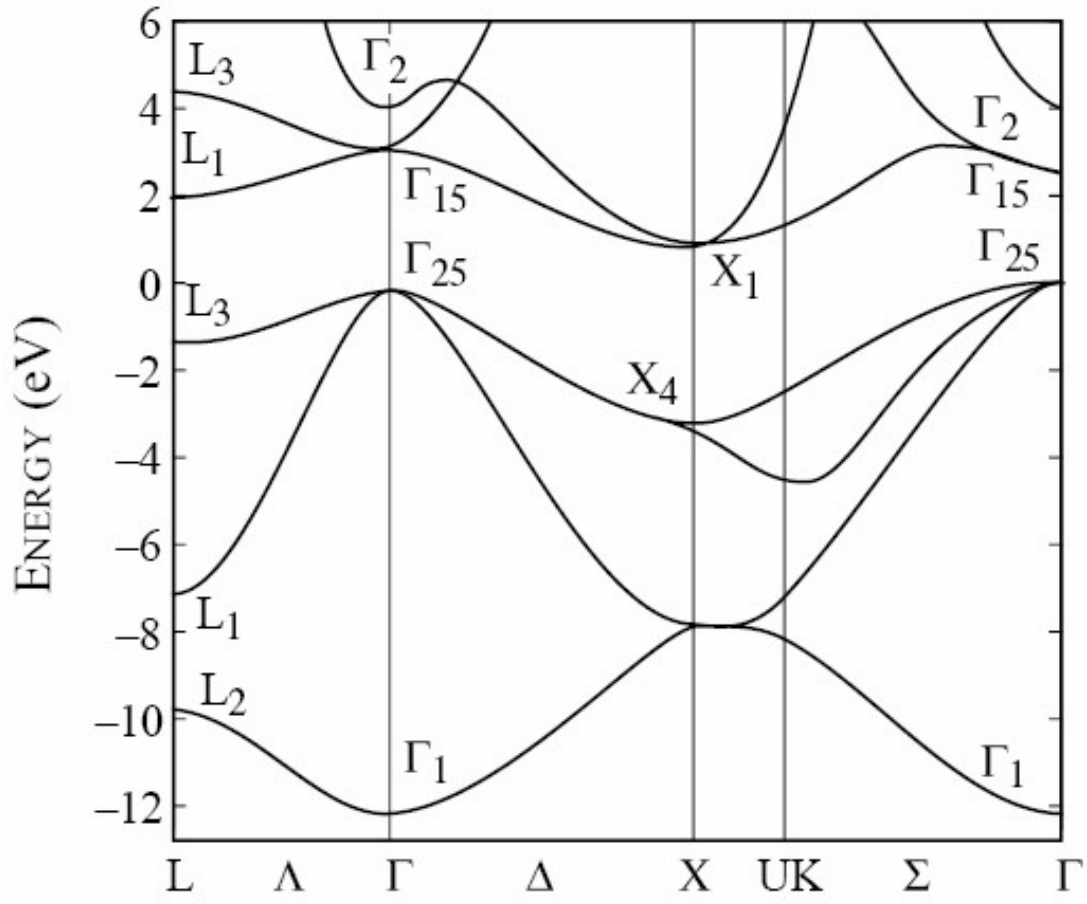
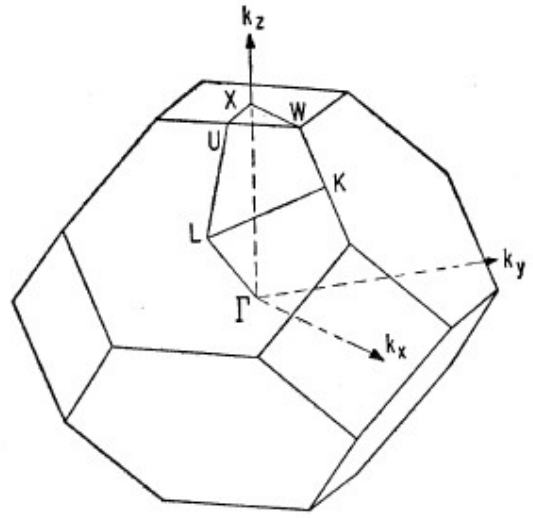
Electron bands

Band Theory, Kittel chapter 7

Calculate the dispersion relation for electrons in a crystal

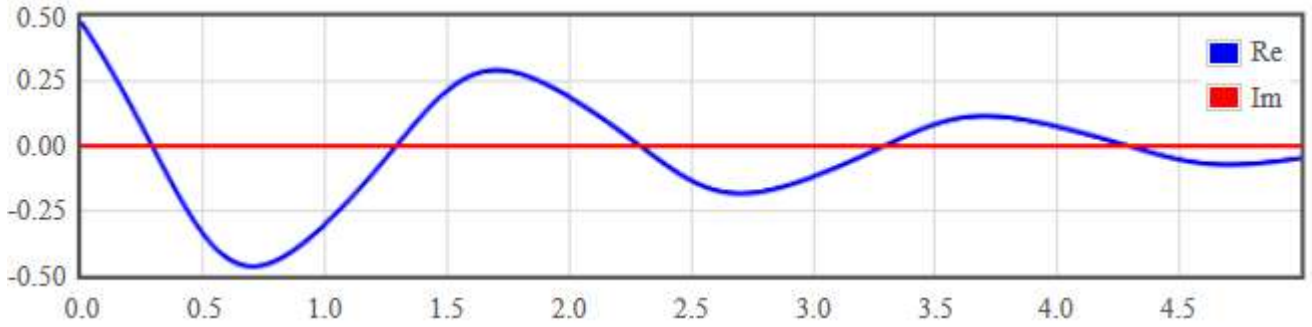




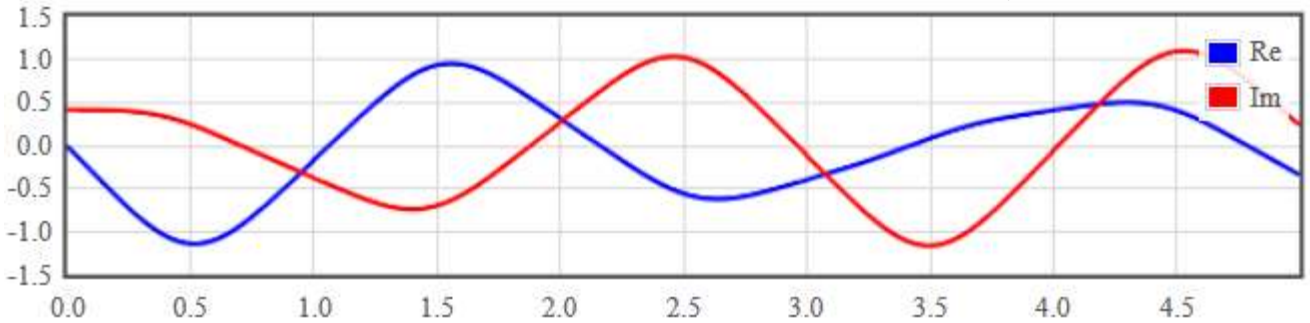
silicon

Linear differential equations with periodic coefficients

Have exponentially decaying solutions,



or solutions of the form $e^{ikx}u_k(x)$

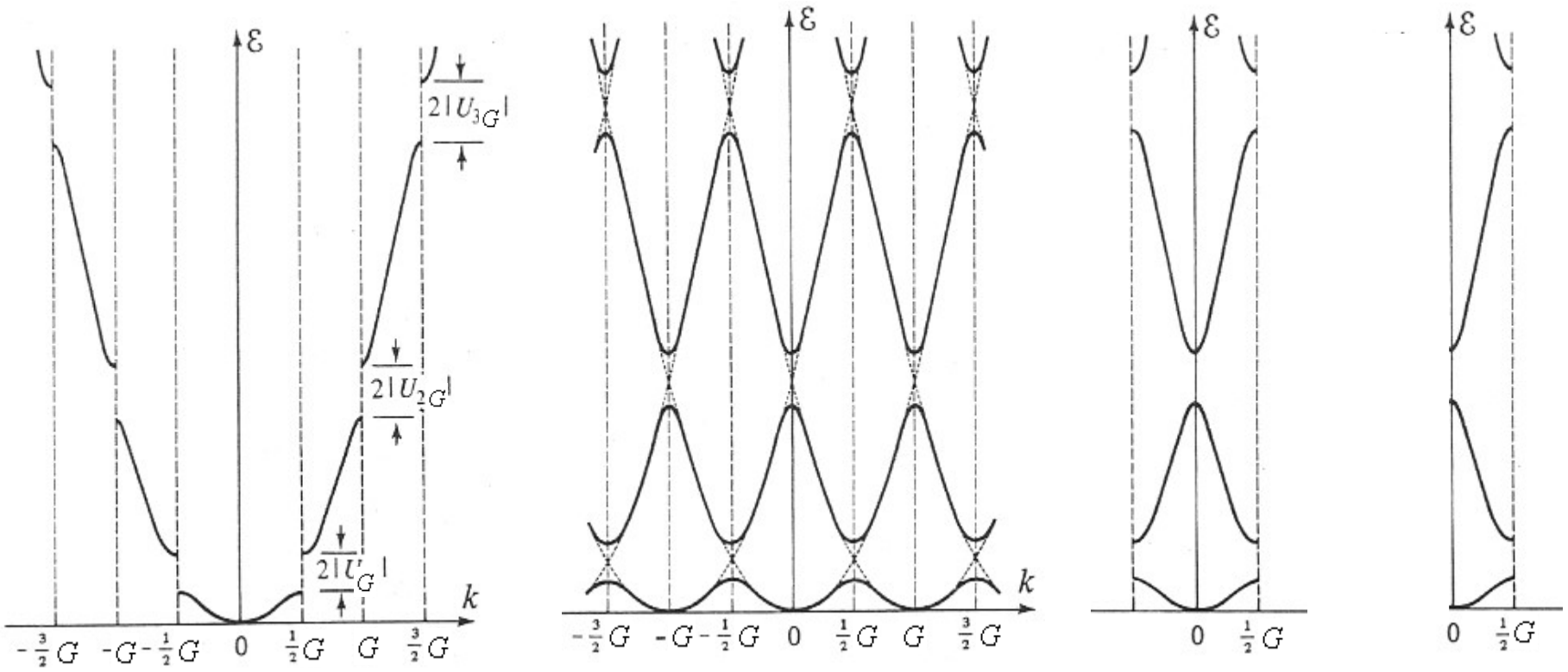


$$T\psi = \lambda\psi$$

$$Te^{ikx}u_k(x) = e^{ik(x+a)}u_k(x+a) = e^{ika}e^{ikx}u_k(x) = e^{ika}\psi$$

$$\lambda = e^{ika}$$

Empty lattice approximation



Extended Repeated Reduced

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \underbrace{e^{i\vec{G}_0\cdot\vec{r}} e^{-i\vec{G}_0\cdot\vec{r}}}_{1} \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\left(\vec{k}+\vec{G}_0\right)\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{G}} e^{i\left(\vec{G}-\vec{G}_0\right)\cdot\vec{r}}$$

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

$$\psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$ ← Any wave function that satisfies periodic boundary conditions

$$\psi(\vec{r}) = \sum_{\vec{k}\in 1Bz} \sum_{\vec{G}} C_{\vec{k}+\vec{G}} e^{i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}}$$

These k's label the symmetries

periodic function

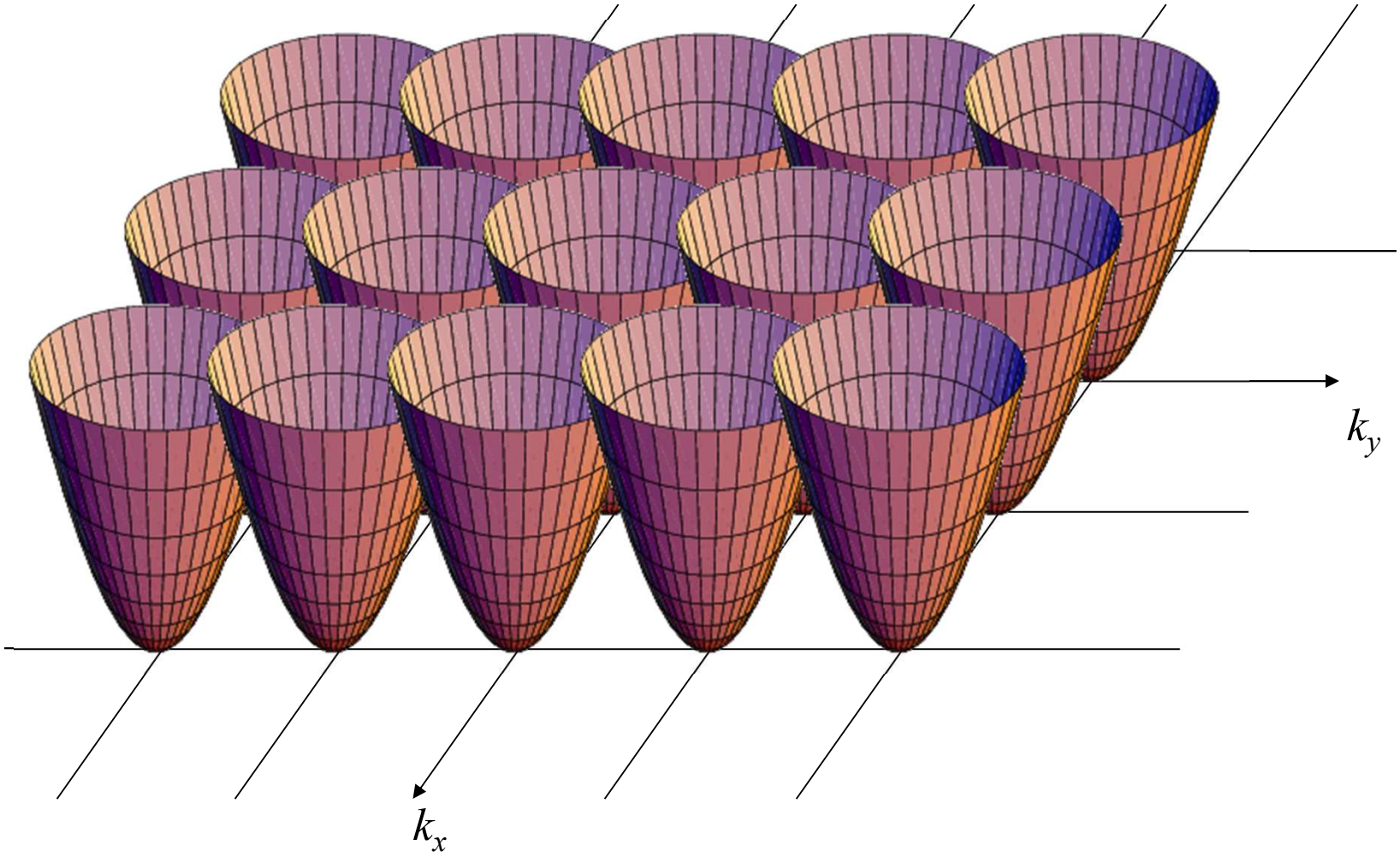
$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}+\vec{G}} e^{i(\vec{k}+\vec{G})\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{k}+\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$$

$$T_{mnl}\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot(\vec{r}+m\vec{a}_1+n\vec{a}_2+l\vec{a}_3)} u_{\vec{k}}(\vec{r}+m\vec{a}_1+n\vec{a}_2+l\vec{a}_3) = e^{i\vec{k}\cdot(m\vec{a}_1+n\vec{a}_2+l\vec{a}_3)}\psi_{\vec{k}}(\vec{r})$$

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

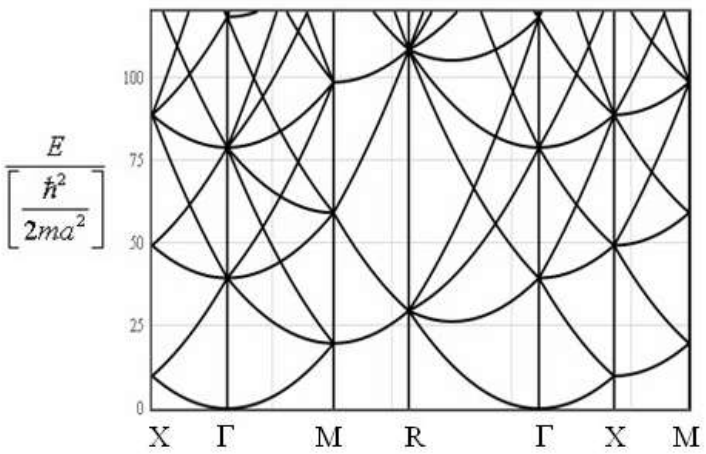
Eigen function solutions of the Schrödinger equation have Bloch form.

Empty lattice approximation



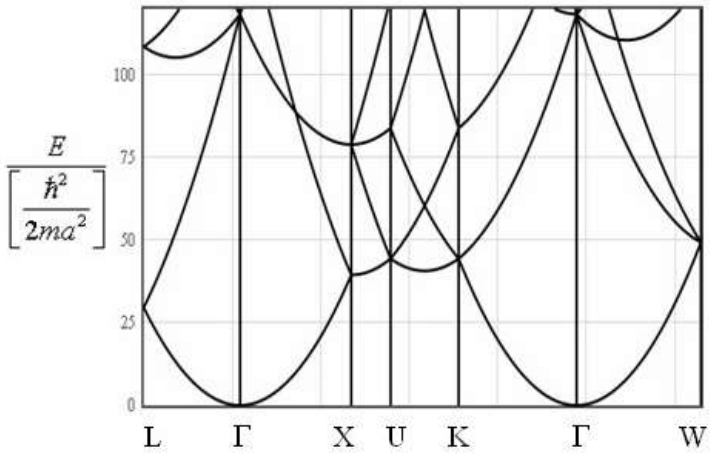
Empty lattice approximation

Simple cubic



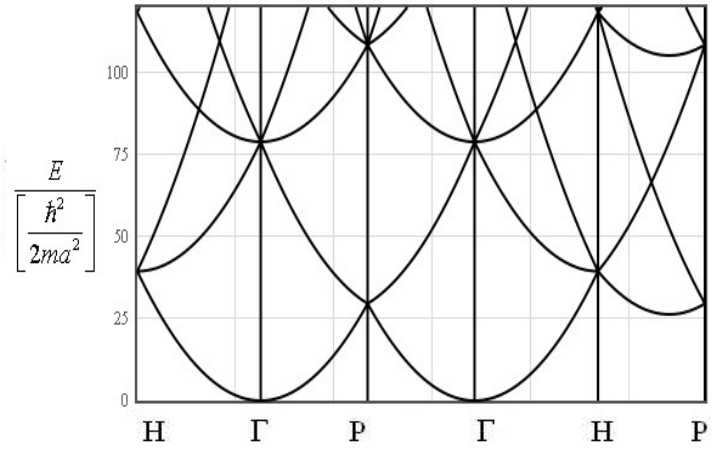
Choose a different order for the symmetry points

Face centered cubic

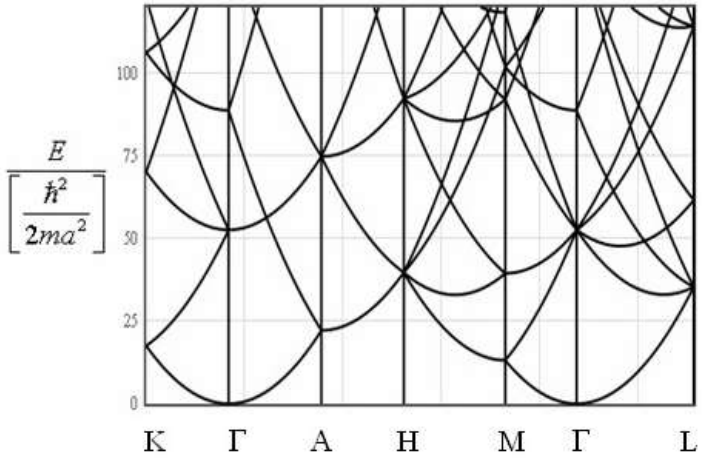


Choose a different order for the symmetry points

Body centered cubic



Hexagonal



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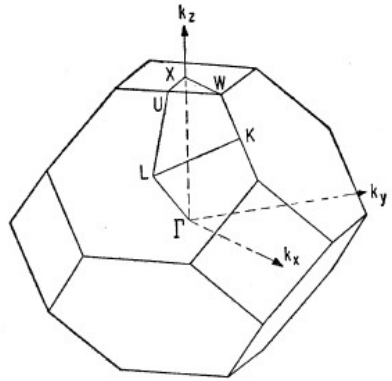
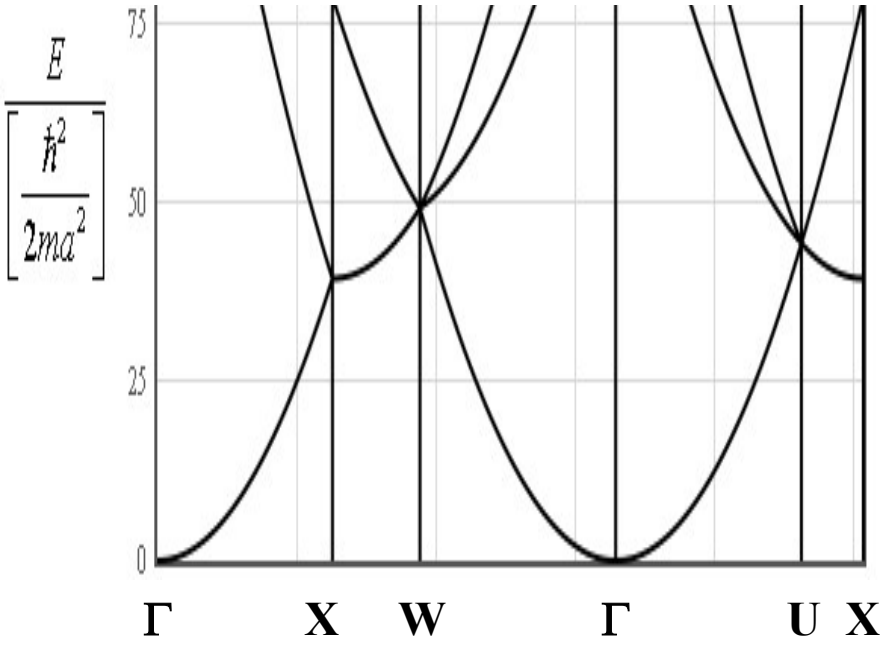
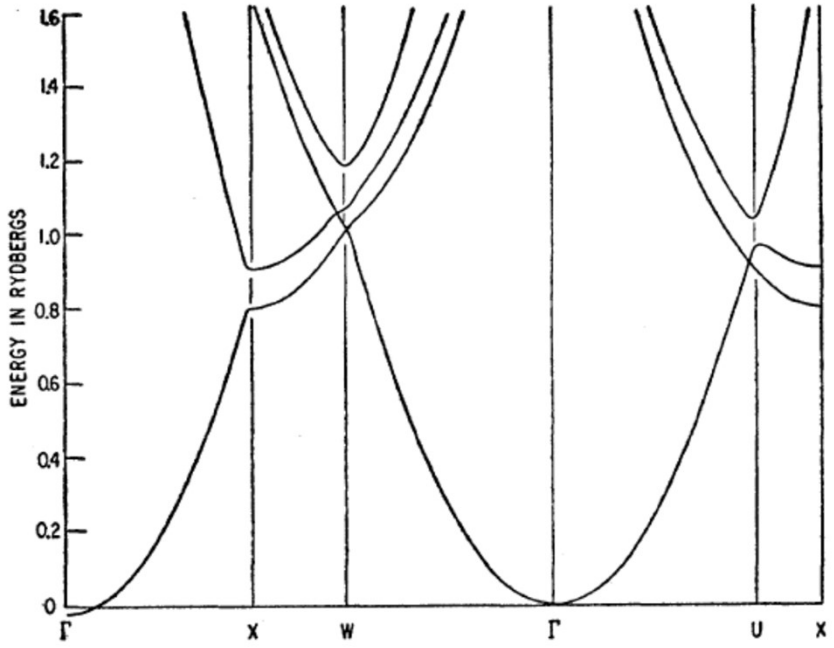
Band Structure of Aluminum

WALTER A. HARRISON
General Electric Research Laboratory, Schenectady, New York

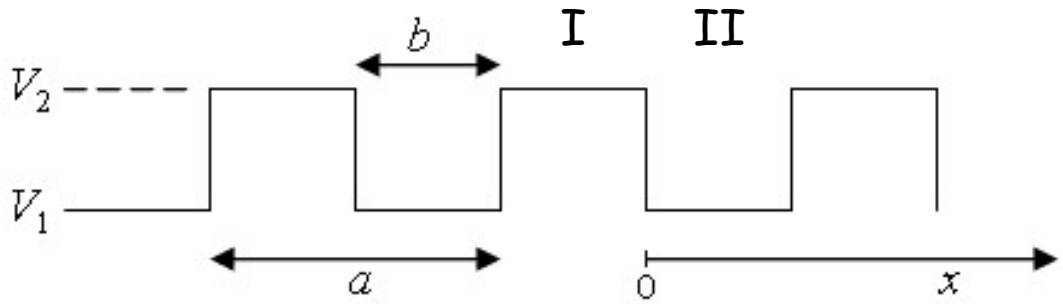


empty lattice approximation





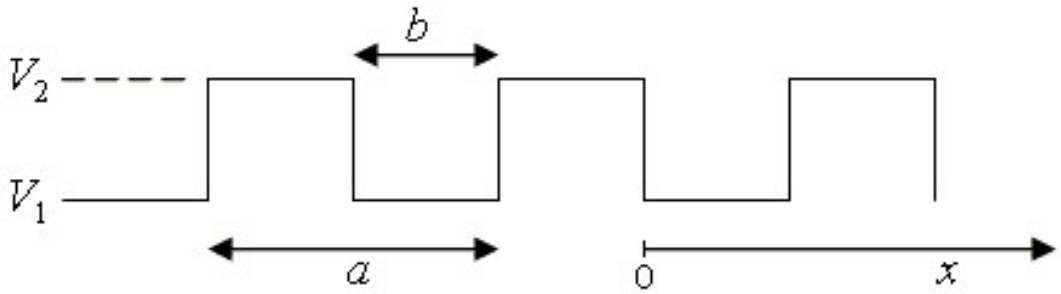
Kronig-Penney model



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

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

Kronig-Penney model

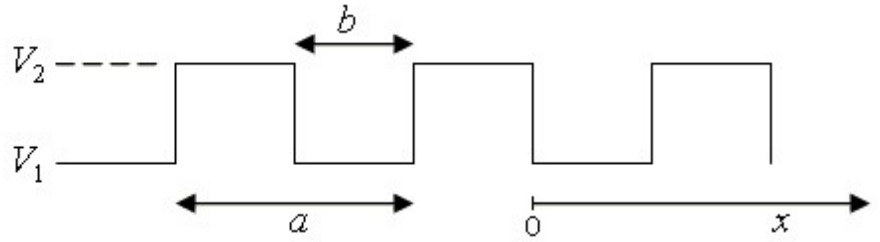


Solutions can be found that are simultaneous eigenfunctions of the Hamiltonian and the translation operator.

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 $b < x < a$

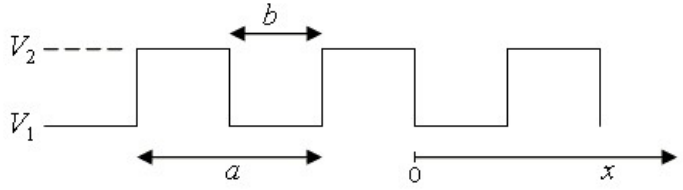
$$\psi_1(x) = \cos(k_2(x-b))\cos(k_1 b) - \frac{k_1 \sin(k_2(x-b))\sin(k_1 b)}{k_2},$$

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

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

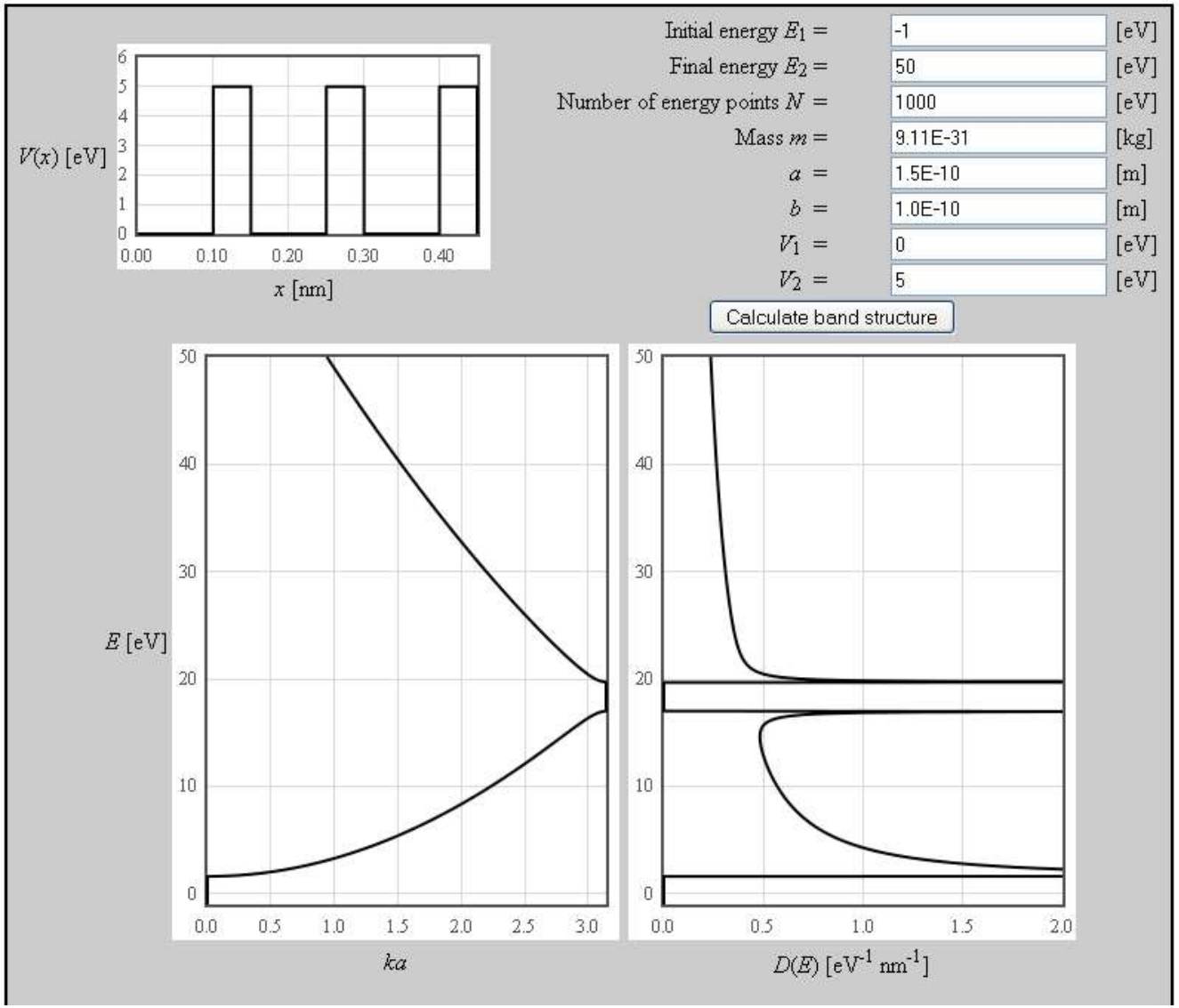
$$\psi_{\pm}(x) = \frac{2\psi_2(a)}{\frac{d\psi_2(a)}{dx} - \psi_1(a) \pm \delta}\psi_1(x) + \psi_2(x), \qquad \lambda\pm = \frac{1}{2}(\alpha \pm \delta),$$

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

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

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

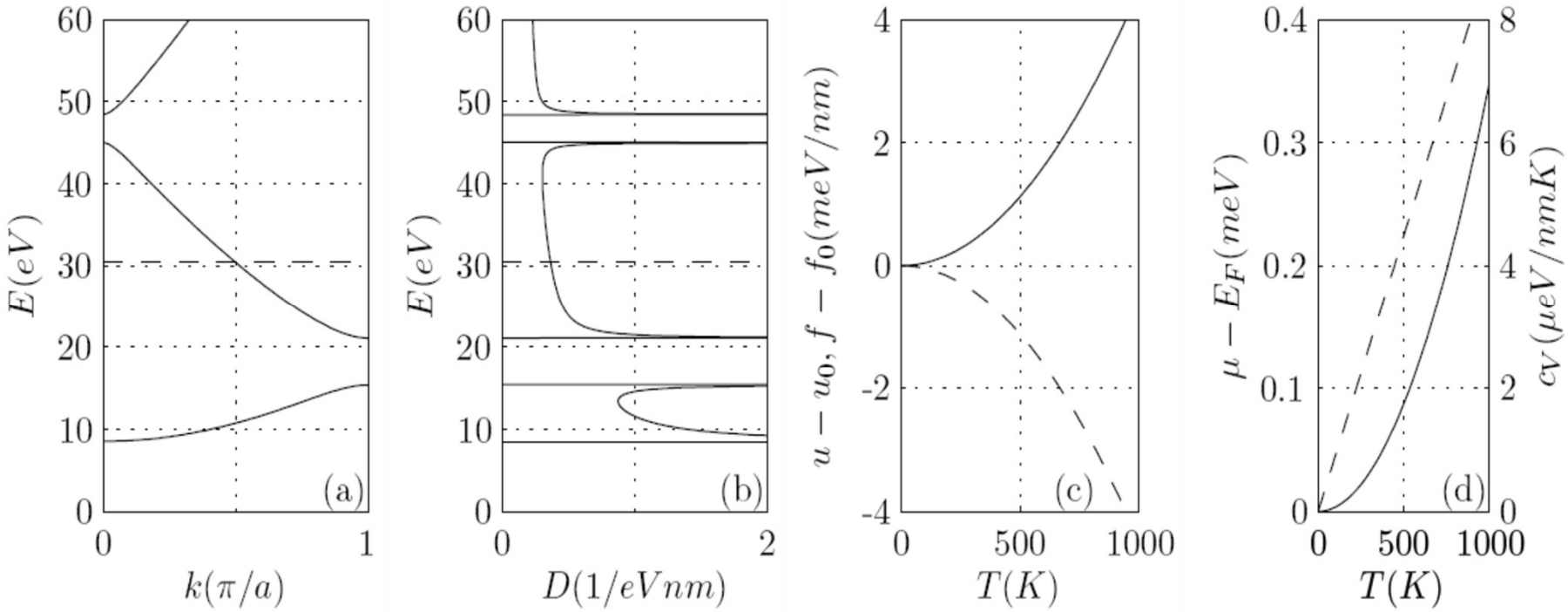
Kronig-Penney model



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

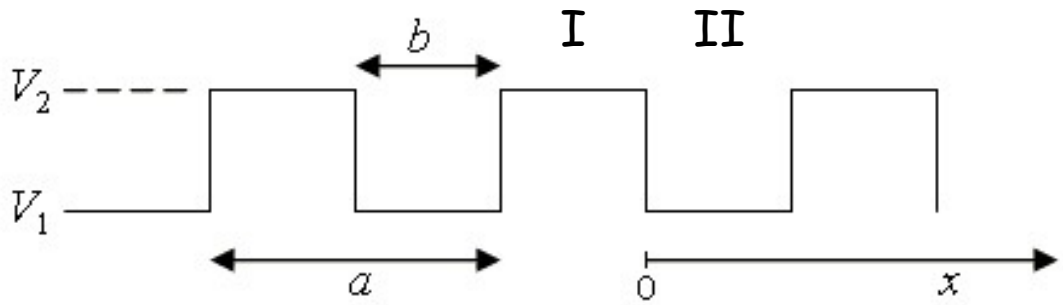
$$k = \pm\frac{1}{a}\tan^{-1}\left(\frac{\sqrt{4-\alpha^2}}{\alpha}\right)$$

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

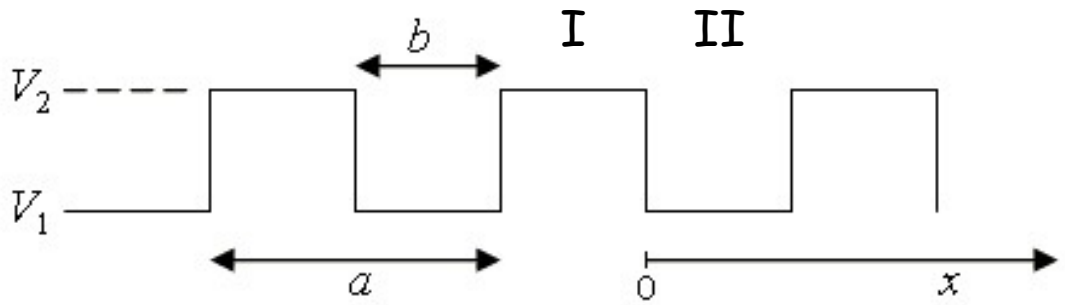


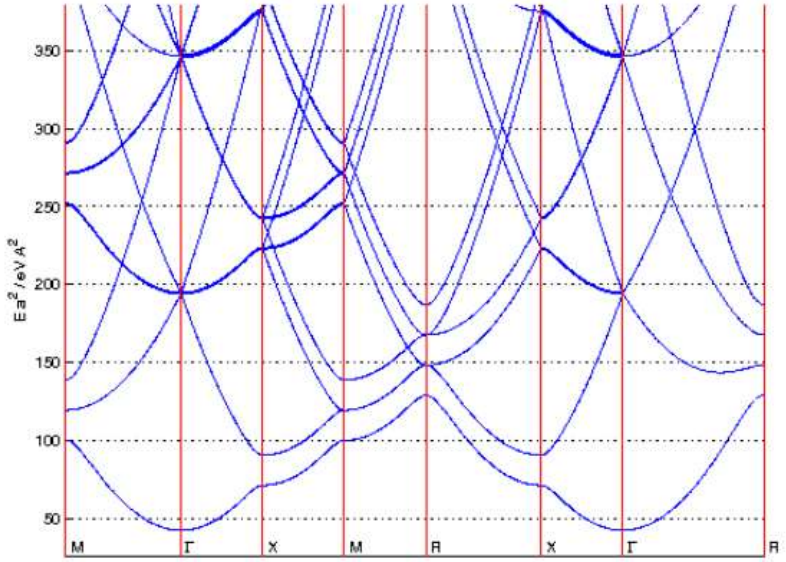
$$-\frac{\hbar^2}{2m}\nabla^2\Psi+(V(x)+V(y)+V(z))\Psi=E\Psi$$

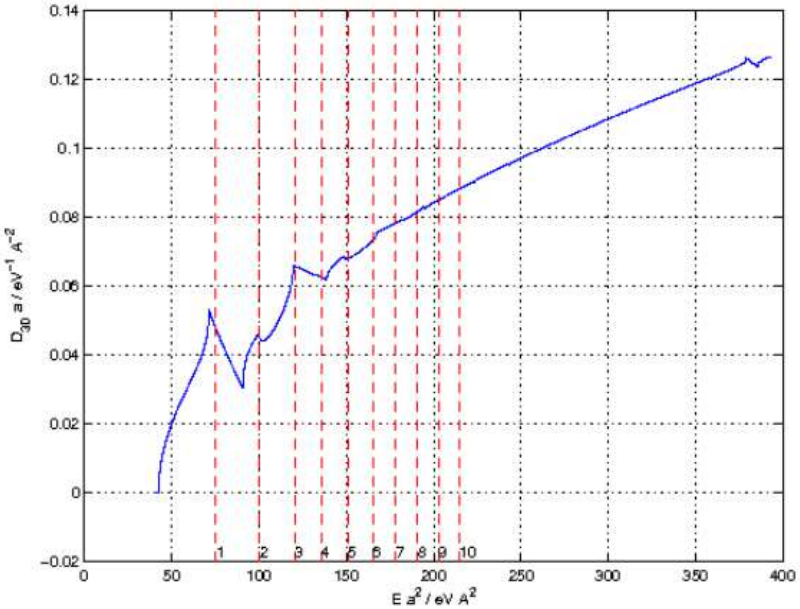
Ψ is the product of the solutions to the Kronig-Penney model.

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

A separable potential

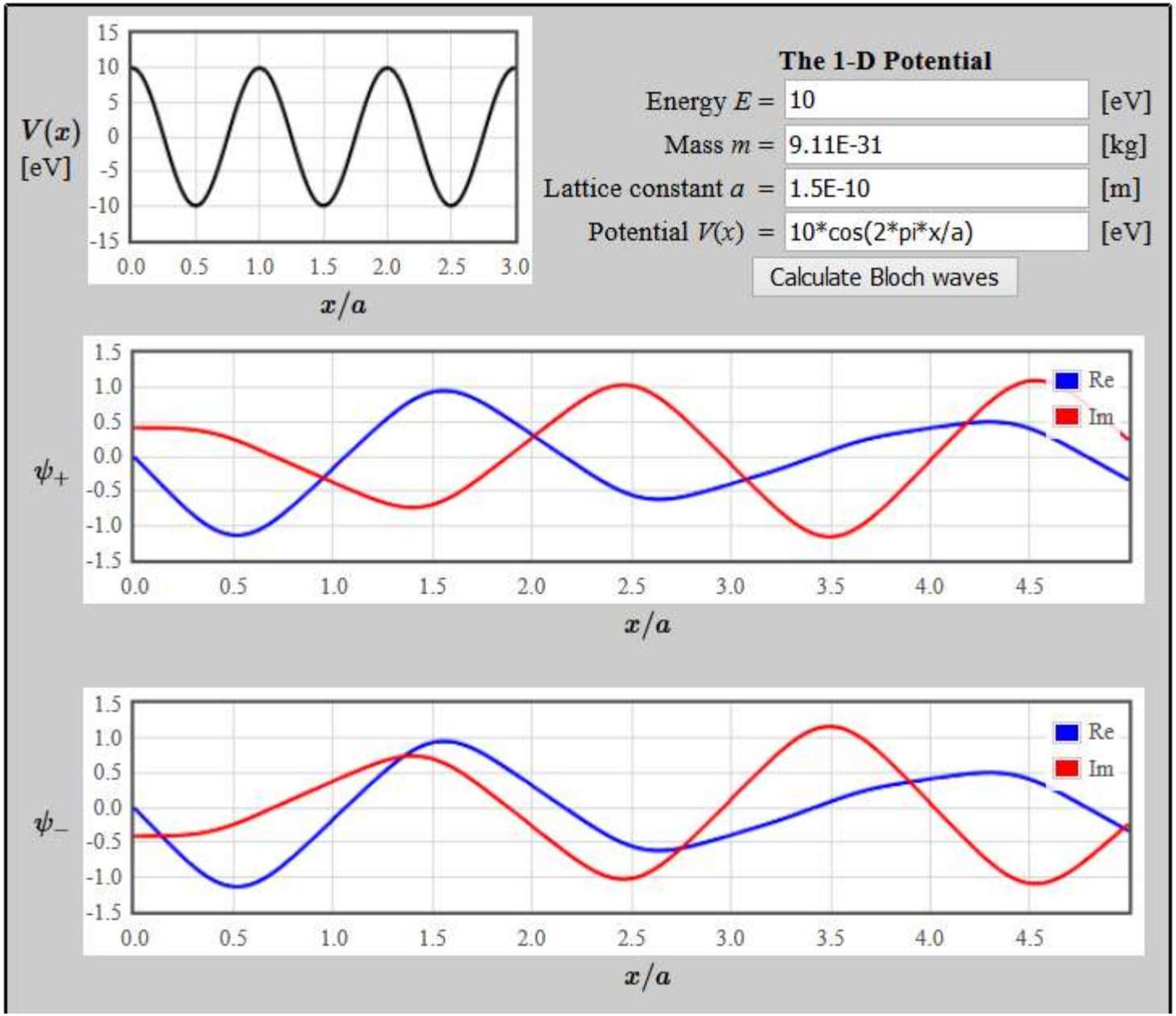






http://lampx.tugraz.at/~hadley/ss1/separablecrystals/thermo.html

Bloch waves in 1-D



Band structure in 1-D