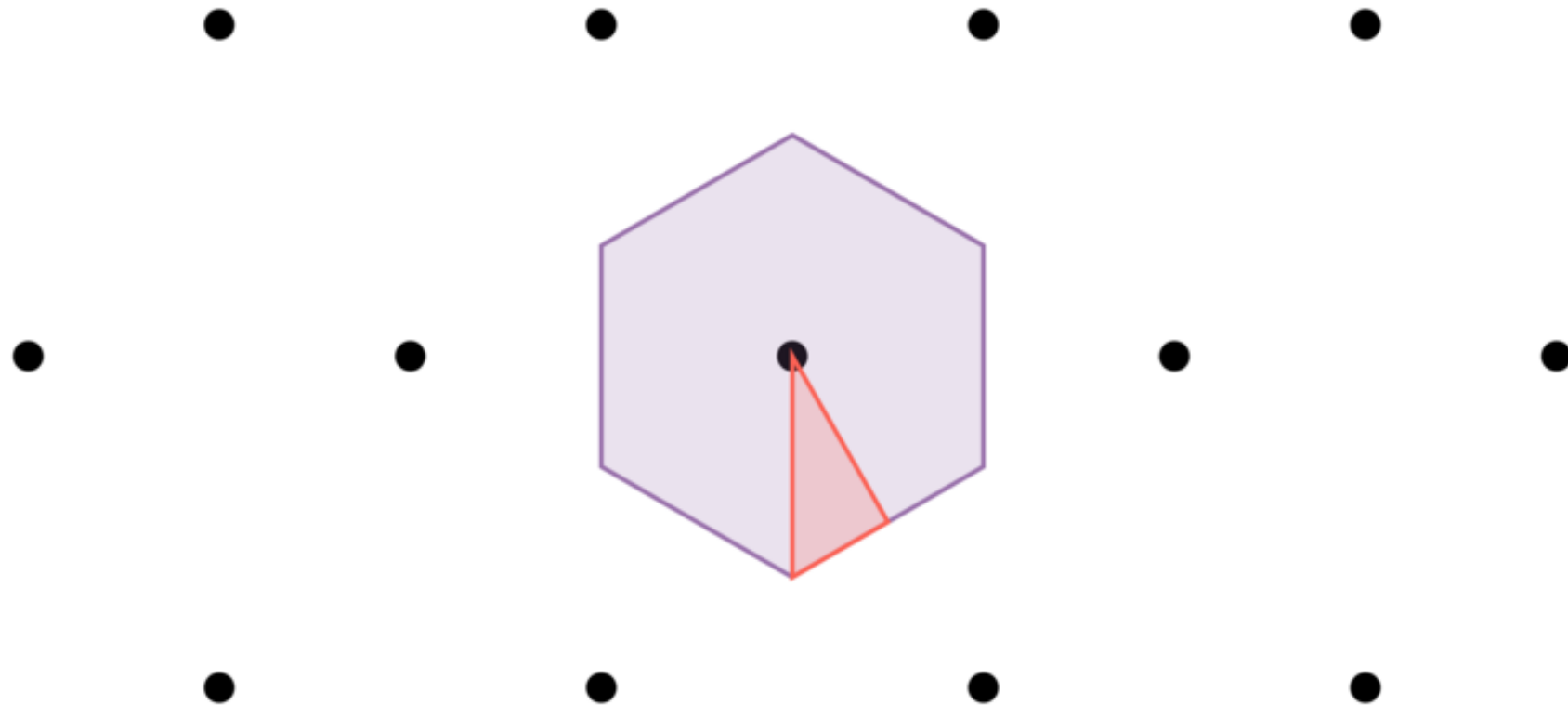
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also see <https://github.com/hedhyw/BrillouinZones>



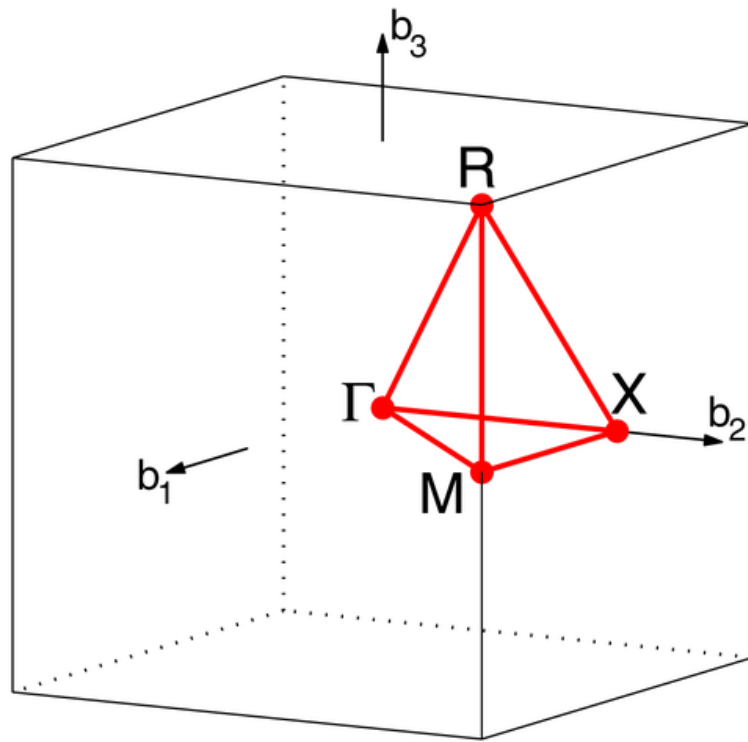
Irreducible Brillouin zone

For 2D hexagonal lattice:

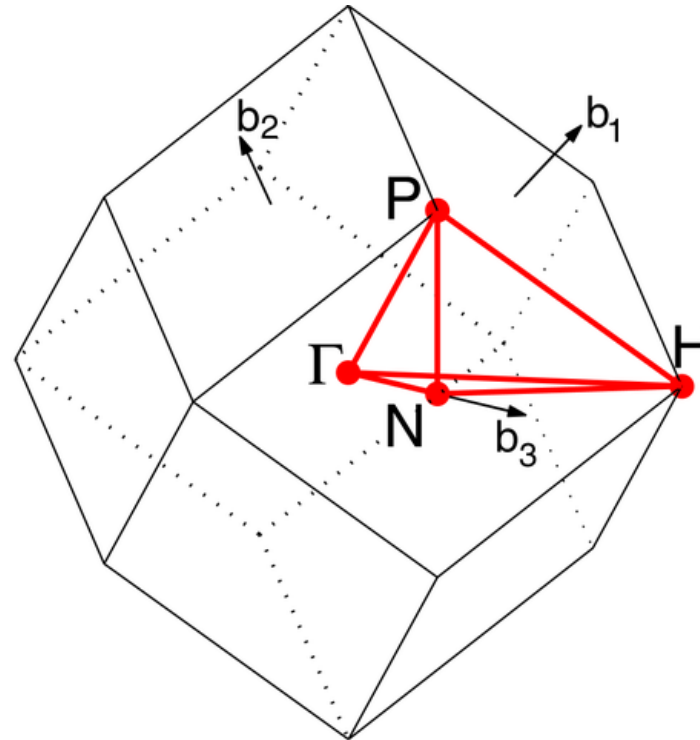


Irreducible Brillouin zone

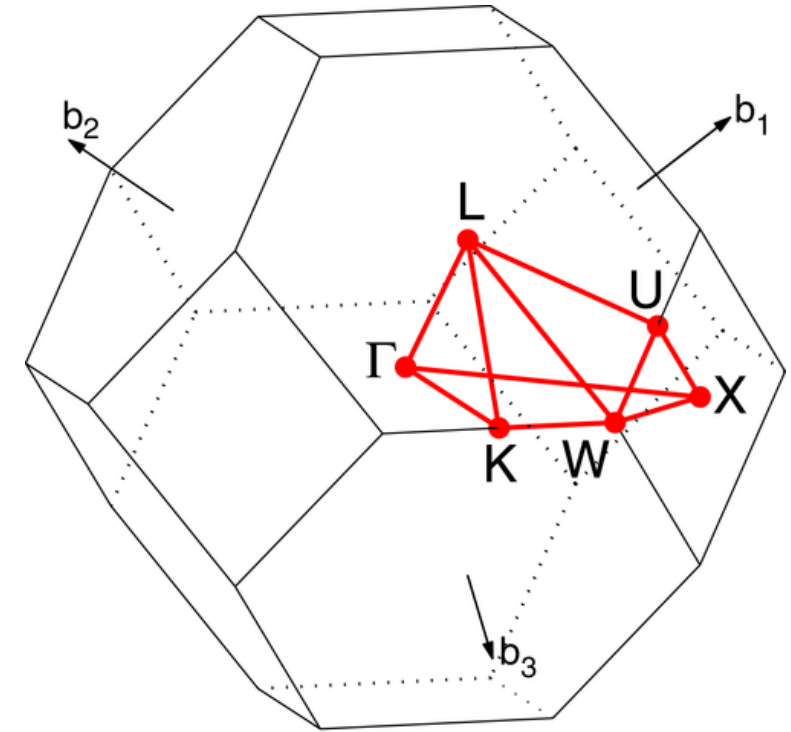
For 3D cubic lattice:



Primitive cubic



Body-centered cubic



Face-centered cubic

Brillouin zone. High-symmetry points

Several points of special interest are called high-symmetry (critical) points:

Γ in the center of the Brillouin zone

X in the center of a face

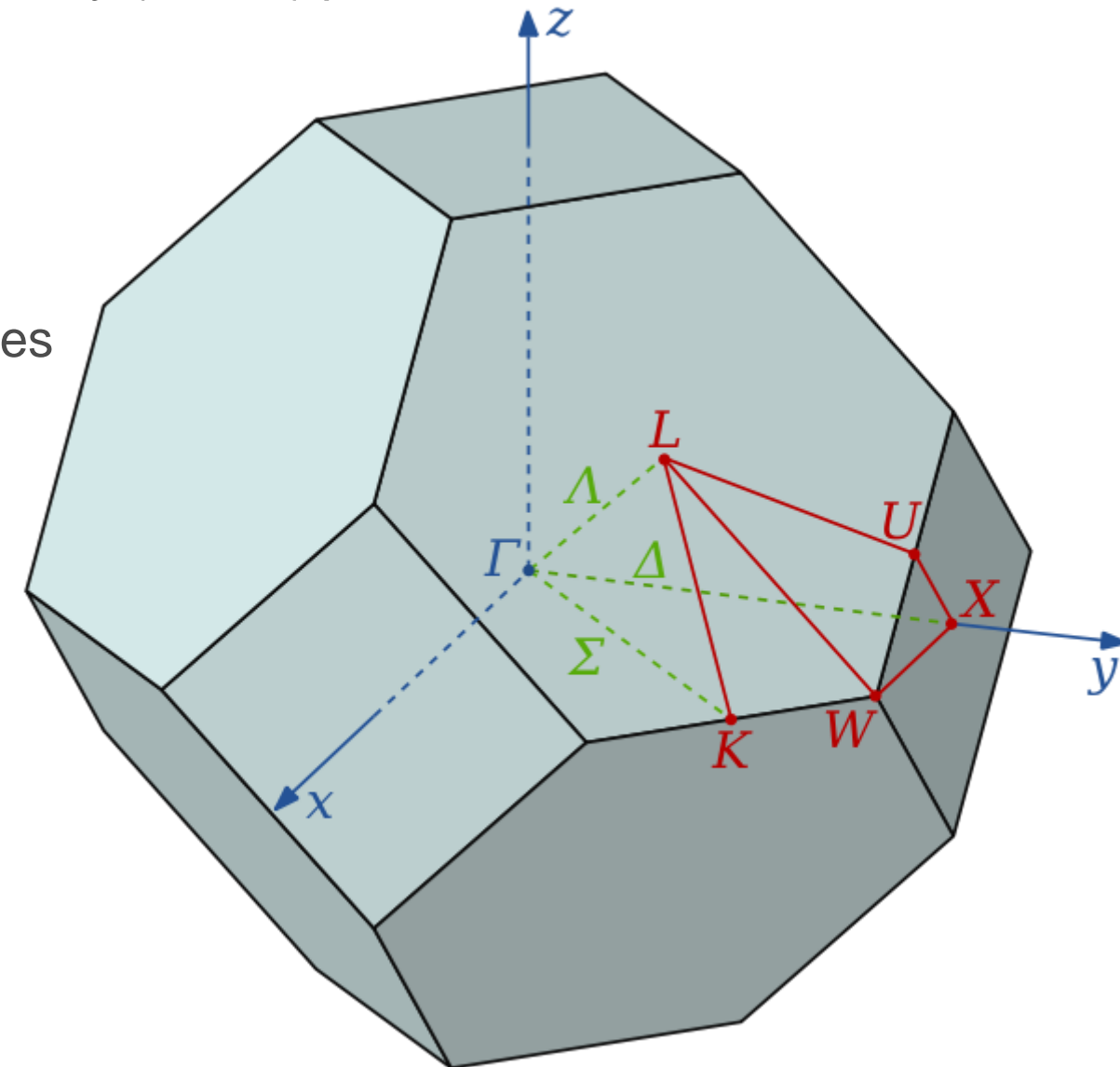
(line from Γ to X is usually indicated as Δ)

L in the center of a hexagonal face

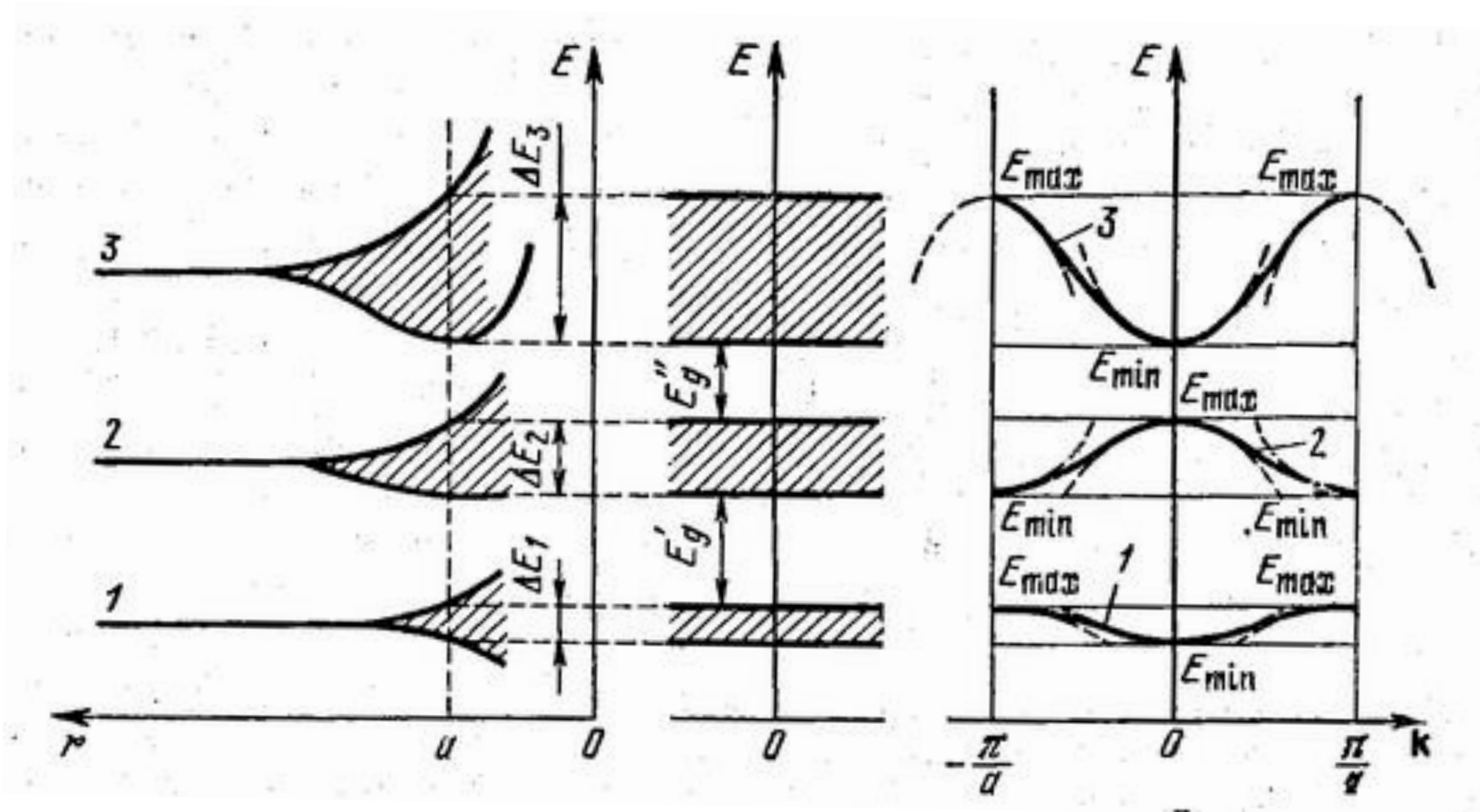
K in the middle of an edge joining two rectangular faces

W in the corner point

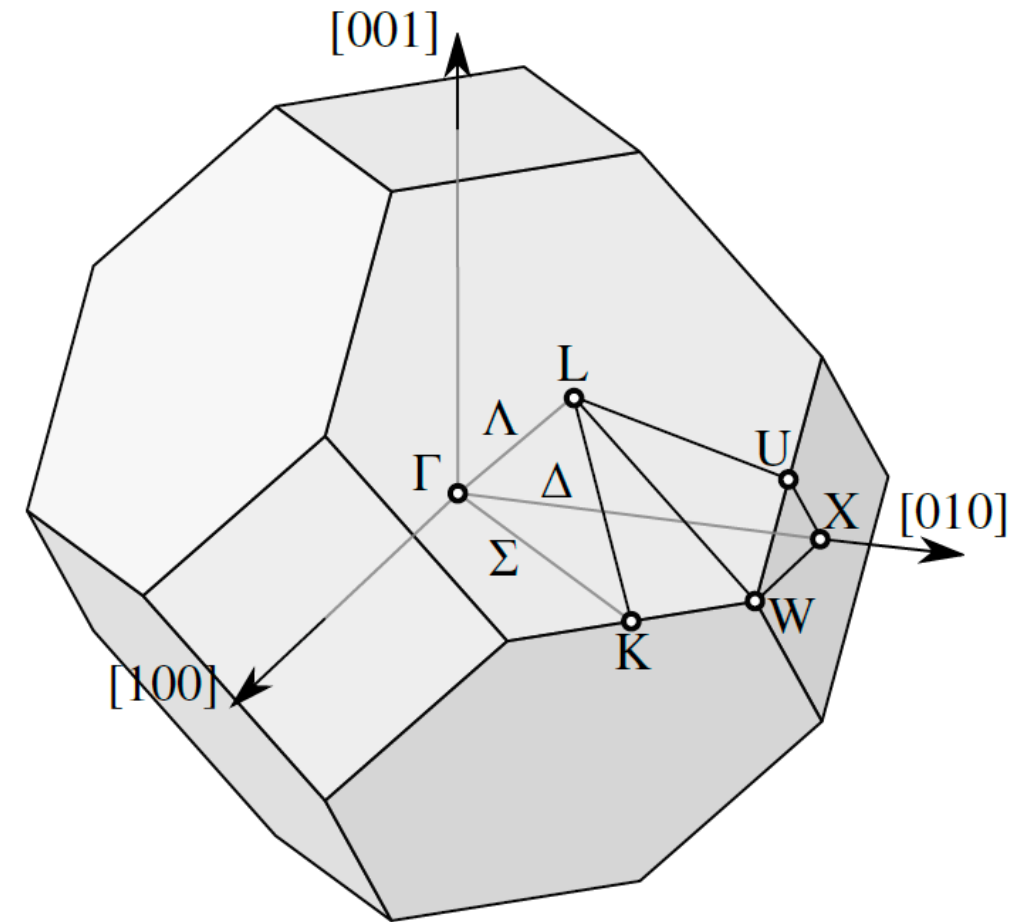
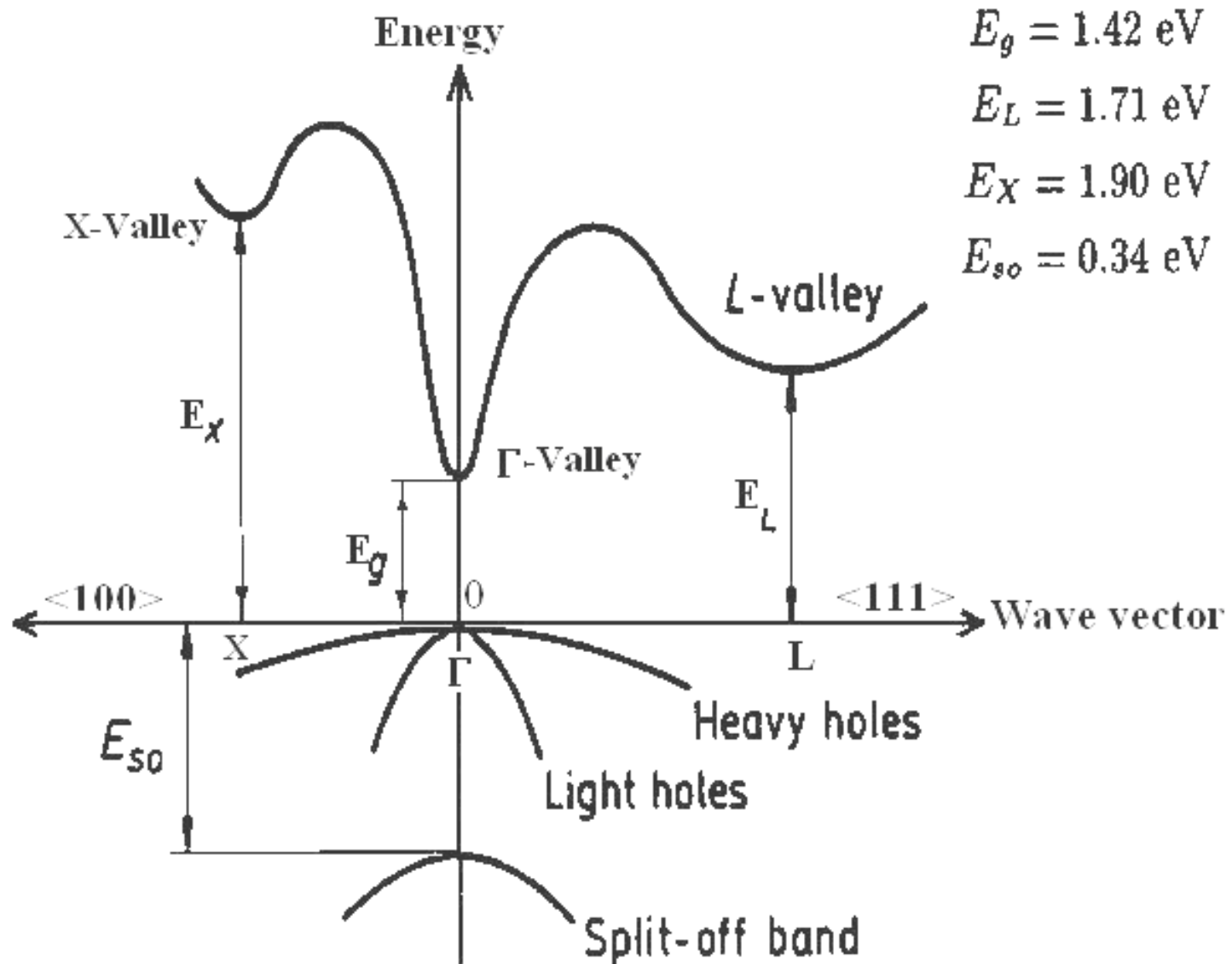
... and other depending on the symmetry



Band structure and Brillouin zone



Band structure and Brillouin zone of GaAs



The electric field of the lattice affects the motion of the electron, which means that its motion determined not by its usual mass m_e (as in vacuum), but by its so-called effective mass m^* .

The effective mass is very important and complex concept, here we will discuss only few moments, for more details see Refs. [1–4].

In the general case, the so-called inertial effective mass (derived *via* Newton's second law) depends on the direction in the crystal and is a tensor. Its components can be found from the dispersion law

$$E = E(\vec{k}): \quad \left(\frac{1}{m_I^*}\right)_{i,j} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} = \begin{pmatrix} m_{xx}^{-1} & m_{xy}^{-1} & m_{xz}^{-1} \\ m_{yx}^{-1} & m_{yy}^{-1} & m_{yz}^{-1} \\ m_{zx}^{-1} & m_{zy}^{-1} & m_{zz}^{-1} \end{pmatrix}$$

In majority of cases the $E(\vec{k})$ can be approximated by using the principal components of the inertial

effective mass tensor and then $m_I^* = 3 \left(\frac{1}{m_x^*} + \frac{1}{m_y^*} + \frac{1}{m_z^*} \right)^{-1}$, which is also defined as conductivity

effective mass m_c^* in the literature since $\sigma = ne^2\tau/m_I^*$ according to the Ohm's law ($\mu_d = \frac{e\tau}{m_I^*}$).



Another useful effective mass is the density of states effective mass (described later):

$$m_d^* = N_v^{2/3} m_b^* = N_v^{2/3} \sqrt[3]{m_x^* m_y^* m_z^*}$$

where N_v is the valley degeneracy factor (number of equivalent extremes), m_b^* is the effective mass of a single valley (for the isotropic spherical case $m_b^* = m_I^*$). The effective mass is frequently used to analyze the transport properties of semiconductors and thermoelectrics in particular. For example, for degenerate semiconductors (majority of thermoelectrics) the Seebeck coefficient is related to the effective mass as:

$$\alpha = \frac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\frac{\pi}{3n}\right)^{2/3} \left(\frac{3}{2} + r\right)$$

where r is the scattering parameter, and m_S^* is the effective mass that contributes to the Seebeck coefficient. In general case, in the framework of the parabolic dispersion and deformation scattering potential ($r = -1/2$) $m_S^* \approx m_d^*$ and is related to the m_I^* through $m_S^* = (N_v^* K^*)^{2/3} m_I^*$, where $N_v^* K^*$ is the Fermi surface complexity factor.^[7]

When only a single band contribute to the transport $m_S^* \approx m_d^* \approx m_I^*$.

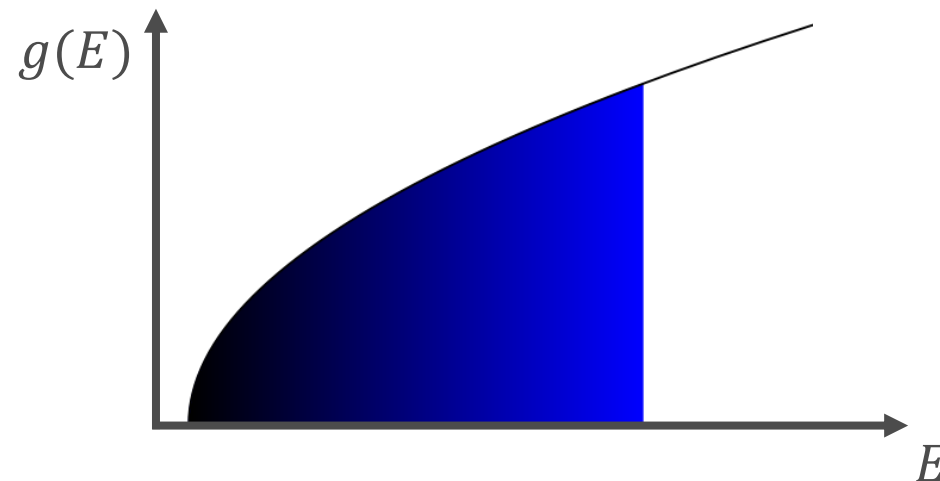


The density of states (DOS) $g(E)$ describes the proportion of states that are to be occupied at each energy. In the case of parabolic dispersion

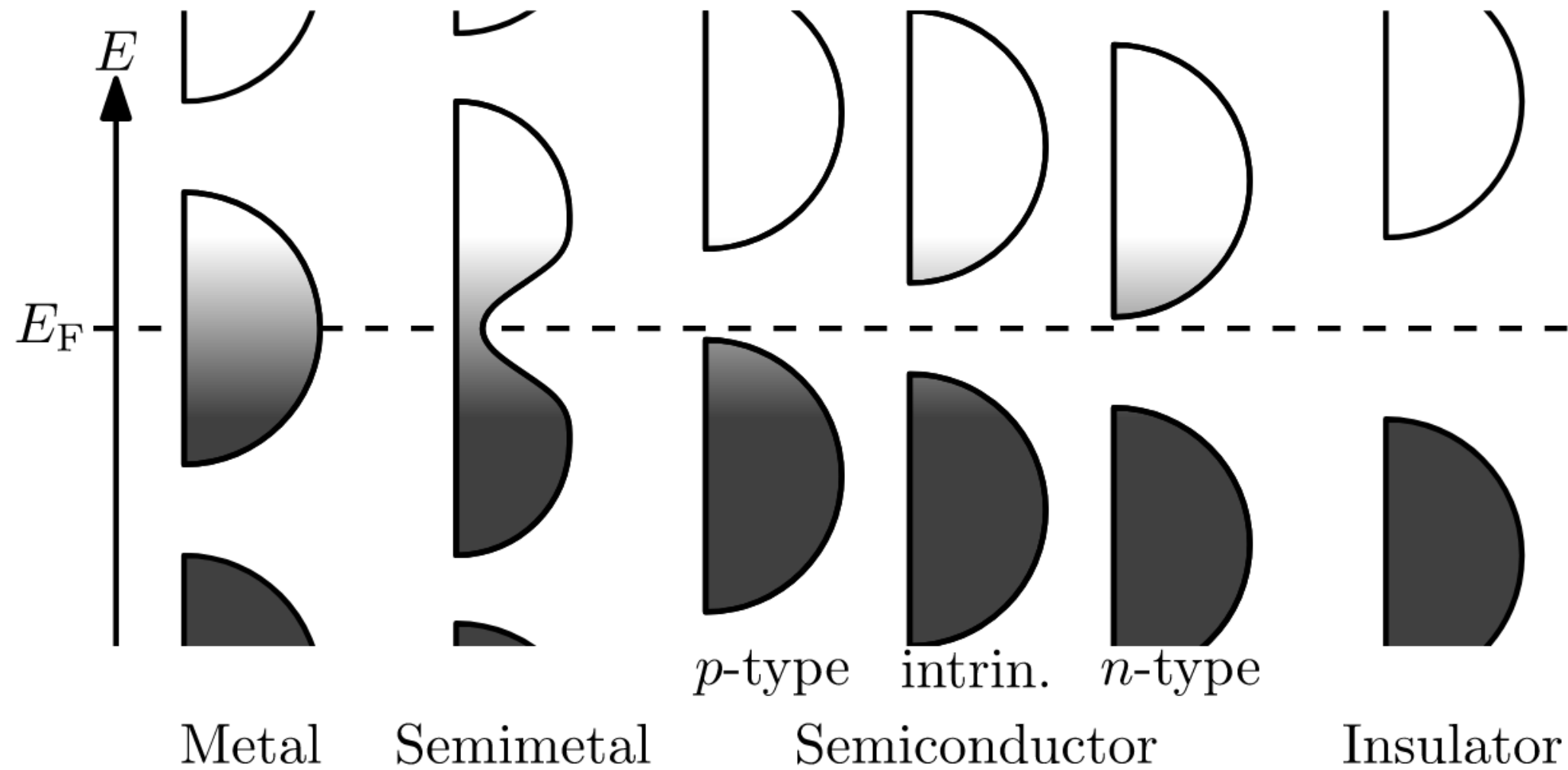
$$g(E) = \frac{N_v}{2\pi^2 \hbar^3} (8m_x^* m_y^* m_z^*)^{1/2} \sqrt{E - E_0}$$

where the density of states effective mass is introduced as $m_d^* = N_v^{2/3} \sqrt[3]{m_x^* m_y^* m_z^*}$, thus

$$g(E) = \frac{1}{2\pi^2} \left(\frac{2m_d^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_0}$$



Density of states



Fermi–Dirac distribution function

The Fermi–Dirac distribution function describes the probability that a level with energy E is occupied. For the equilibrium state of the system, quantum statistics leads to the following relation:

$$f_0(E, T) = \frac{1}{e^{\frac{E-F}{k_B T}} + 1}$$

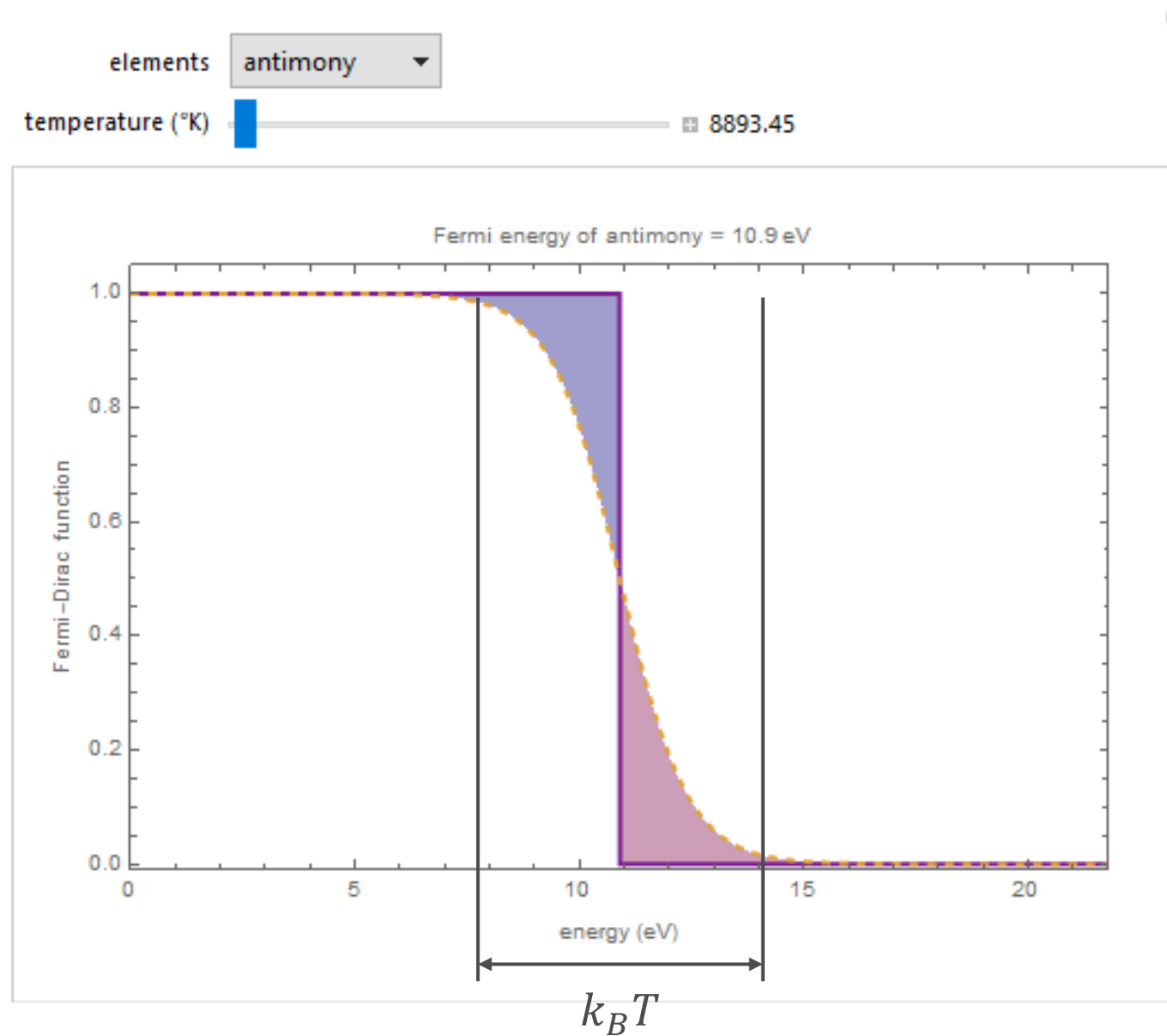
where E is the total energy of the charge carrier, T is the absolute temperature, k_B is the Boltzmann constant, F is the Fermi energy.



Hence the Fermi energy can be considered as

- the maximum energy that electrons have at absolute zero temperature
- the Fermi level separates occupied energy levels from non occupied
- the Fermi energy is the Gibbs thermodynamic potential per particle (chemical potential)

Fermi–Dirac distribution function



Fermi–Dirac distribution function

Two extremes are possible, so-called degenerate and non-degenerate cases. Let's consider $\eta = \frac{E-F}{k_B T}$, then if $\eta < -1$ a semiconductor can be considered as non-degenerate (Fermi level lies higher than valence band maxima for $k_B T$ at least or lower than conduction band minima for $k_B T$ at least), if $\eta > 5$ a semiconductor can be considered as degenerate (Fermi level is in the valence (conduction) band for at least $5k_B T$ lower than its maxima (higher than its minima)).

For degenerate system (Fermi–Dirac statistics):

$$f_0(\eta) = \frac{1}{e^\eta + 1} \approx e^{-\eta}$$

For non-degenerate system (Maxwell–Boltzmann statistics):

$$f_0(E, T) \approx e^{\frac{F}{k_B T}} \cdot e^{-\frac{E}{k_B T}}$$



Carrier concentration and Fermi integral

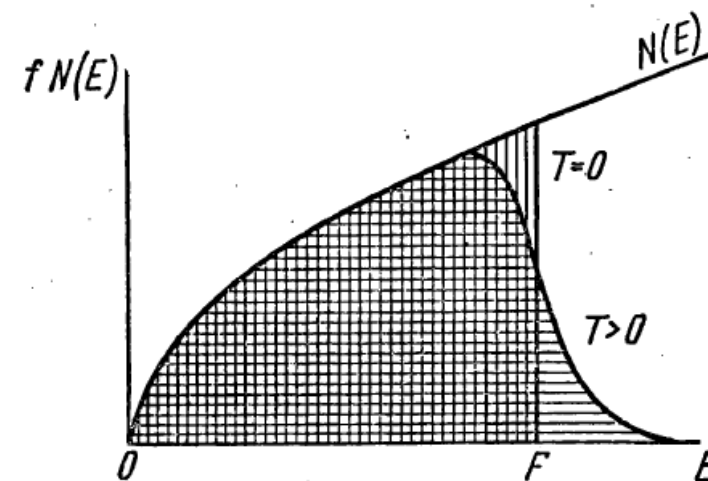
Considering all the above the charge carrier concentration can be calculated as:

$$n = 2 \int_{E_c}^{\infty} f_0(E, T) g(E) dE$$

$$f_0(E, T) = \frac{1}{e^{\frac{E-F}{k_B T}} + 1} \text{ and } g(E) = 2\pi \left(\frac{2m_d^*}{h^2} \right)^{3/2} \sqrt{E - E_c}$$

$$\text{using } \varepsilon = \frac{E - E_c}{k_B T} \text{ and } \eta = \frac{F - E_c}{k_B T}$$

$$n = 2 \int_{E_c}^{\infty} \frac{2\pi \left(\frac{2m_d^*}{h^2} \right)^{3/2} \sqrt{E - E_c}}{e^{\frac{E-F}{k_B T}} + 1} dE = 4\pi \left(\frac{2m_d^* k_B T}{h^2} \right)^{3/2} \int_0^{\infty} \frac{\varepsilon^{1/2}}{1 + e^{\varepsilon - \eta}} d\varepsilon$$



Carrier concentration and Fermi integral

For electrons:

$$n = 4\pi \left(\frac{2m_d^* k_B T}{h^2} \right)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2}}{1 + e^{\varepsilon - \eta}} d\varepsilon = \frac{2}{\sqrt{\pi}} N_c F_{1/2}(\eta)$$

For holes:

$$p = 4\pi \left(\frac{2m_d^* k_B T}{h^2} \right)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2}}{1 + e^{\varepsilon - \eta}} d\varepsilon = \frac{2}{\sqrt{\pi}} N_v F_{1/2}(\eta)$$

here N_c and N_v are the so-called effective density of states:

$$N_c = 2 \left(\frac{2\pi m_{d,n}^* k_B T}{h^2} \right)^{3/2} \text{ and } N_v = 2 \left(\frac{2\pi m_{d,p}^* k_B T}{h^2} \right)^{3/2}$$

(the effective masses of electrons ($m_{d,n}^*$) and holes ($m_{d,p}^*$) are not the same!)

$F_{1/2}(\eta)$ is the Fermi integral of order 1/2.

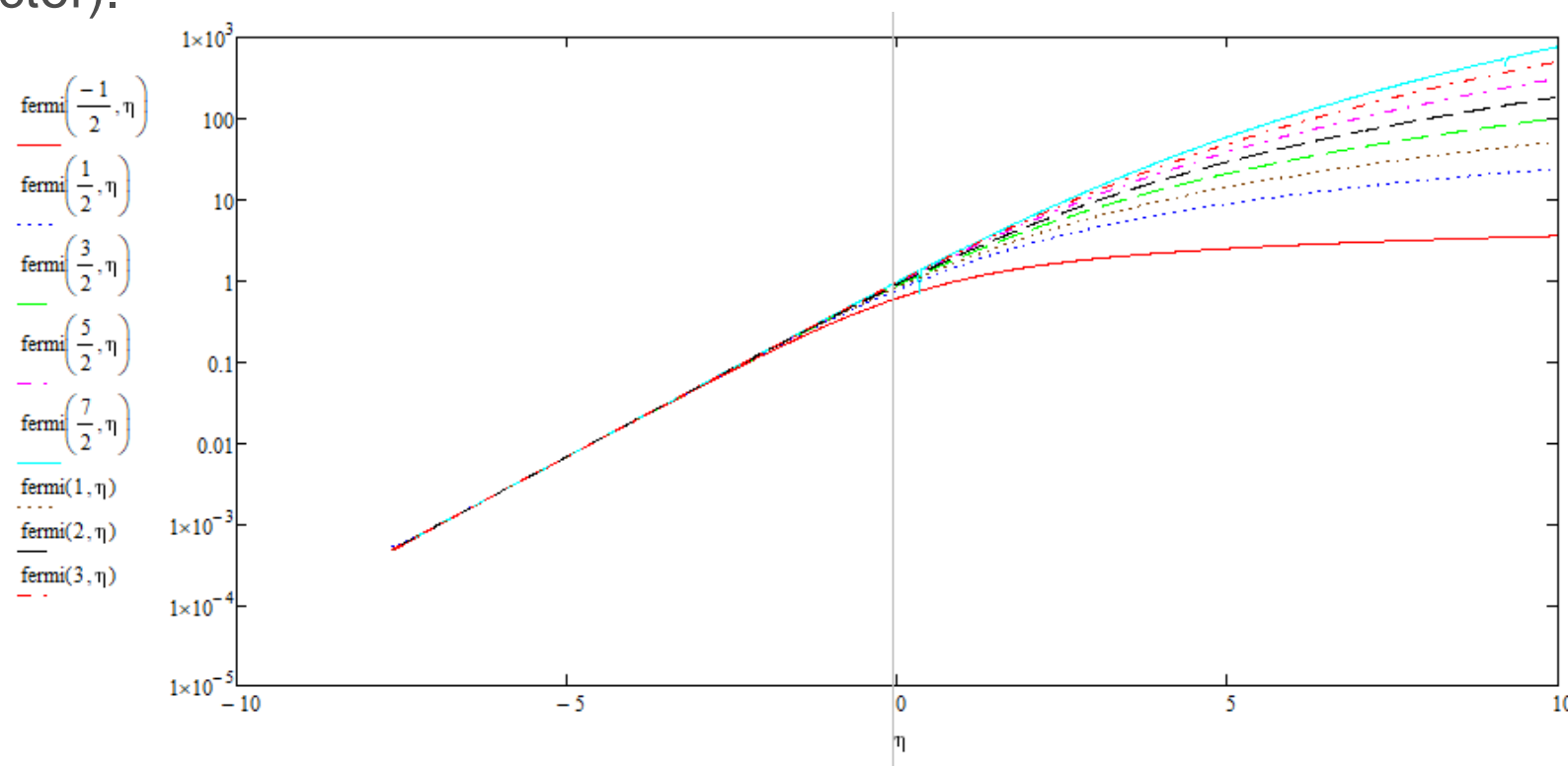


Fermi integral

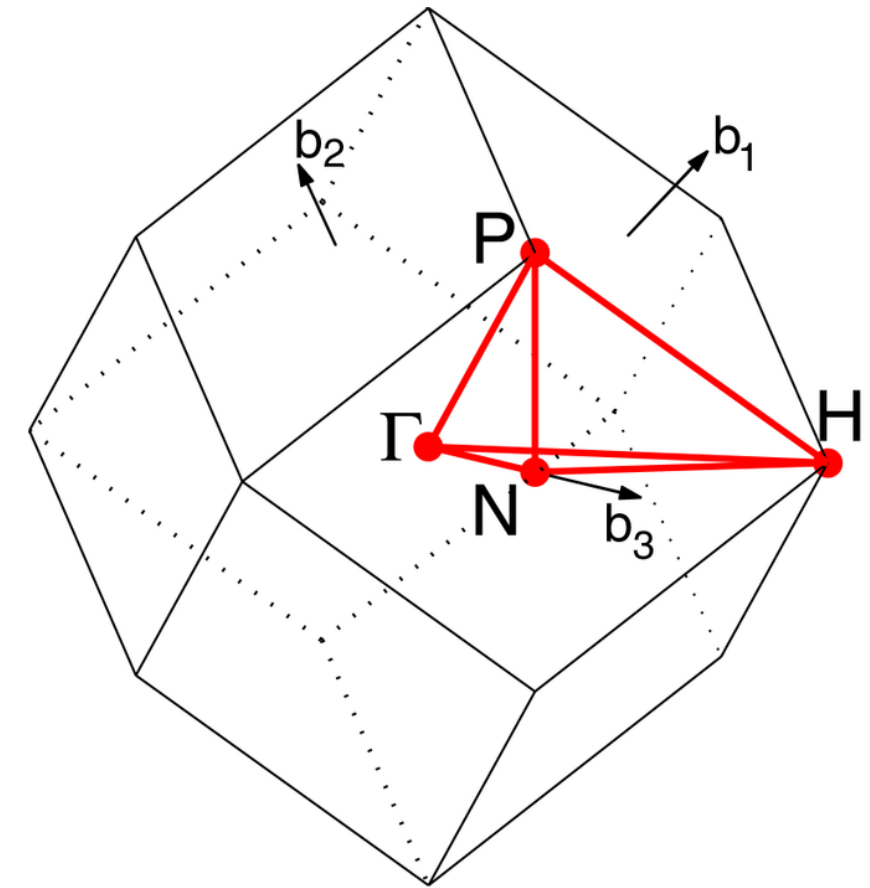
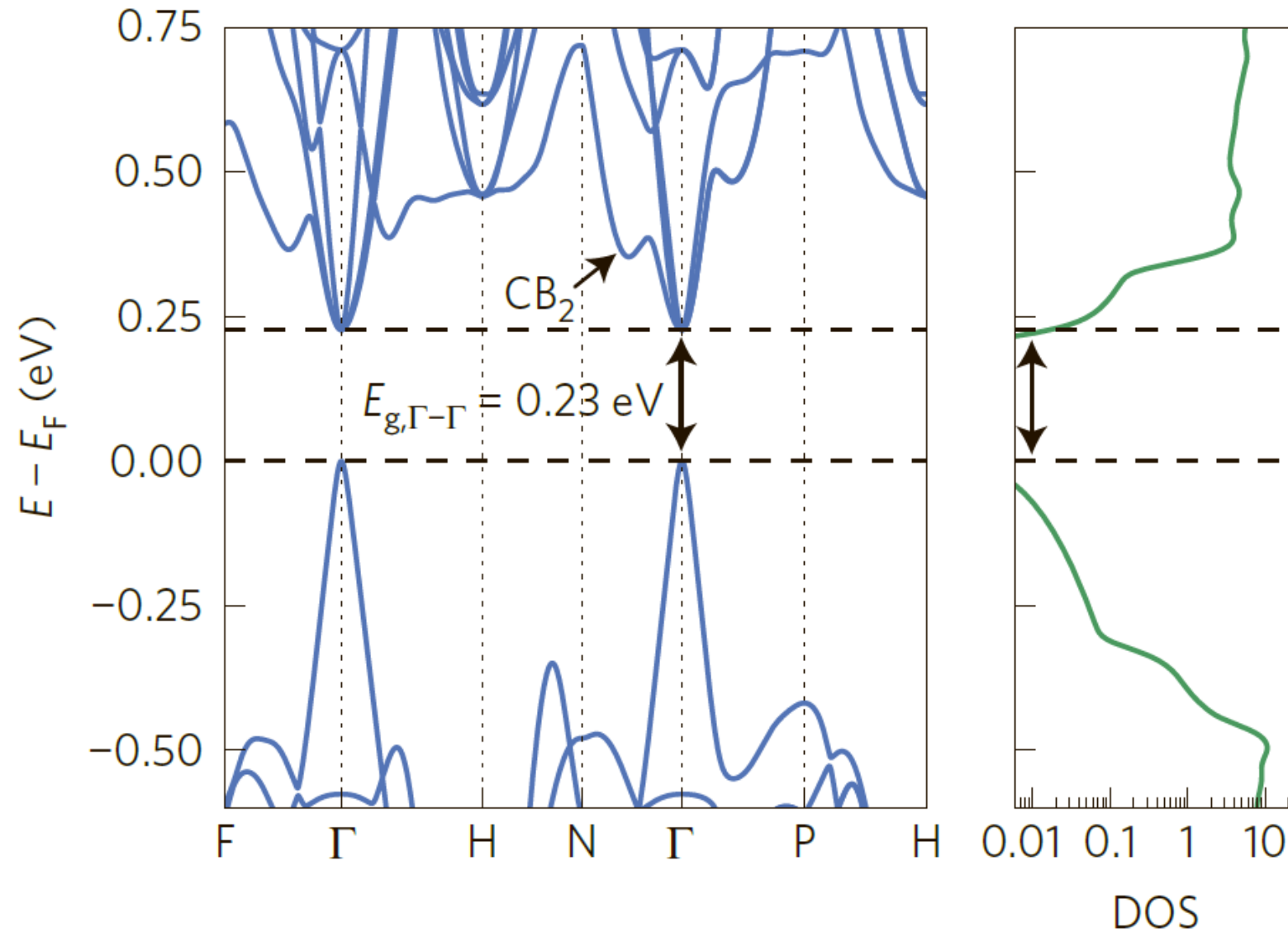
In general:

$$F_j(\eta) = \int_0^{\infty} \frac{\varepsilon^j}{1 + e^{\varepsilon - \eta}} d\varepsilon$$

where j is the order (index) of the integral, η is the reduced Fermi level, ε is the reduced energy of an electron (i.e., the distance to the conduction band or to the valence band, depending on the type of semiconductor).



Band structure of the CoSb₃ skutterudite



BCC path: $\Gamma-H-N-\Gamma-P-H|P-N$

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