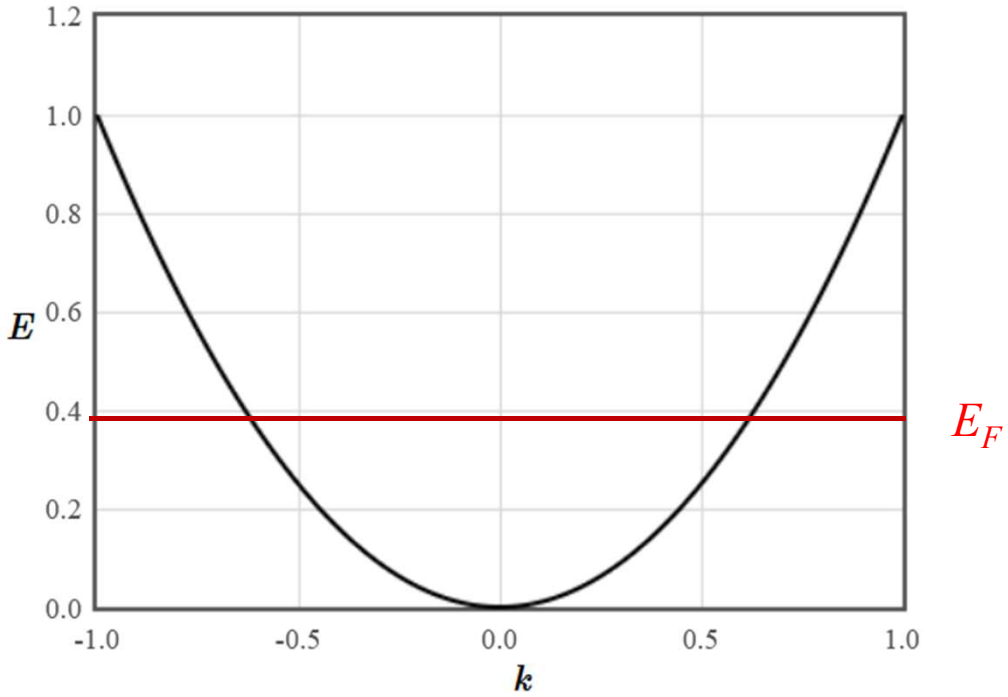
Electron bands

Extra exercise exams

Exercise exams (1 & 2) Friday 28 June 10:00 – 10:45 P2

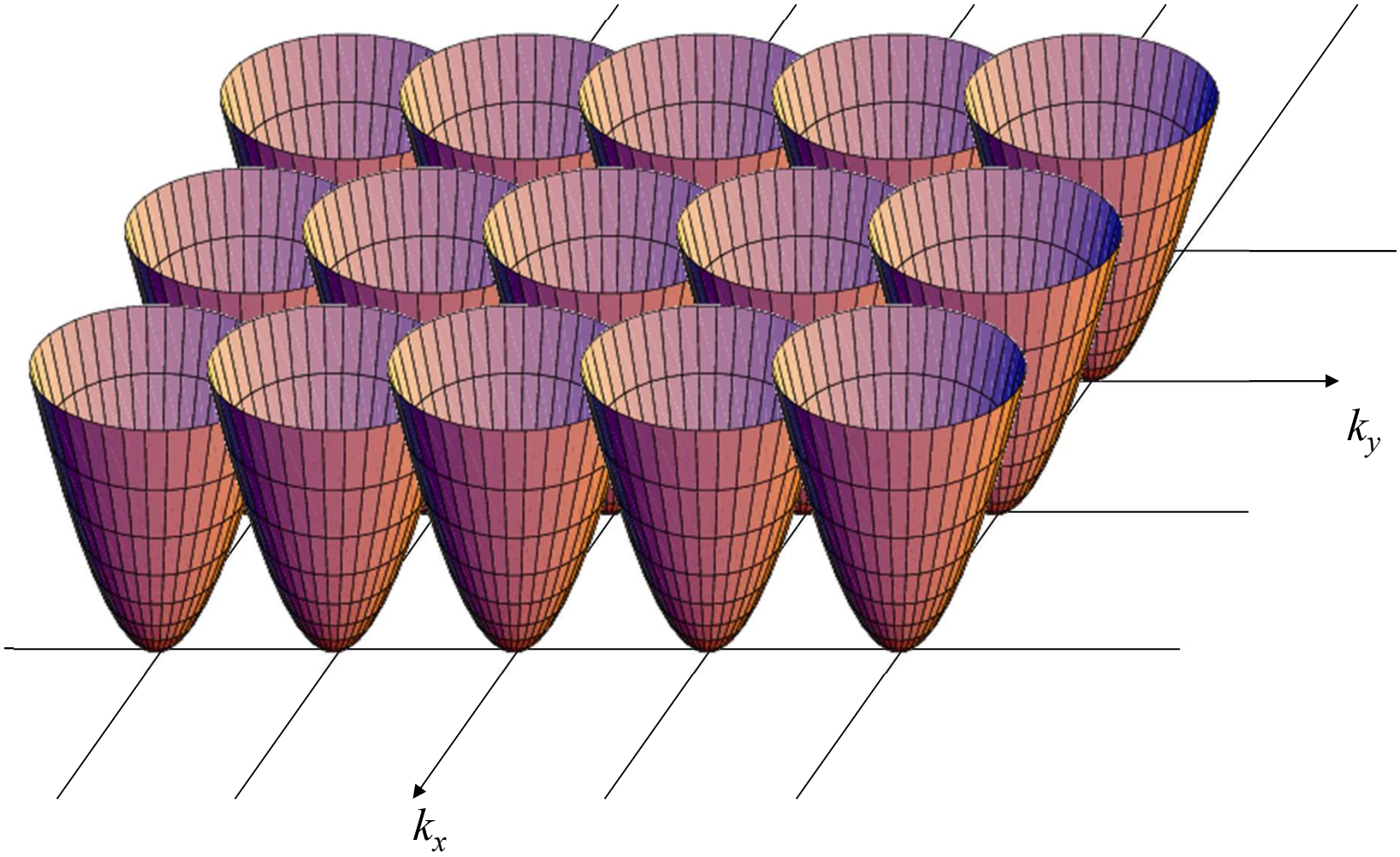
Combined exam Friday 4 October 14:00 – 15:00 P2

Free electrons



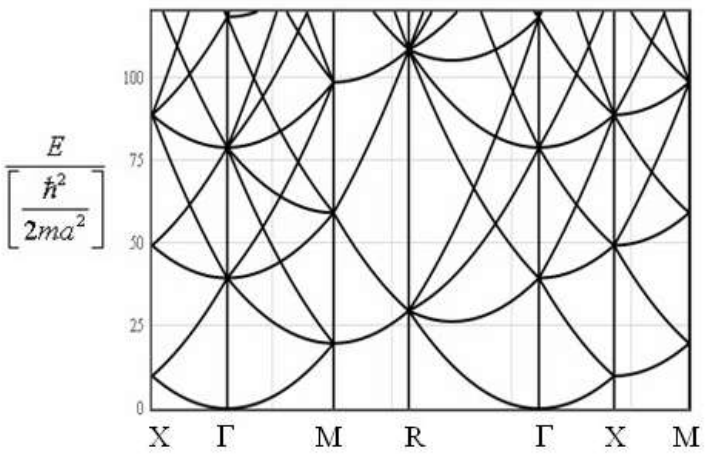
Free electrons can’t absorb a photon

Empty lattice approximation



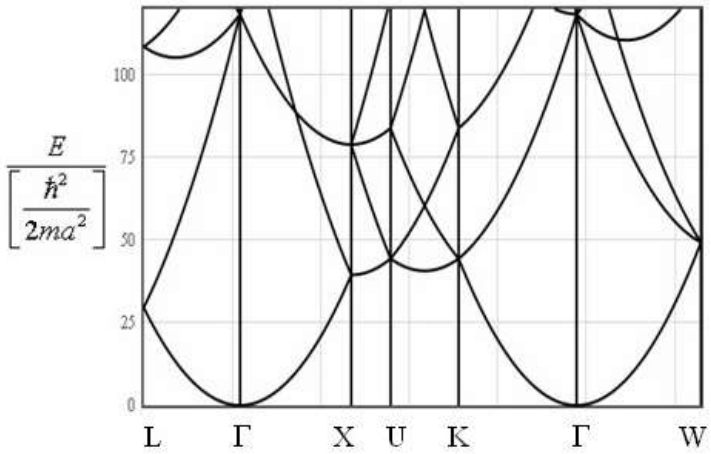
Empty lattice approximation

Simple cubic



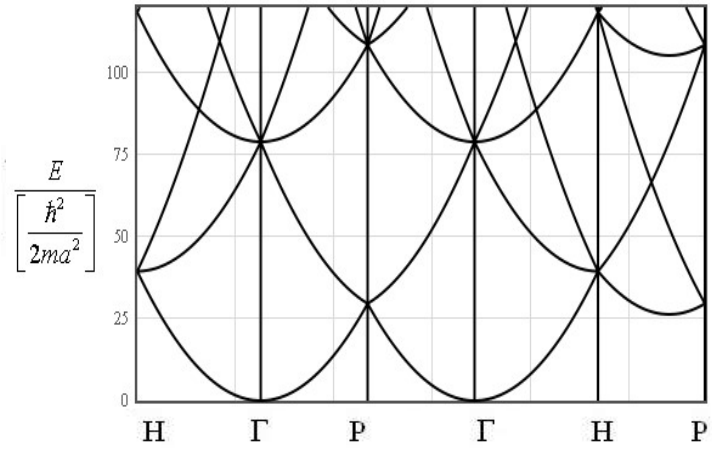
Choose a different order for the symmetry points

Face centered cubic

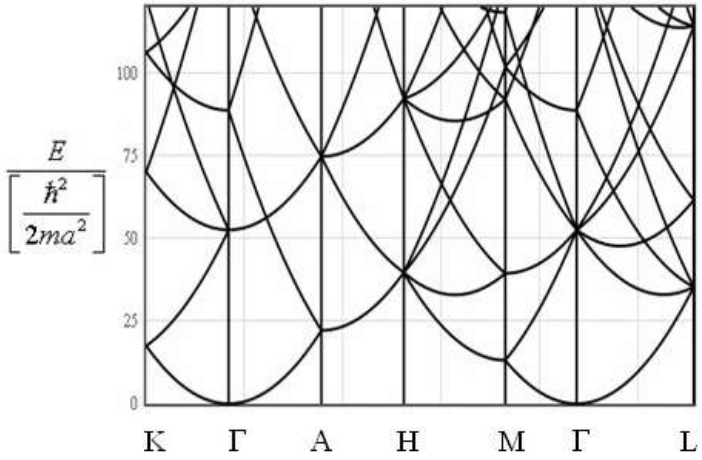


Choose a different order for the symmetry points

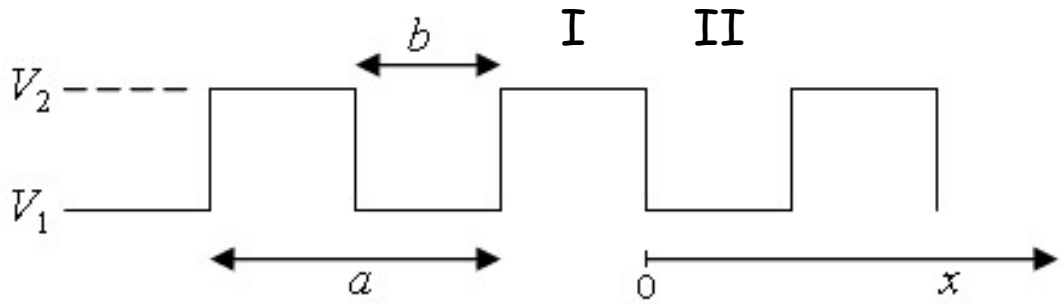
Body centered cubic



Hexagonal



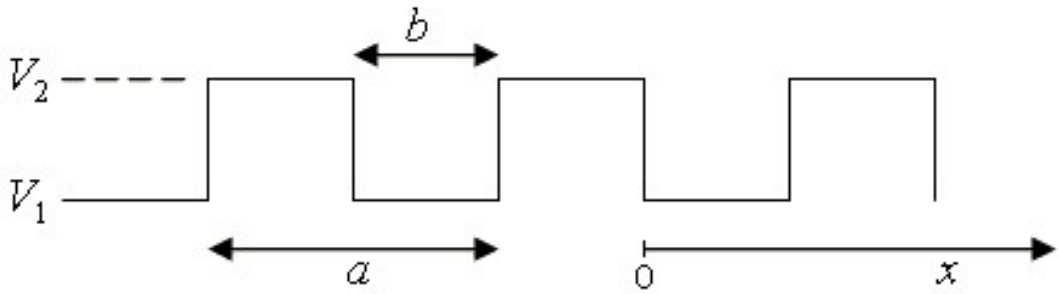
Kronig-Penney model



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi$$

Solutions can be found in region I and region II
Match boundary conditions

Kronig-Penney model

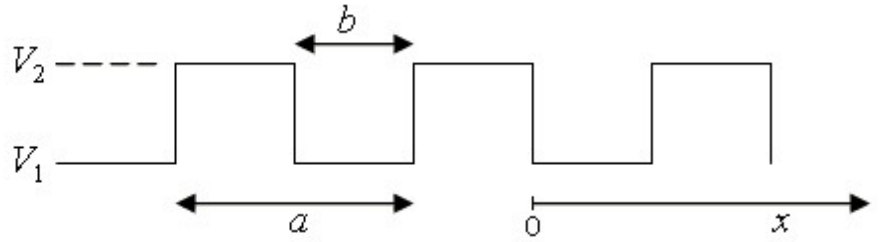


Solutions can be found that are simultaneous eigenfunctions of the Hamiltonian and the translation operator.

Eigenfunctions of the translation operator can be found in terms of any two linearly independent solutions. A convenient choice is:

$$\psi_1(0)=1, \qquad \frac{d\psi_1}{dx}(0)=0, \qquad \psi_2(0)=0, \qquad \frac{d\psi_2}{dx}(0)=1.$$

Kronig-Penney model



for $0 < x < b$

$$\psi_1(x) = \cos(k_1 x), \qquad \psi_2(x) = \frac{\sin(k_1 x)}{k_1}$$

for $b < x < a$

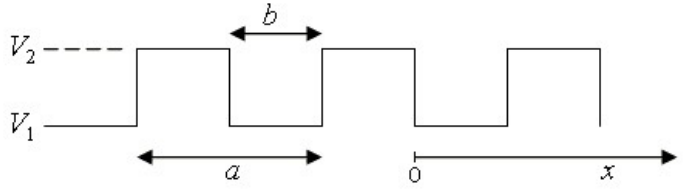
$$\psi_1(x) = \cos(k_2(x-b))\cos(k_1 b) - \frac{k_1 \sin(k_2(x-b))\sin(k_1 b)}{k_2},$$

$$\psi_2(x) = \frac{\cos(k_2(x-b))\sin(k_1 b)}{k_1} + \frac{\sin(k_2(x-b))\cos(k_1 b)}{k_2}.$$

Except for the coefficients, these are the same solutions as we found for light in a layered material.

Kronig-Penney model

at $x = a$



$$\psi_1(a) = \cos(k_2(a-b))\cos(k_1 b) - \frac{k_1 \sin(k_2(a-b))\sin(k_1 b)}{k_2},$$

$$\psi_2(a) = \frac{\cos(k_2(a-b))\sin(k_1 b)}{k_1} + \frac{\sin(k_2(a-b))\cos(k_1 b)}{k_2}.$$

The translation operator translates the function a distance *a*.

$$\begin{bmatrix} \psi_1(x+a) \\ \psi_2(x+a) \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix}.$$

The elements of the translation operator can be evaluated at $x = a$.

Kronig-Penney model

$$\begin{bmatrix} \psi_1(x+a) \\ \psi_2(x+a) \end{bmatrix} = \begin{bmatrix} \psi_1(a) & \frac{d\psi_1}{dx}(a) \\ \psi_2(a) & \frac{d\psi_2}{dx}(a) \end{bmatrix} \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix}$$

The eigen functions and eigen values are

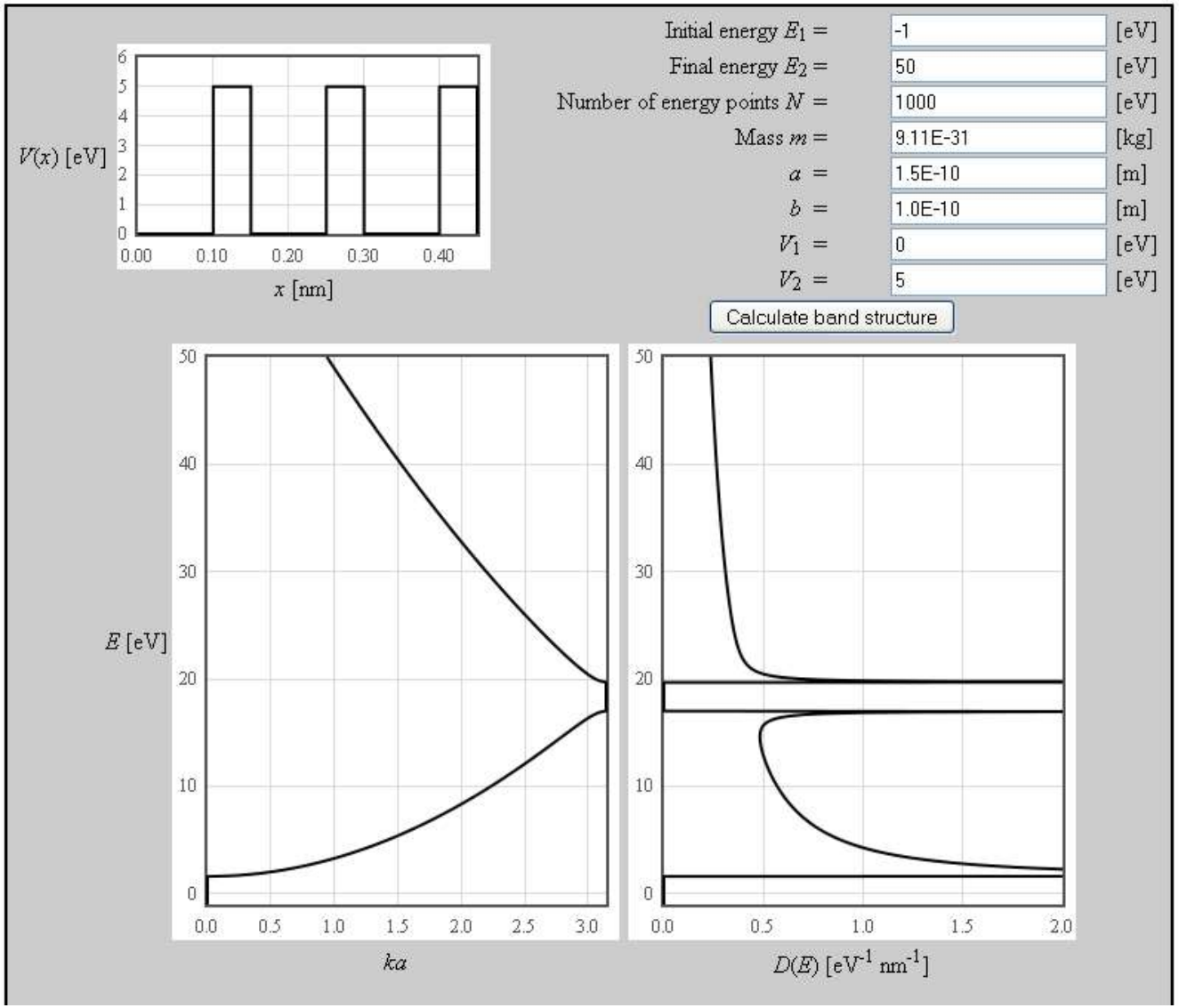
$$\psi_{\pm}(x) = \frac{2\psi_2(a)}{\frac{d\psi_2(a)}{dx} - \psi_1(a) \pm \delta}\psi_1(x) + \psi_2(x), \qquad \lambda\pm = \frac{1}{2}(\alpha \pm \delta),$$

$$\delta = \sqrt{\alpha^2 - 4}$$

$$\alpha = \psi_1(a) + \frac{d\psi_2(a)}{dx} = 2\cos\left(k_2(a-b)\right)\cos(k_1 b) - \left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right)\sin\left(k_2(a-b)\right)\sin(k_1 b).$$

If $\alpha > 2$, the potential acts like a mirror for electrons

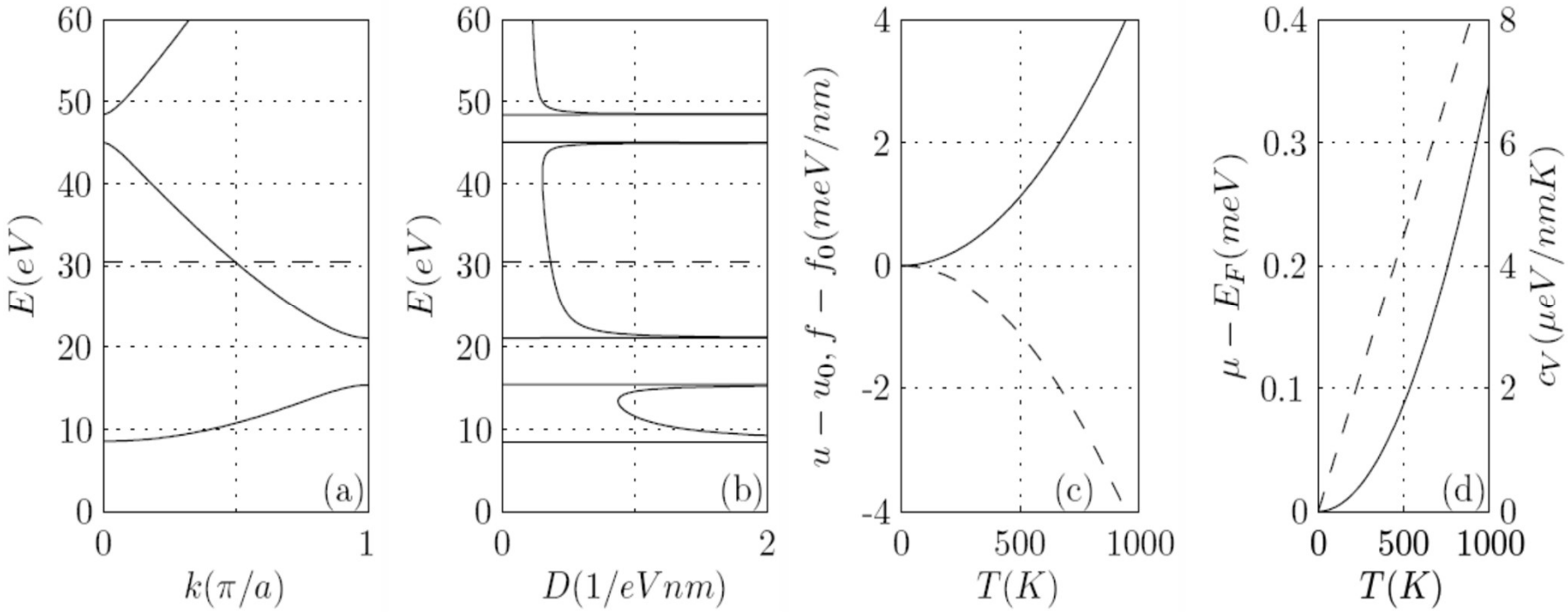
Kronig-Penney model



$$\alpha(E, V_1, V_2, a, b)$$

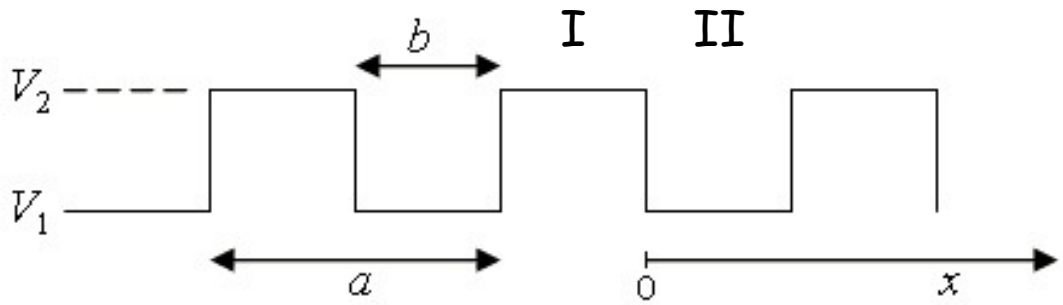
$$k = \pm\frac{1}{a}\tan^{-1}\left(\frac{\sqrt{4-\alpha^2}}{\alpha}\right)$$

Kronig-Penney model



(a) The energy-wave number dispersion relation. The dashed line is the Fermi energy. (b) The density of states. (c) The internal energy density (solid line) and Helmholtz free energy density (dashed line). (d) The chemical potential (solid line) and the specific heat (dashed line). All of the plots were drawn for a square wave potential with the parameters: $V = 12.5$ eV, $a = 2 \times 10^{-10}$ m, $b = 5 \times 10^{-11}$ m, and an electron density of $n = 3$ electrons/primitive cell.

A separable potential

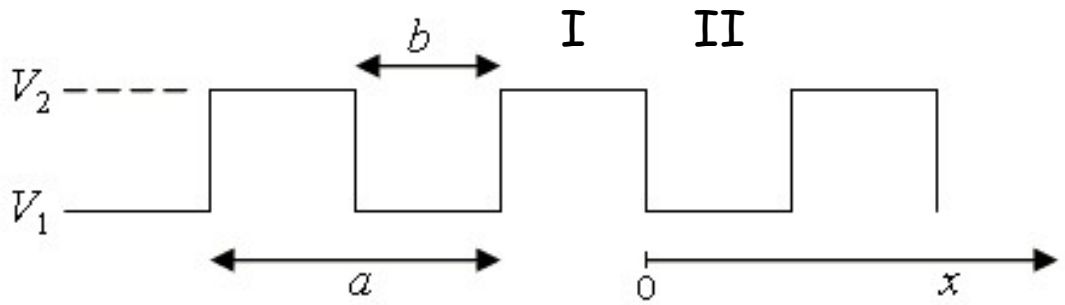


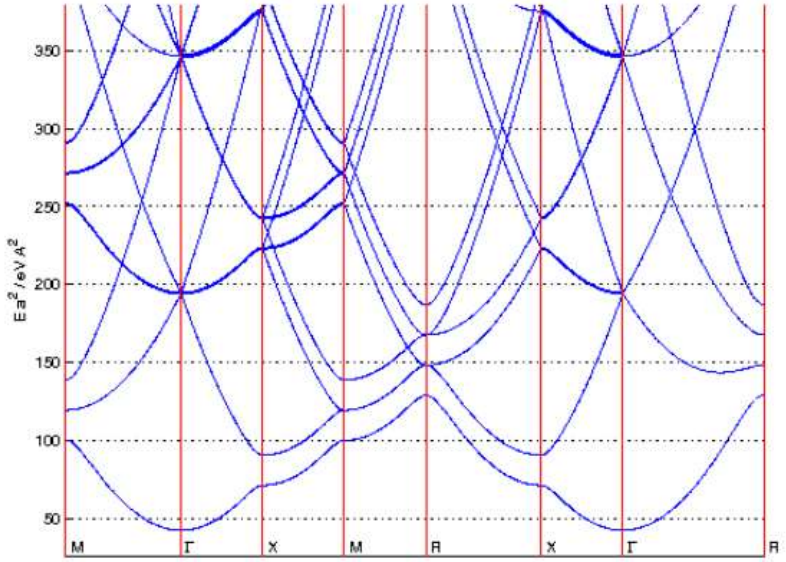
$$-\frac{\hbar^2}{2m}\nabla^2\Psi+(V(x)+V(y)+V(z))\Psi=E\Psi$$

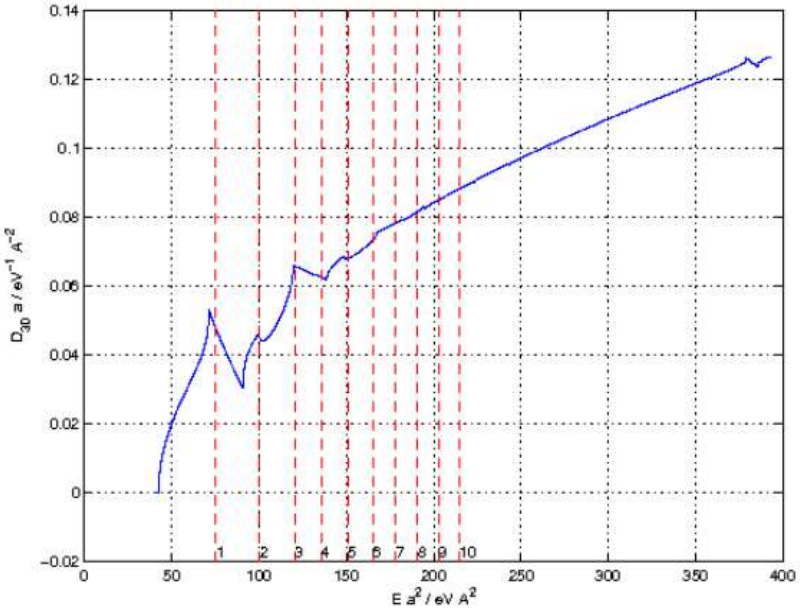
Ψ is the product of the solutions to the Kronig-Penney model.

$$\Psi(x,y,z)=\psi_{KP}(x)\psi_{KP}(y)\psi_{KP}(z)$$

A separable potential







http://lampx.tugraz.at/~hadley/ss1/separablecrystals/thermo.html

2N electron states/band

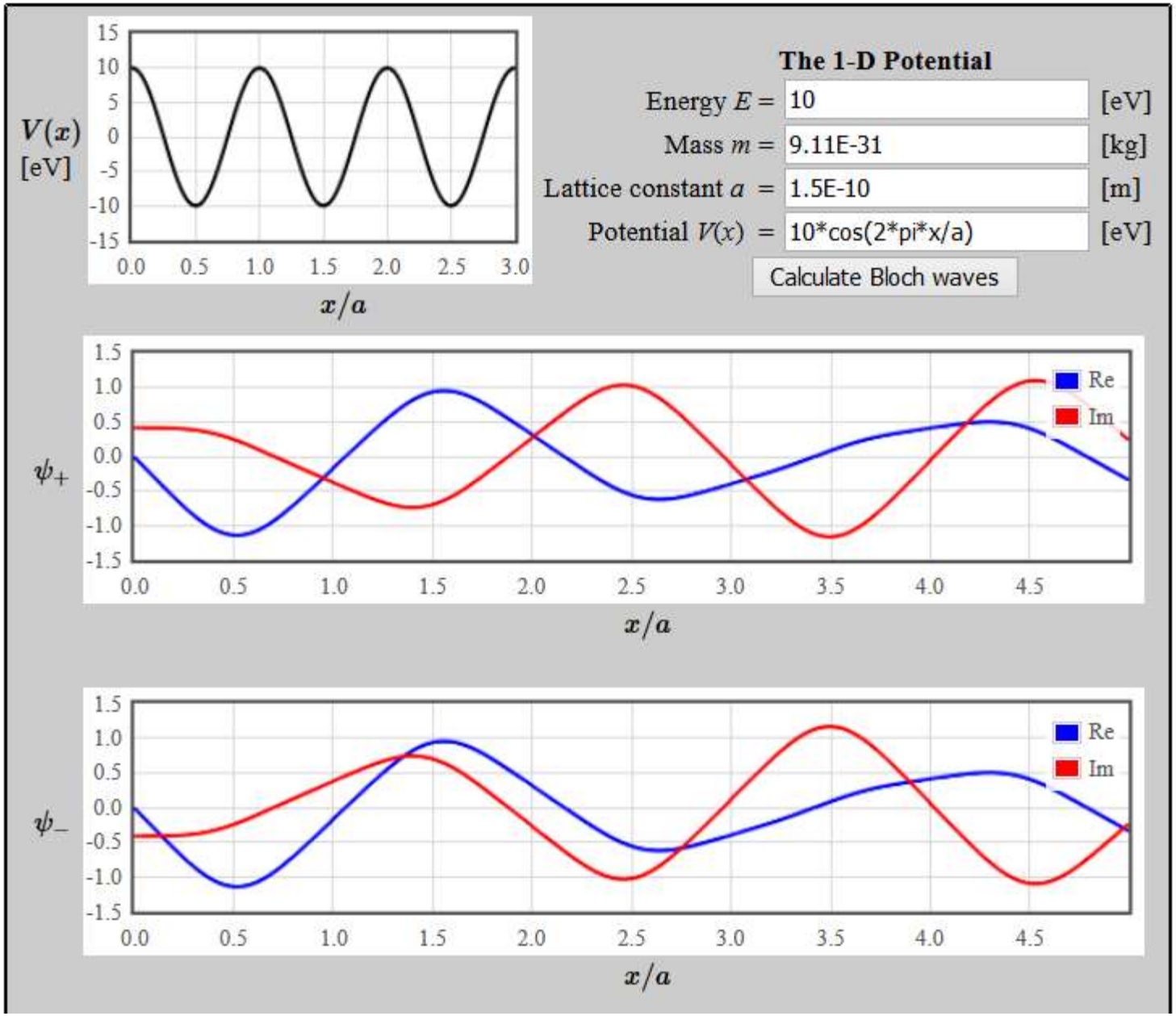
N primitive unit cells = k-states in 1st Bz

Each band can hold $2N$ electrons

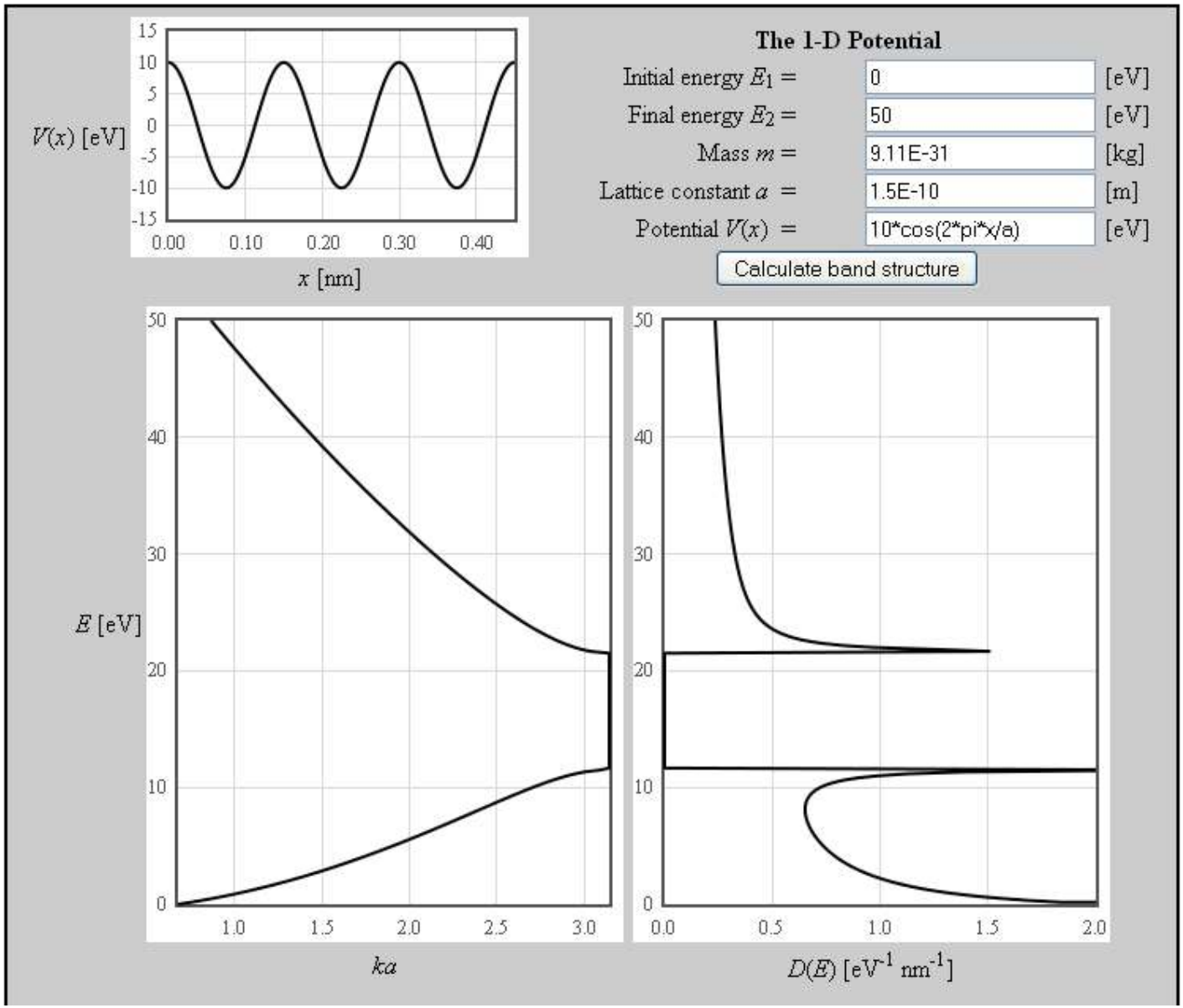
A primitive unit cell contains p electrons

There are enough electrons to fill $pN/(2N)$ bands

Bloch waves in 1-D



Band structure in 1-D



Band structure calculations

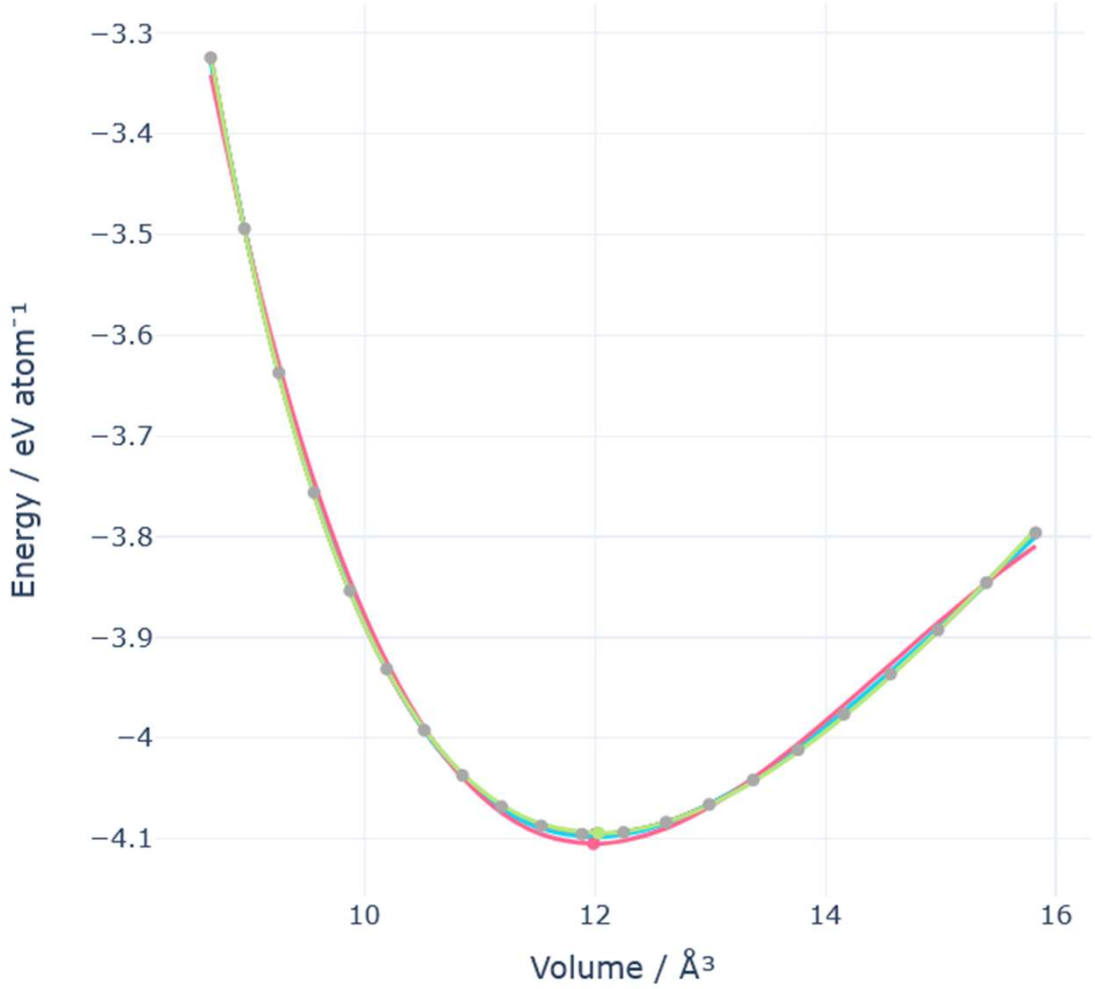
Knowing how the atoms are arranged, calculate the electron states

Density Functional Theory (DFT)
Plane wave method
Tight binding

$$H| = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_a \frac{\hbar^2}{2m_a}\nabla_a^2 - \sum_{a,i} \frac{Z_a e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_a|} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_j|} + \sum_{a<b} \frac{Z_a Z_b e^2}{4\pi\epsilon_0|\vec{r}_a - \vec{r}_b|}$$

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

Band structure calculations



Bloch Theorem

Bloch form $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$

Eigenfunction solutions of the Schrödinger equation have Bloch form.

k is a wave vector in the 1st Brillouin zone

$u_{\vec{k}}(\vec{r})$ is a periodic function

Plane wave method

$$-\frac{\hbar^2}{2m}\nabla^2\psi_{\vec{k}} + U(\vec{r})\psi_{\vec{k}} = E\psi_{\vec{k}}.$$

The potential is periodic $$U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Bloch form $$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}'} C_{\vec{G}'} e^{i\vec{G}'\cdot\vec{r}}$$

$$\sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = \sum_{\vec{G}'} C_{\vec{G}'} e^{i\vec{G}'\cdot\vec{r}}$$

We can relabel the reciprocal lattice vectors since we sum over them.