7th IIC-EMTCCM
European Master in Theoretical Chemistry and Computational Modelling
7th International Intensive Course

Lecture 1

Periodicity and Spatial Confinement

Crystal structure
Translational symmetry
Energy bands
k·p theory and effective mass
Theory of invariants
Heterostructures

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SUMMARY (keywords)

Lattice → **Wigner-Seitz unit cell**

Periodicity → **Translation group** → **wave-function in Block form**

Reciprocal lattice → **k-labels within the 1rst Brillouin zone**

Schrodinger equation → **BCs depending on k; bands E(k); gaps**

Gaps → **metal, isolators and semiconductors**

Machinery: kp Theory → effective mass **J character table**

Theory of invariants: $\Gamma \otimes \Gamma \ni A_1$; $H = \sum N_i^{\Gamma} k_i^{\Gamma}$

Heterostructures: EFA

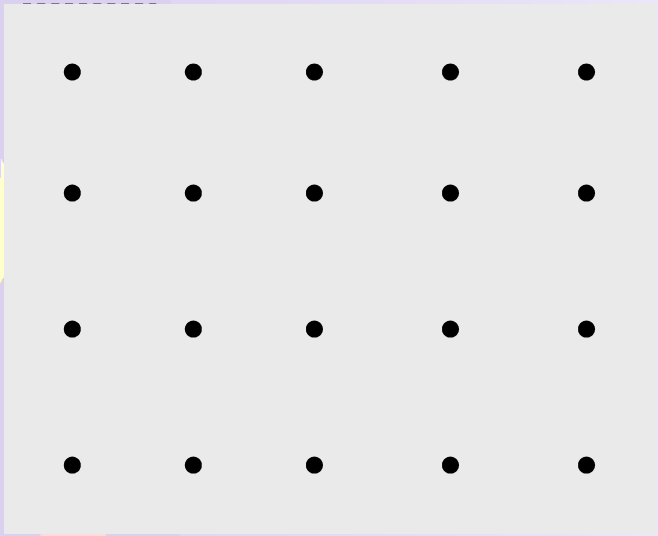
$$k \rightarrow \hat{p} = -i\nabla$$

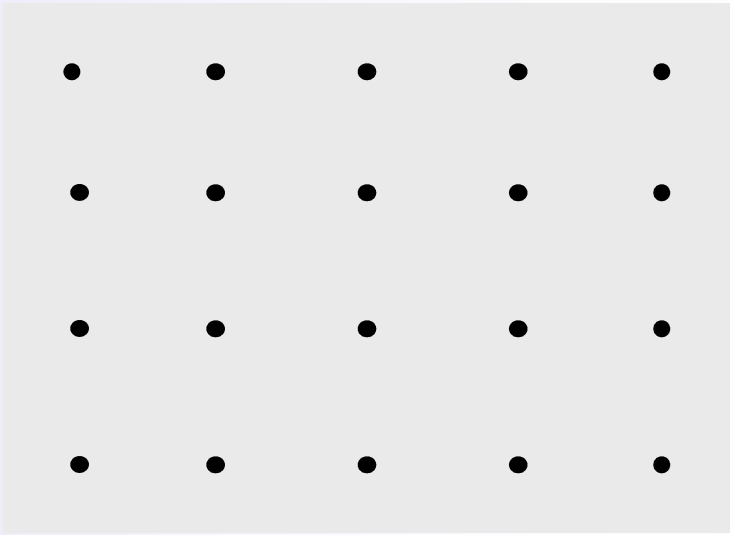
$$confinement \rightarrow V_c = band\ \ offset$$

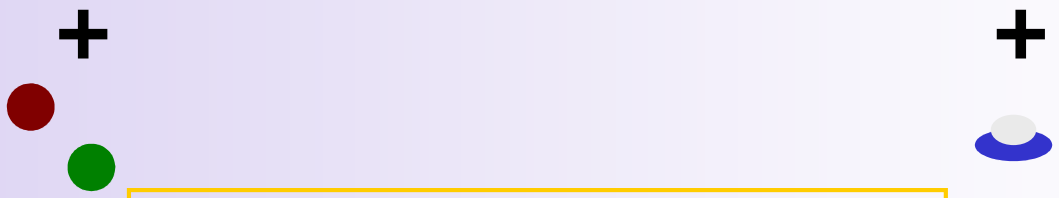
QWell QWire QDot

Crystal structure

A crystal is solid material whose constituent atoms, molecules or ions are arranged in an orderly repeating pattern

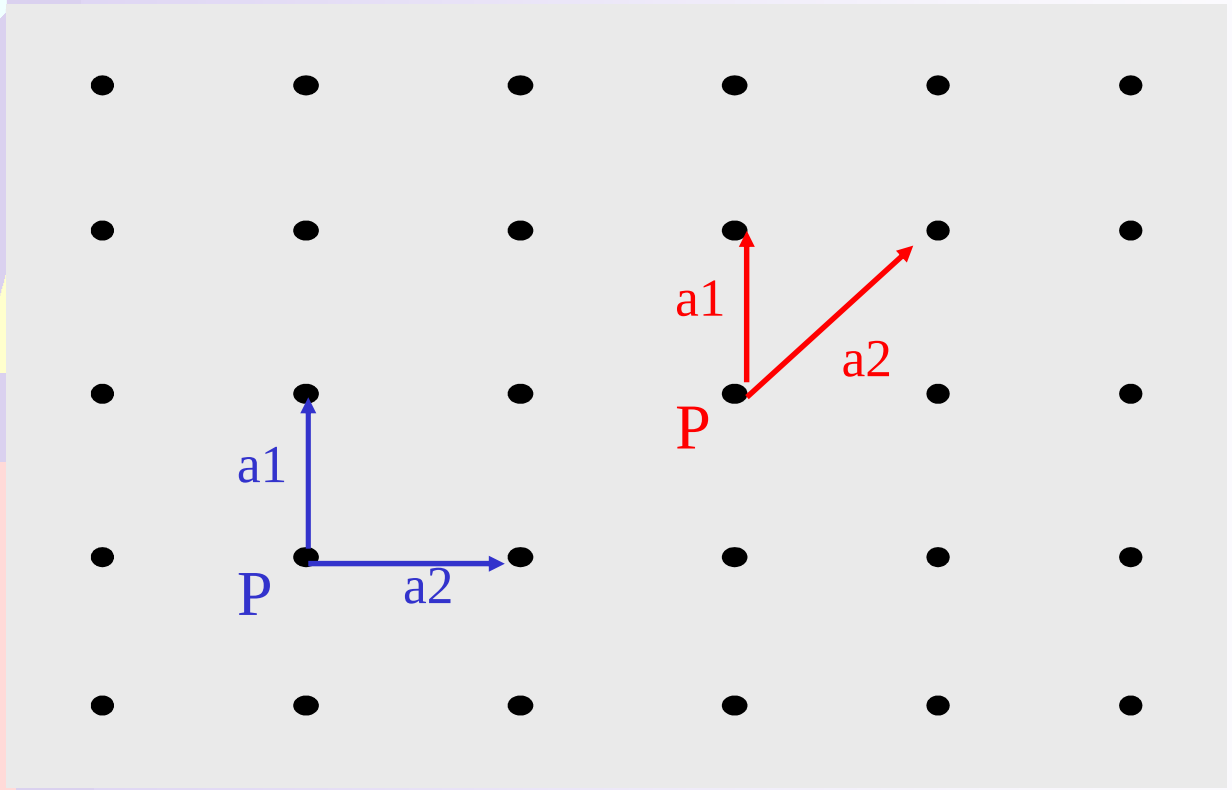






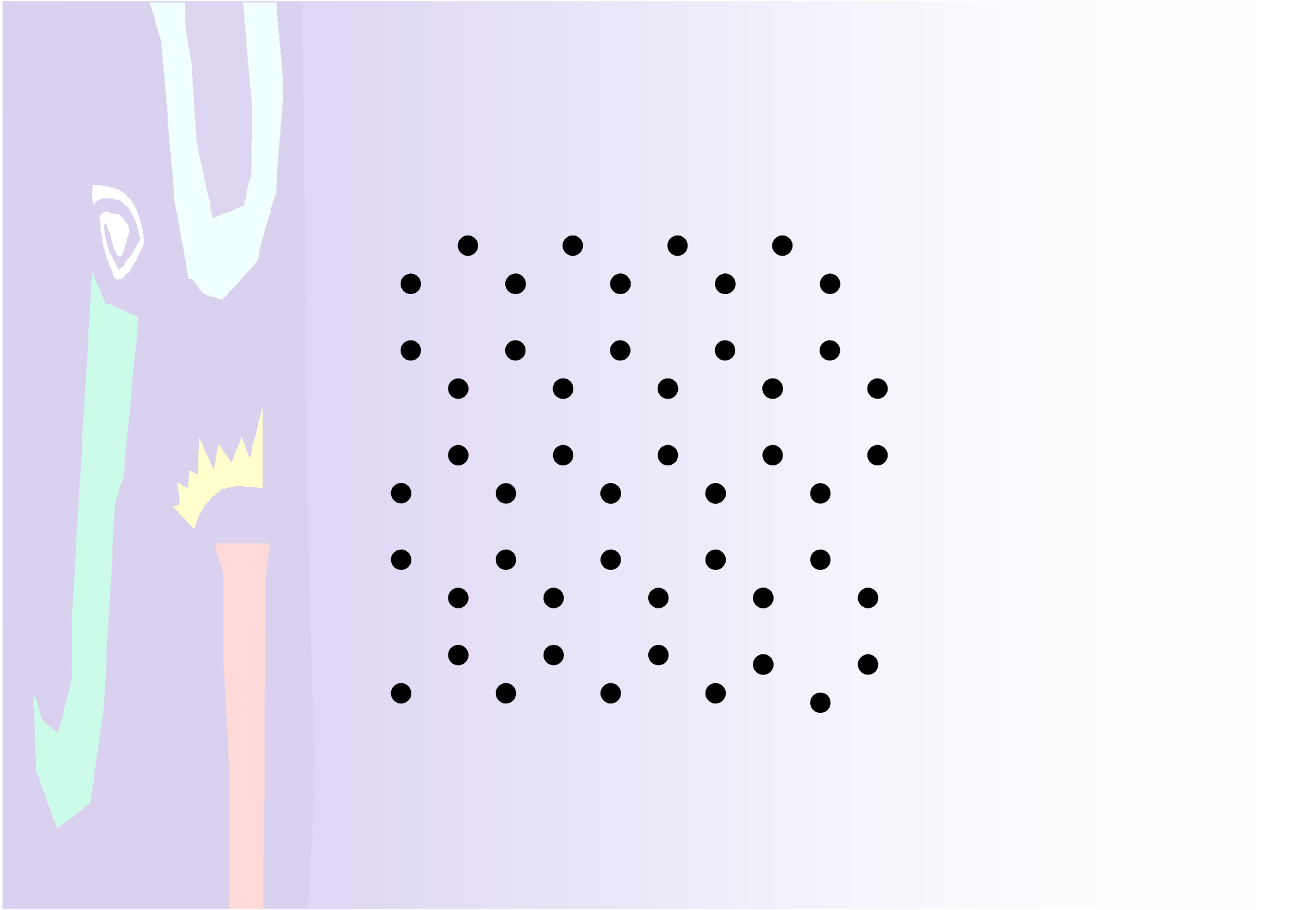
Crystal = lattice + basis

Bravais lattice: the lattice looks the same when seen from *any* point

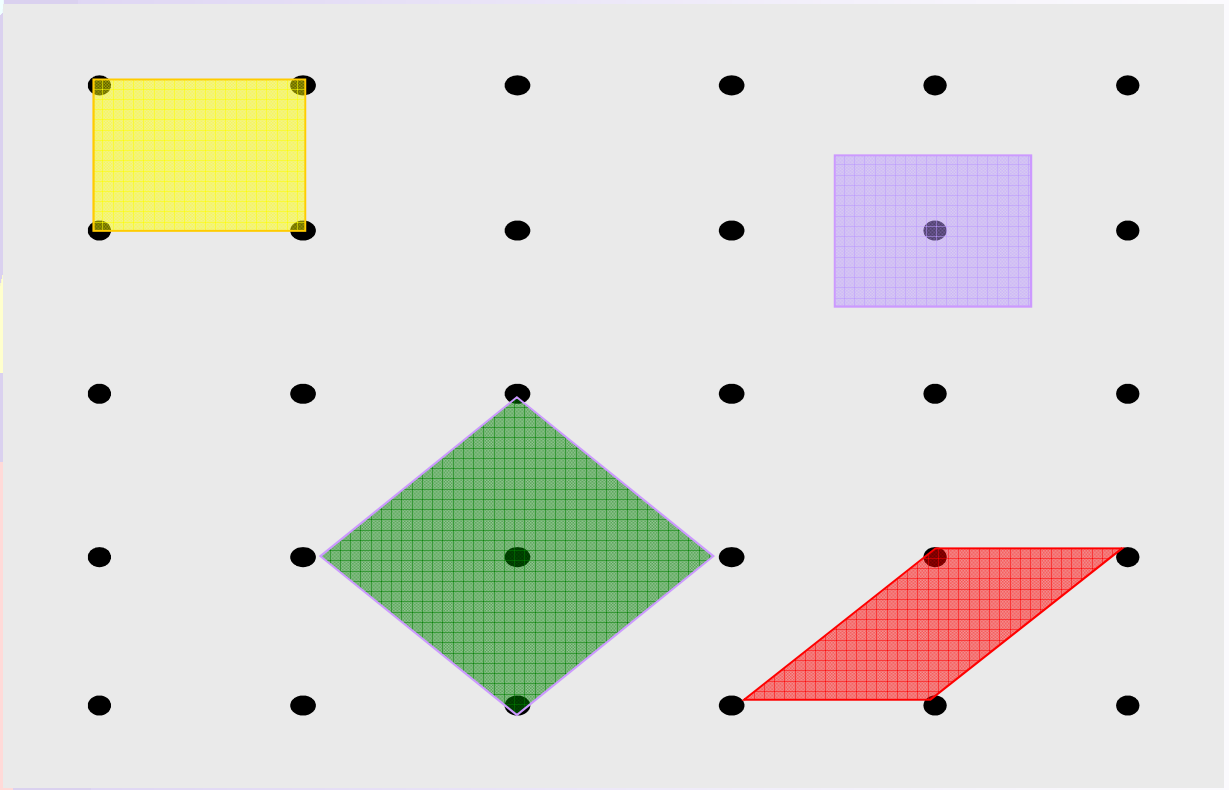


$$P' = P + (m,n,p) * (a1,a2,a3)$$

integers



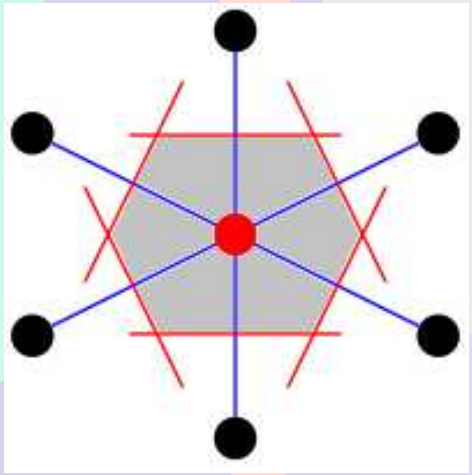
Unit cell: a region of the space that fills the entire crystal by translation

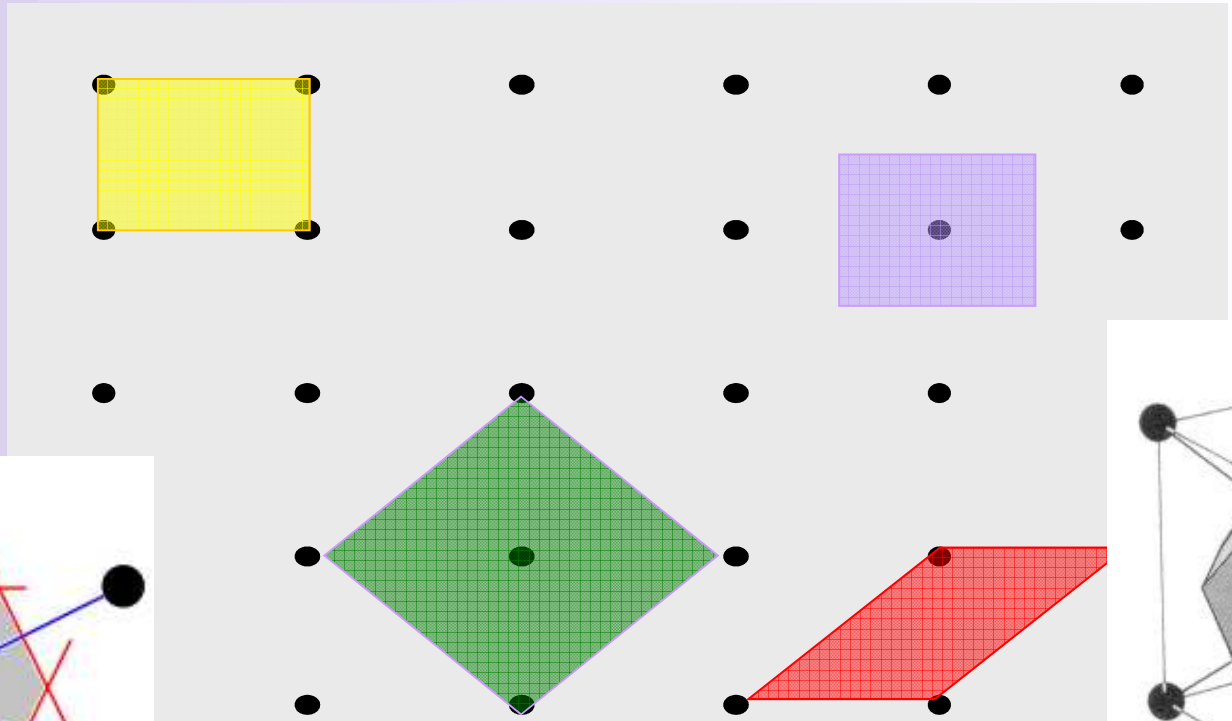


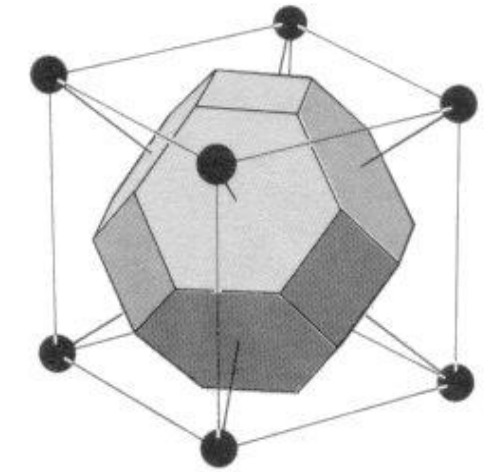
Primitive: smallest unit cells (1 point)

Wigner-Seitz unit cell: primitive and captures the point symmetry

Centered in one point. It is the region which is closer to that point than to any other.



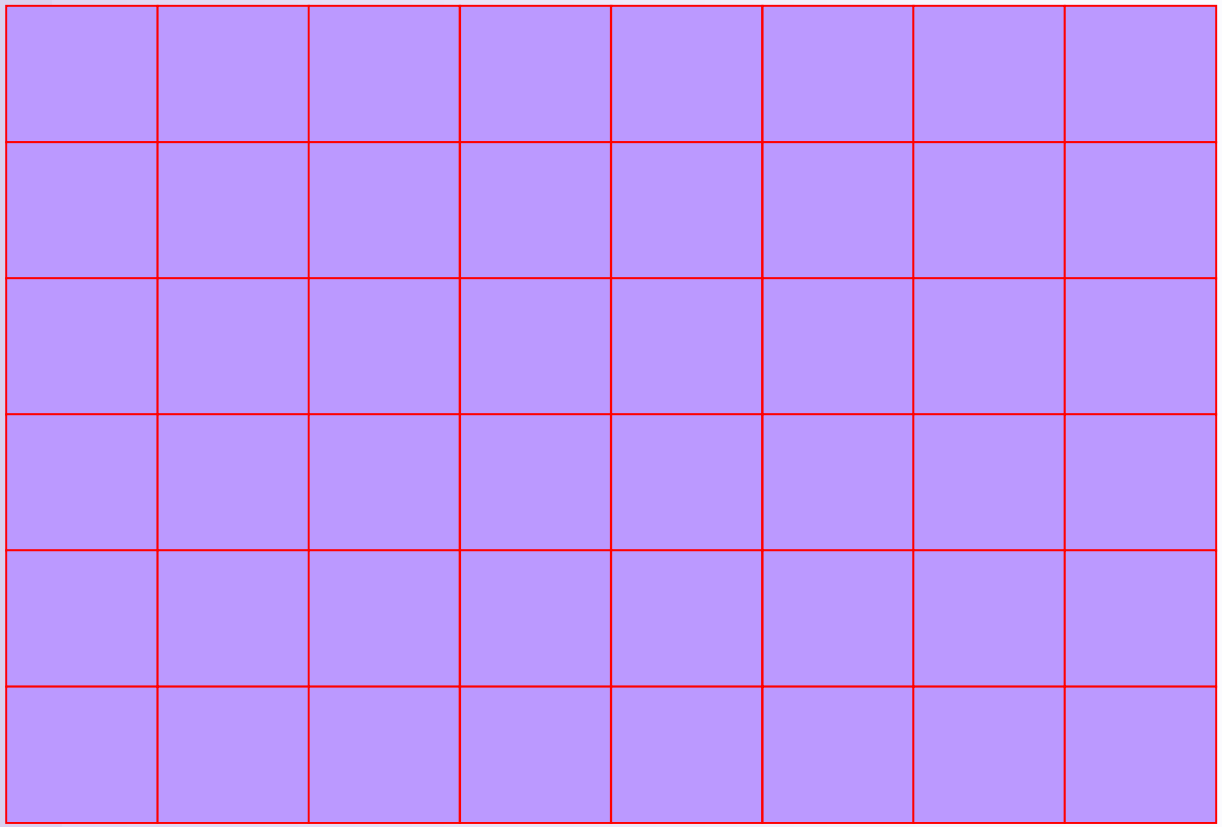




Body-centered cubic

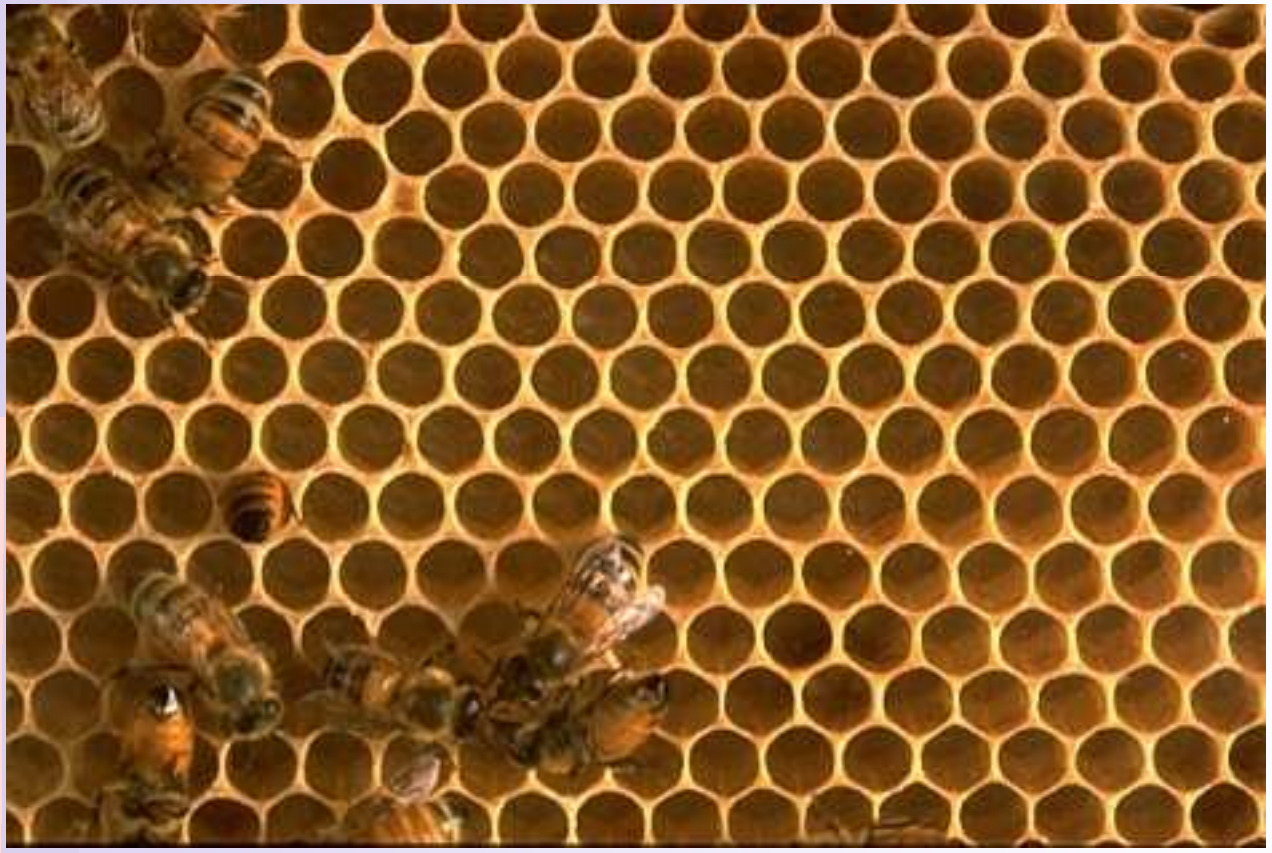
How many types of lattices exist?

C_4?



How many types of lattices exist?

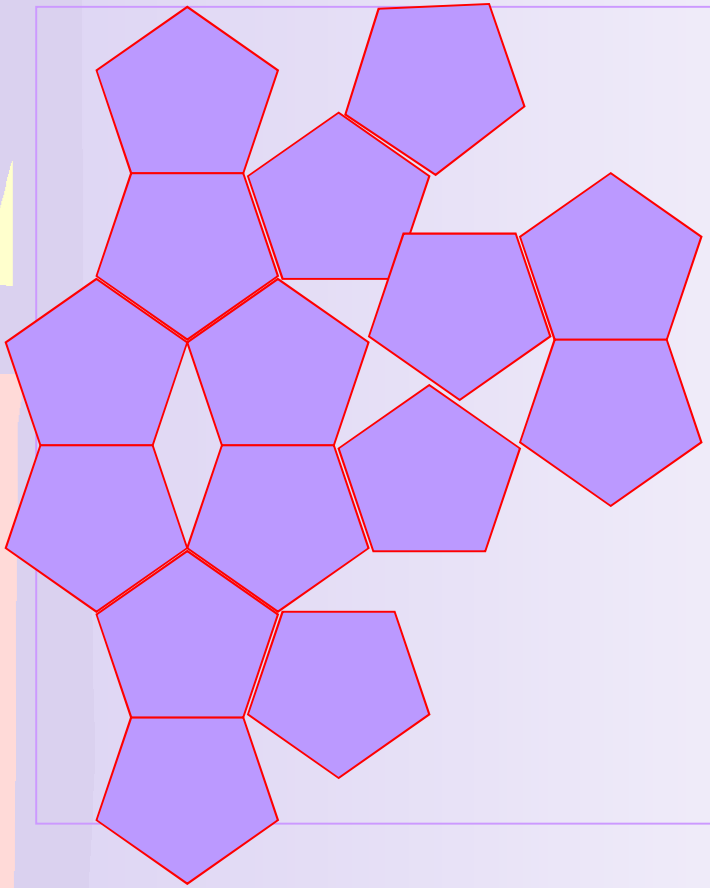
C_6?



How many types of lattices exist?

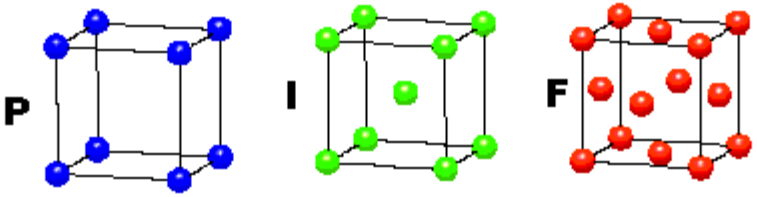
14 (in 3D)

C_5?

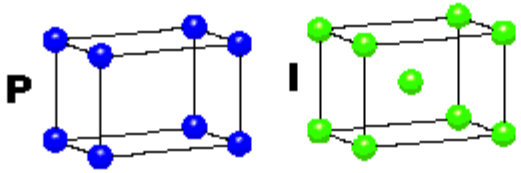


Bravais Lattices

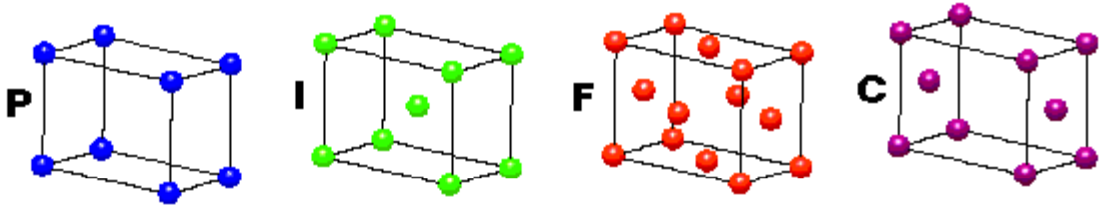
CUBIC
$a = b = c$
$\alpha = \beta = \gamma = 90°$



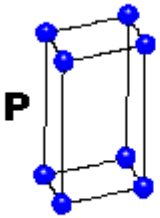
TETRAGONAL
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$



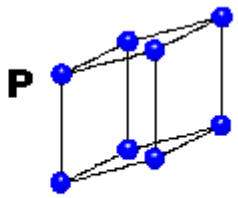
ORTHORHOMBIC
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



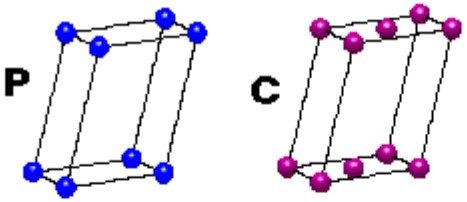
HEXAGONAL
$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$



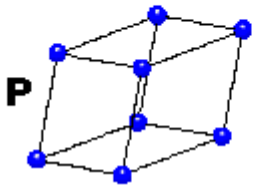
TRIGONAL
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$



MONOCLINIC
$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$



TRICLINIC
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

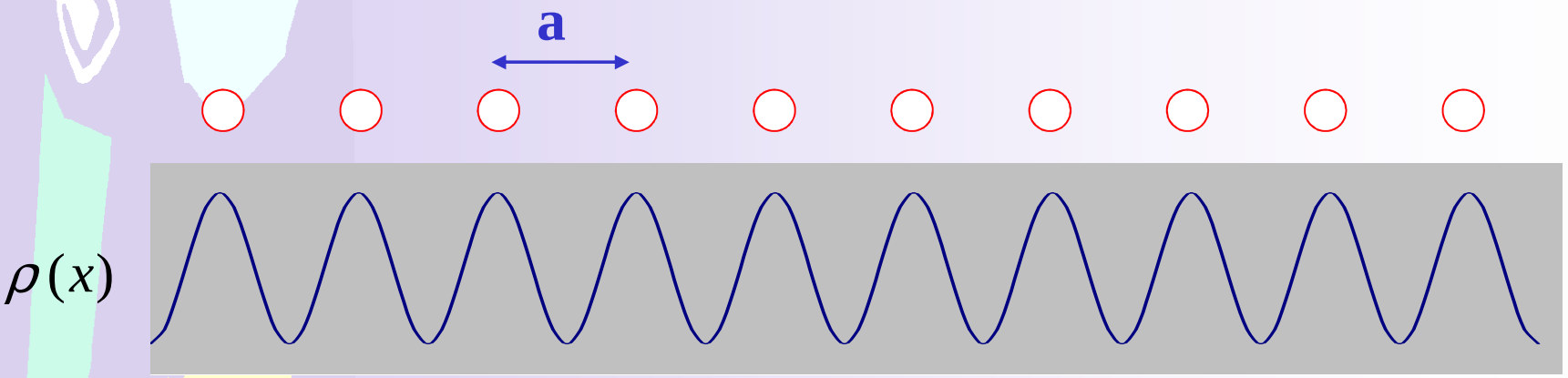


4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Translational symmetry

We have a periodic system.

Is there a simple function to approximate its properties?



$$\rho(x)=\rho(x+na)\Leftrightarrow|f(x)|^2=|f(x+na)|^2\Rightarrow f(x+na)=e^{i\phi}f(x)$$

$$T_n f(x)=f(x+na)\rightarrow \qquad \{T_n\}\rightarrow Translation\ \ Group$$

$$[T_n,T_m]=0\rightarrow Abelian\ Group$$

$$T_n=e^{i\,a\,n\,\hat{p}}=\sum_q\frac{(i\,a\,n)^q}{q!}\hat{p}^q$$

$$T_n f(x)=e^{ian\hat{p}}f(x)=\sum_q\frac{(ian)^q}{q!}(-i)^q\frac{d^q f}{dx^q}=f(x+an)$$

Eigenfunctions of the linear momentum basis of translation group irreps

$$T_n e^{ikx} = e^{ian\hat{p}} e^{ikx} = e^{iank} e^{ikx}$$

	E	$\cdots$	T_n	$\cdots$	
$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\cdots$	$\vdots$
k	1	$\cdots$	e^{ikna}	$\cdots$	e^{ikx}
$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\cdots$	$\vdots$

$$T_n = e^{i\,a\,n\,\hat{p}} = \sum_q \frac{(i\,a\,n)^q}{q!}\hat{p}^q$$

Range of k and 3D extension

$$k \sim k' = k + \frac{2\pi}{a} m, \quad m \in Z$$ **same character:** $$e^{i[k+\frac{2\pi}{a}m]na} = e^{ikna}$$

$$k \in [-\frac{\pi}{a}, \frac{\pi}{a}]; \quad \mathrm{k} = 0 \quad \text{labels the fully symmetric } \mathrm{A}_1 \text{ irrep}$$

3D extension $\begin{cases} \mathrm{x} \to \boldsymbol{r} \\ k \to \boldsymbol{k} \end{cases}$

Bloch functions as basis of irreps:

$$\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}} u(\boldsymbol{r}); \quad u(\boldsymbol{r}+\boldsymbol{a}) = u(\boldsymbol{r})$$

$$T_{\boldsymbol{a}}\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\,\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{a})} u(\boldsymbol{r}+\boldsymbol{a}) = \underbrace{e^{i\,\boldsymbol{k}\cdot\boldsymbol{a}}}_{character}\; e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}} u(\boldsymbol{r})$$

Reciprocal Lattice

$$1D:\ k \sim k' \rightarrow k'-k = K = \frac{2\pi}{a}:\ e^{iKa} = 1$$

$$3D:\ \boldsymbol{k} \sim \boldsymbol{k}' \rightarrow \boldsymbol{k}'-\boldsymbol{k} = \boldsymbol{K}:\ e^{i\,\boldsymbol{K}\cdot\boldsymbol{a}_i} = 1, \quad \boldsymbol{a}_i = \boldsymbol{a},\boldsymbol{b},\boldsymbol{c}\ \textit{(lattice vectors)}$$

$$\boldsymbol{K}? \qquad \boldsymbol{K} = \mathrm{p}_1\boldsymbol{k}_1 + \mathrm{p}_2\boldsymbol{k}_2 + \mathrm{p}_3\boldsymbol{k}_3, \qquad \boldsymbol{k}_\mathrm{i} = 2\pi\,\frac{(\boldsymbol{a}_\mathrm{j}\times\boldsymbol{a}_\mathrm{k})}{(\boldsymbol{a}_\mathrm{j}\times\boldsymbol{a}_\mathrm{k})\boldsymbol{a}_\mathrm{i}}, \qquad \mathrm{p_i} \in Z$$

$$\boldsymbol{K}\cdot\boldsymbol{a}_\mathrm{i} = 2\pi\ p_i \qquad \{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3\} \ \rightarrow\ \textit{reciprocal lattice}$$

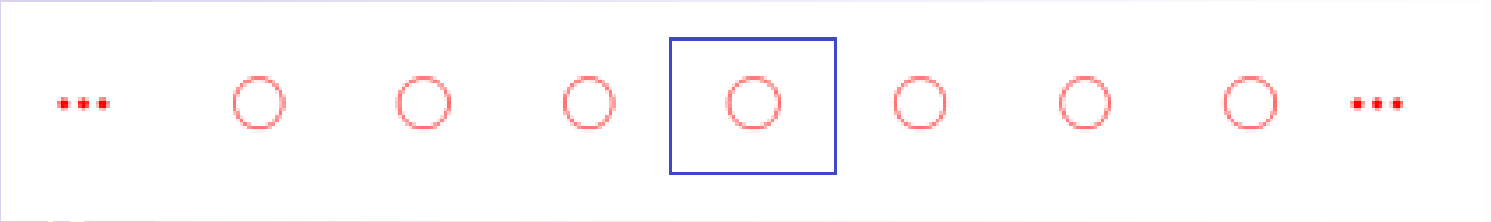
$$\Gamma:\ \boldsymbol{k} = 0, \qquad \boldsymbol{k} = \mathrm{x}\boldsymbol{k}_1 + \mathrm{y}\boldsymbol{k}_2 + \mathrm{z}\boldsymbol{k}_3, \qquad \mathrm{x,y,z} \in (-1/2,1/2)$$

First Brillouin zone: Wigner-Seitz cell of the reciprocal lattice

Solving Schrödinger equation: Von-Karman BCs

Crystals are infinite... How are we supposed to deal with that?

We use periodic boundary conditions



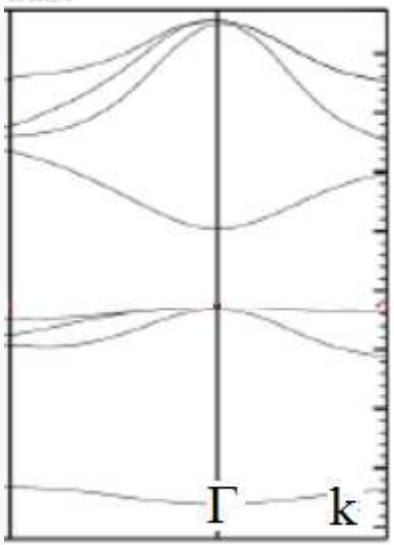
Group of translations:

$$T_a \Psi_k(r) = e^{i k \cdot a} \Psi_k(r)$$

$$\Psi_k(-a/2) = e^{i\phi} \Psi_k(a/2), \quad \phi \in [-\pi, \pi]$$

k is a quantum number due to translational symmetry

1rst Brillouin zone



We solve the Schrödinger equation ***for each k value****:*

The plot $E_n(k)$ *represents an* ***energy band***

How does the wave function look like?

$[\hat{T}, \hat{H}] = 0$ Hamiltonian eigenfunctions are basis of the T_n group irreps

We require $\hat{T}\Psi = e^{i\vec{k}\vec{t}}\,\Psi$

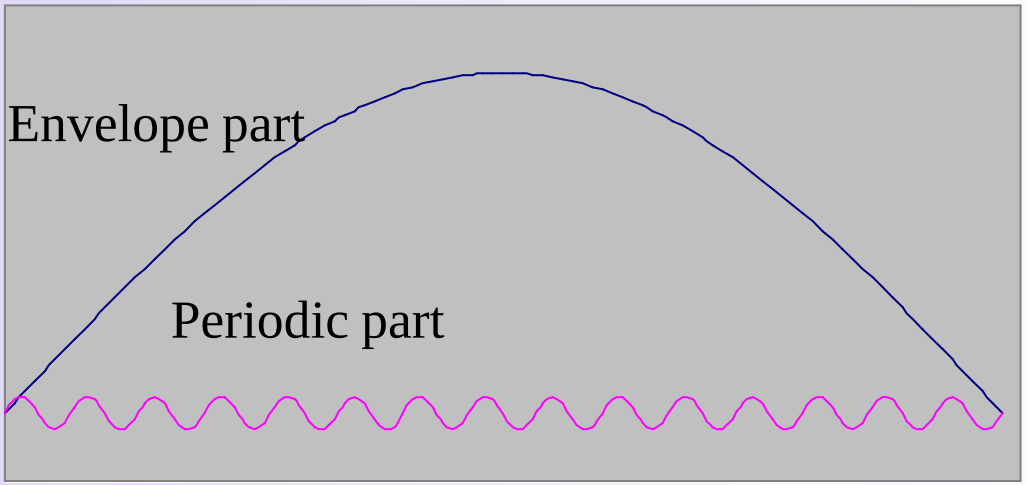
$$\Psi_k(\vec{r}) = e^{i\vec{k}\vec{r}}\,u_k(\vec{r})$$

Bloch function

Envelope part

Periodic (unit cell) part

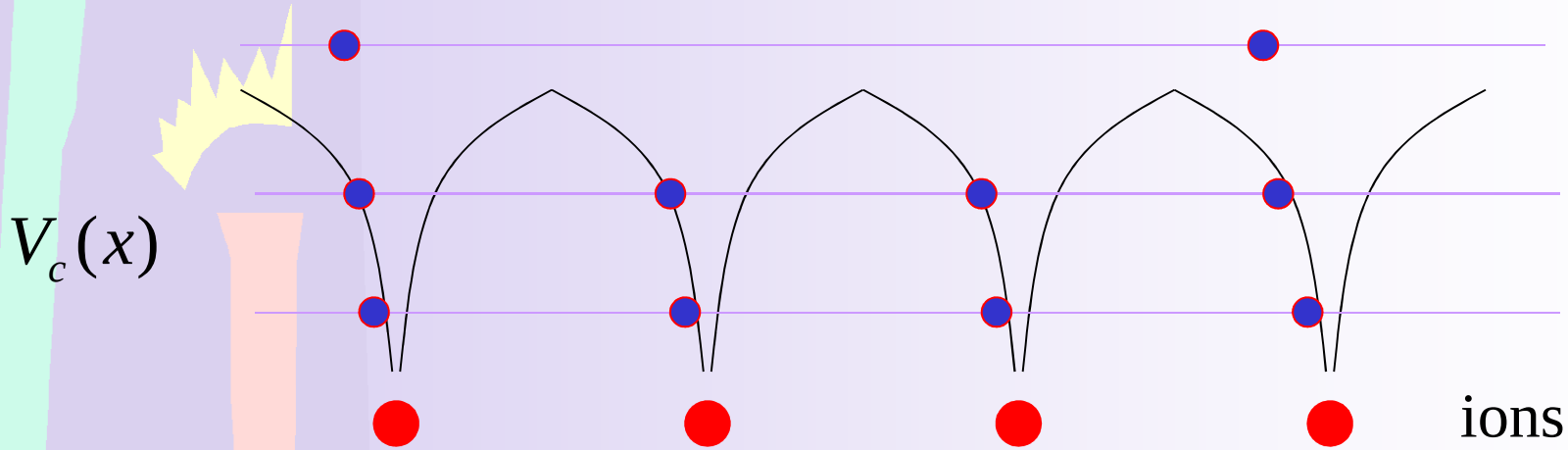
$$u_k(\vec{r}+\vec{t}) = u_k(\vec{r})$$



Energy bands

How do electrons behave in crystals?

quasi-free electrons



$$\left(\frac{p^2}{2m} + V_c(x)\right)\Psi_k(x) = \varepsilon_k\,\Psi_k(x)$$

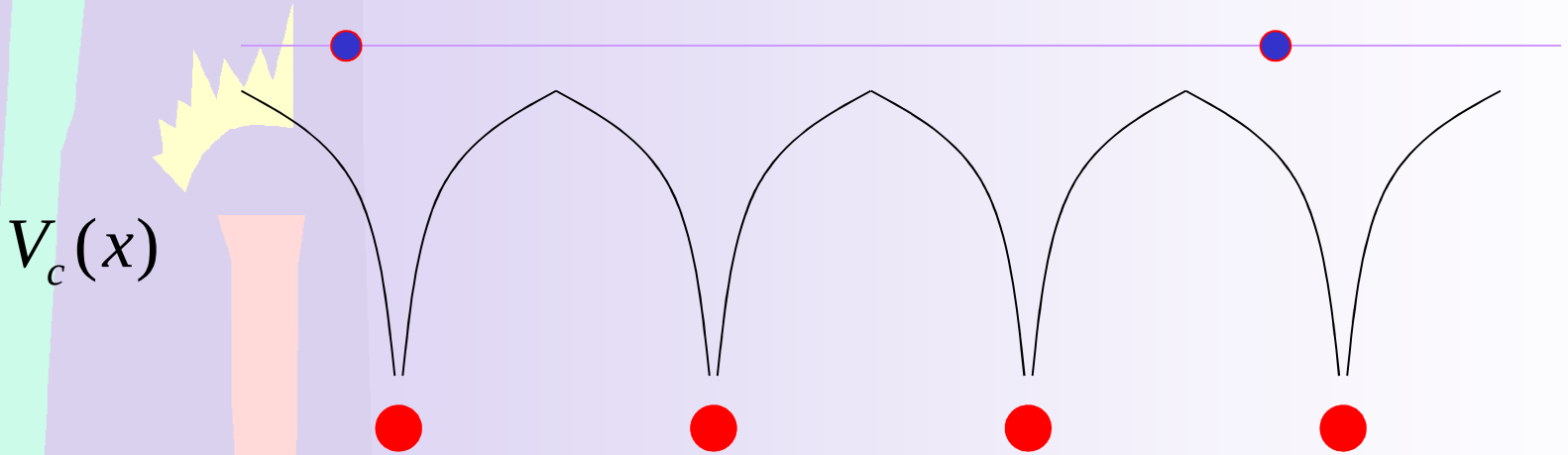
$$BC: \Psi_k(x+a) = e^{ika}\,\Psi_k(x) \qquad \varepsilon_k >> V_c(x)$$

Empty lattice

$$\Psi_k(x) = N\,e^{ikx}$$

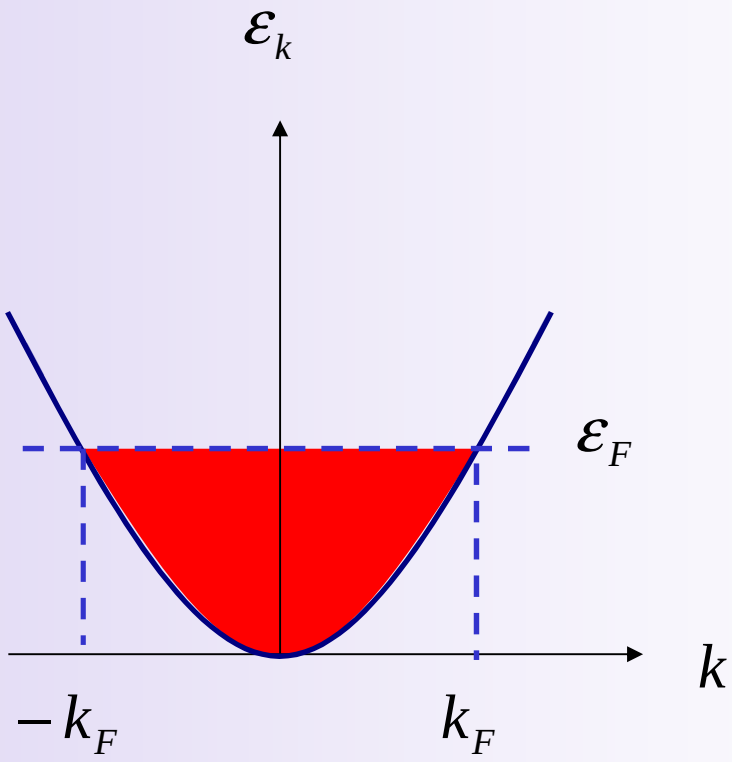
$$k = \frac{2\pi\,p}{a}$$

Plane wave



$$\hat{p}\,\Psi_k(x) = \hbar\,k\,\Psi_k(x)$$

$$\varepsilon_k = \frac{\hbar^2\,k^2}{2m}$$

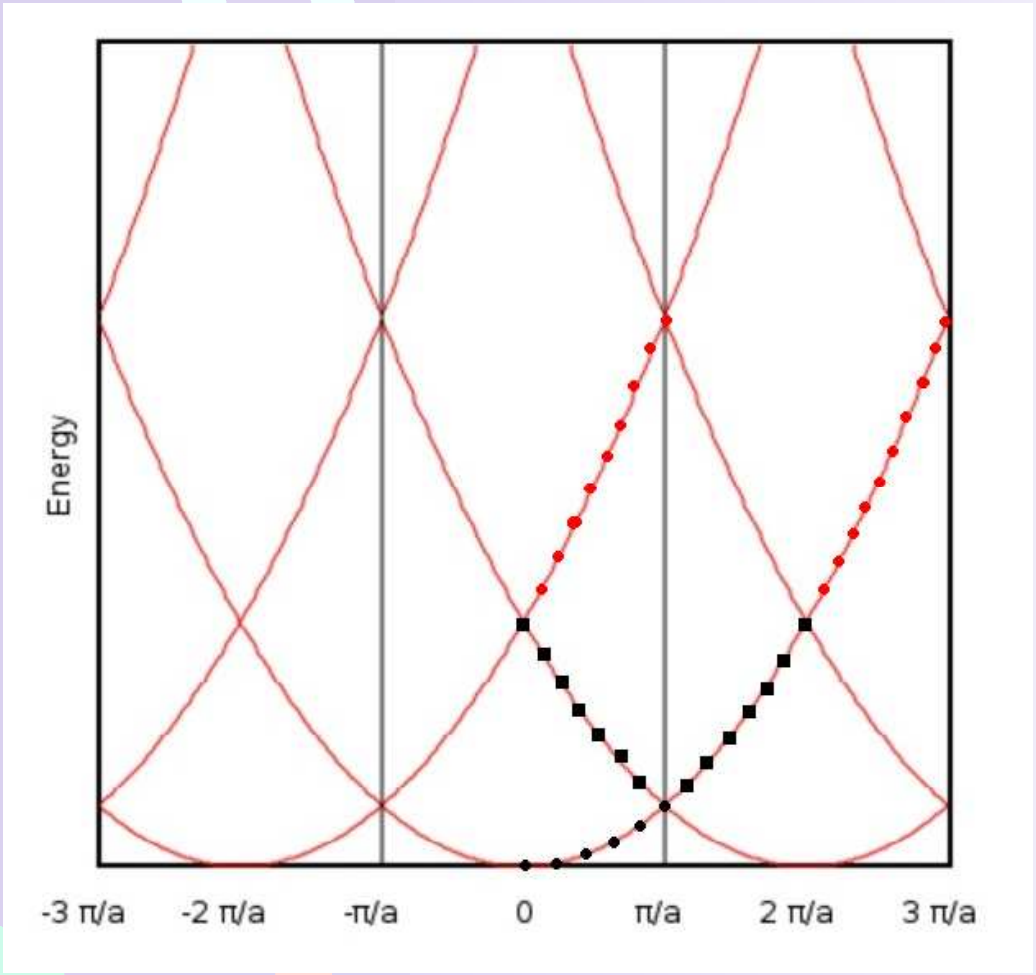


T=0 K

Fermi energy

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

Band folded into the first Brillouin zone



$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

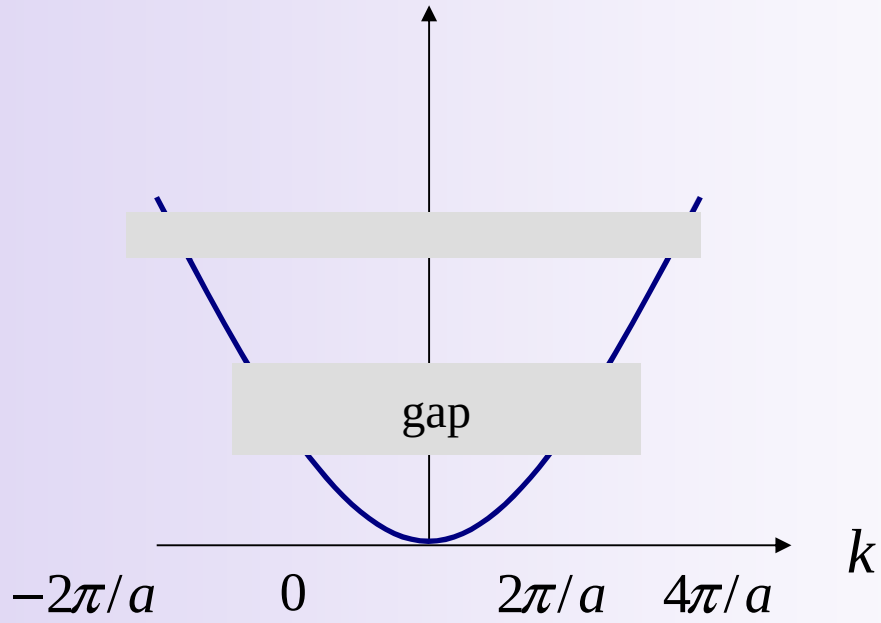
$\varepsilon(k)$: **single parabola**

$$BC: \Psi_k(x+a) = e^{ika}\,\Psi_k(x)$$

$$k \sim k' \rightarrow k' - k = K = \frac{2\pi}{a}: \quad e^{iKa} = 1$$

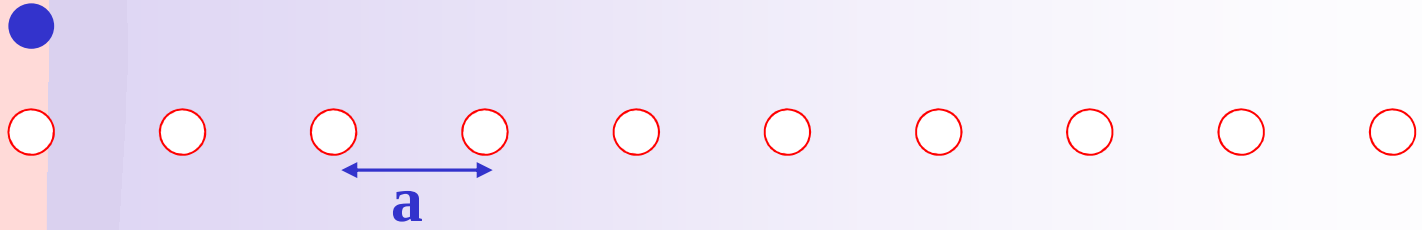
folded parabola

$$\left(\frac{p^2}{2m} + V_c(x) \right) \Psi_k(x) = \varepsilon_k \Psi_k(x)$$

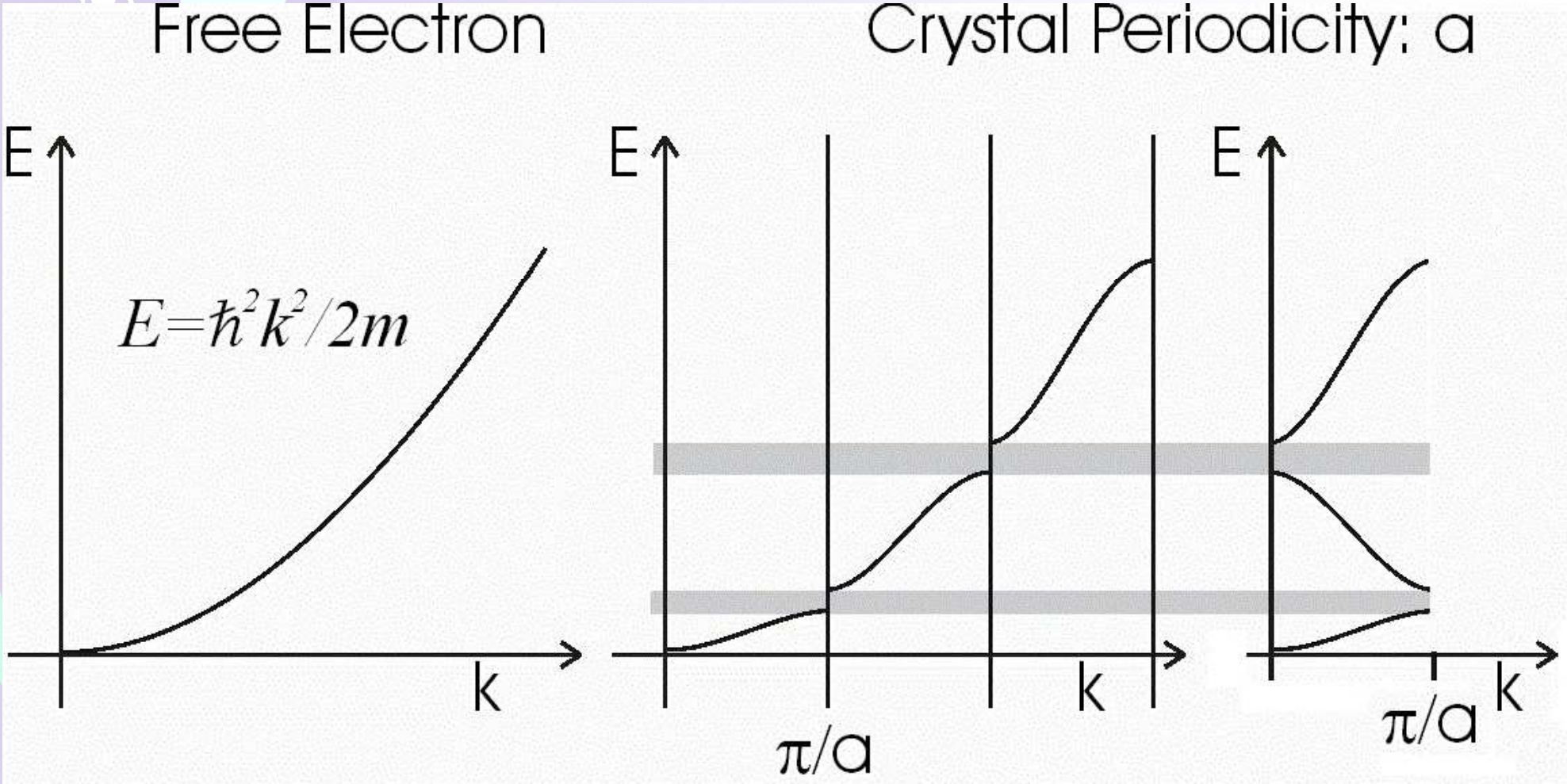


Bragg diffraction

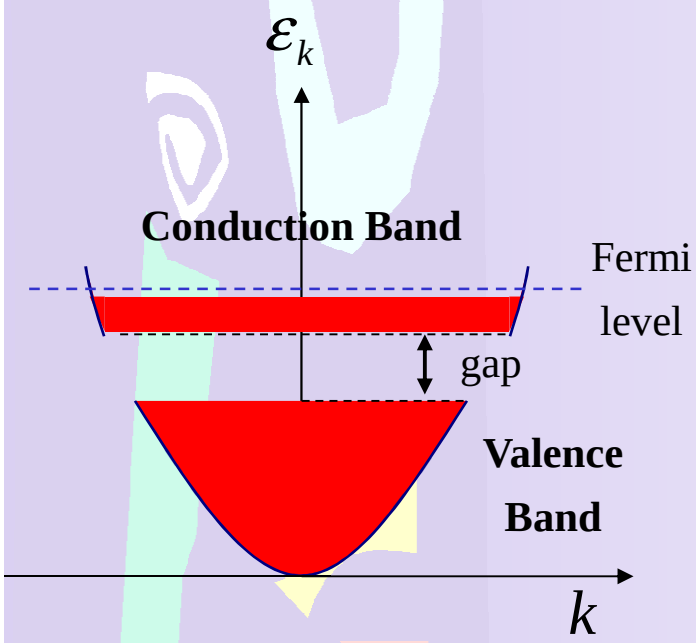
$$a\,k = 2\pi\,n, \quad n \in Z$$



$$\left(\frac{p^2}{2m}+V_c(x)\right)\Psi_k(x)=\varepsilon_k\,\Psi_k(x)$$

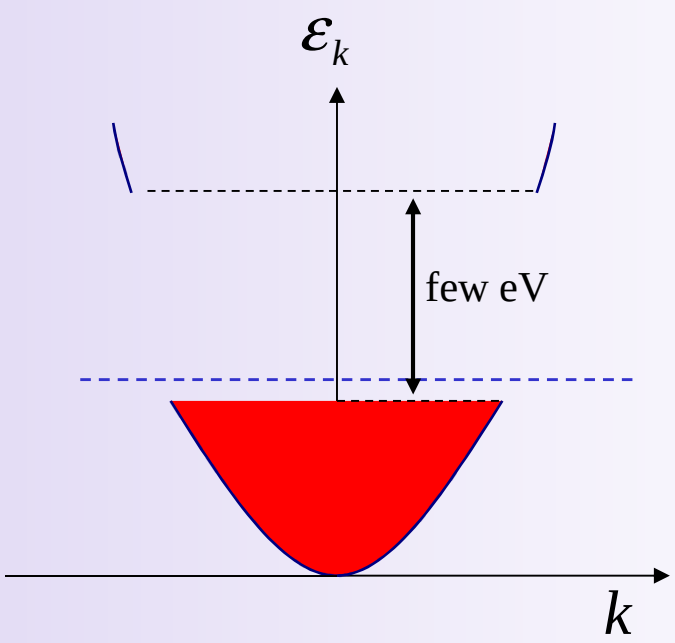


Types of crystals



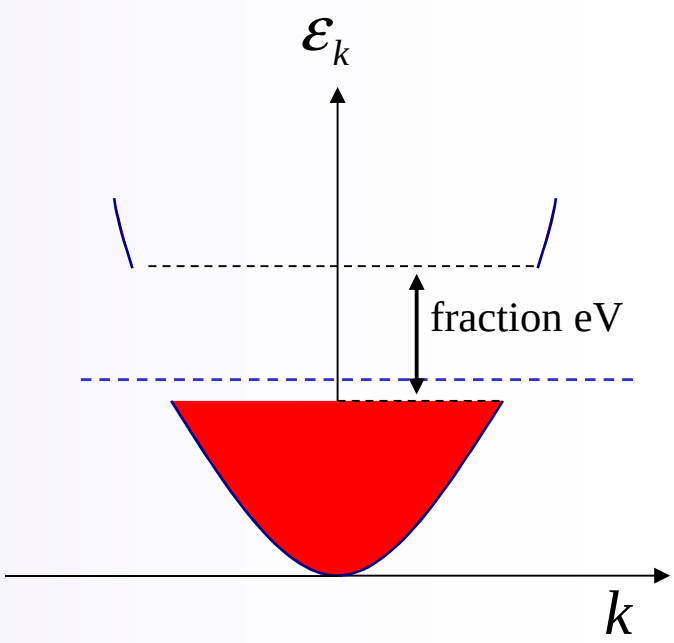
Metal

• Empty orbitals available at low-energy: high conductivity



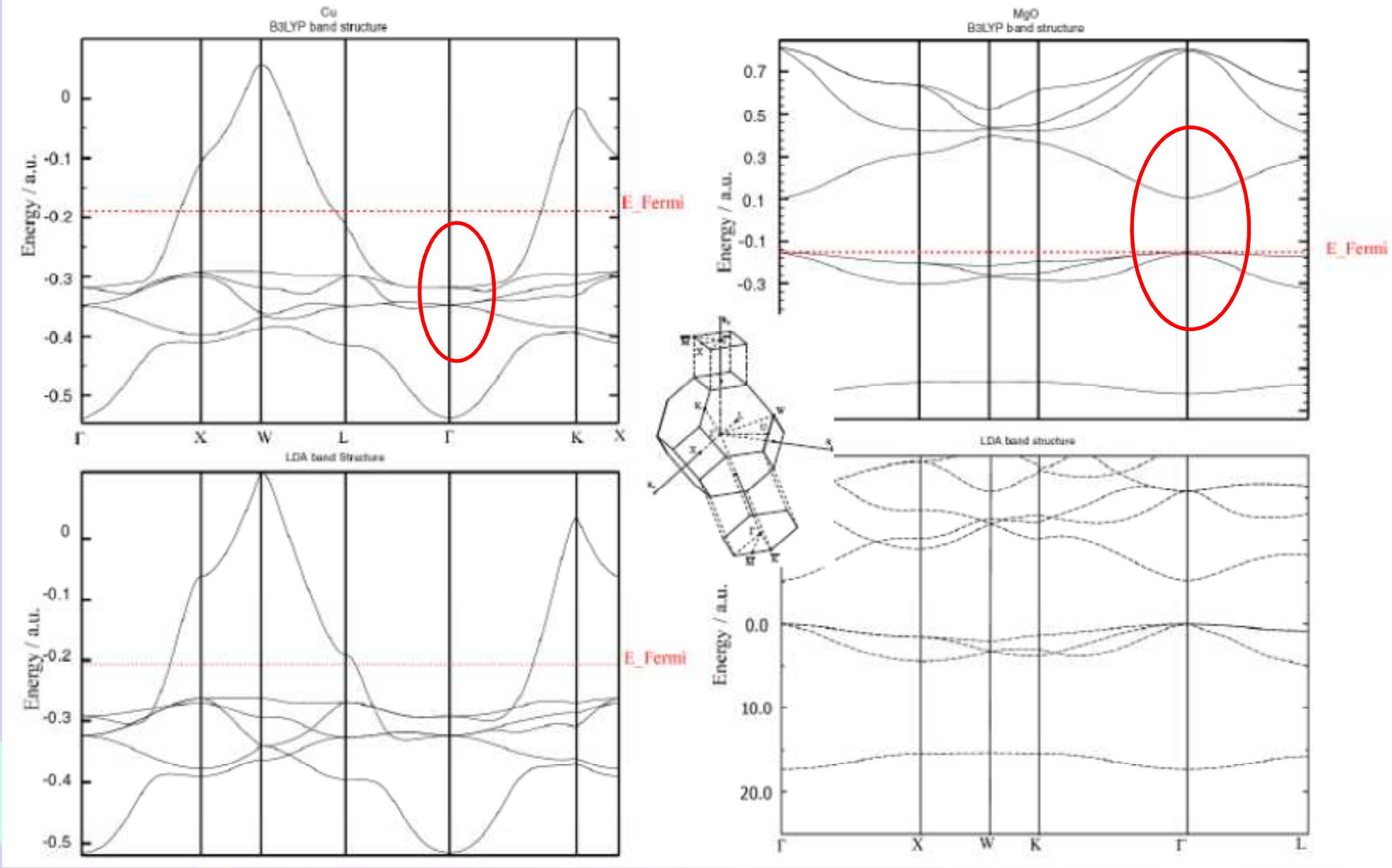
Insulator

• Low conductivity



Semiconductor

• Switches from conducting to insulating at will


Cu
B3LYP band structure
Energy / a.u.
0
-0.1
-0.2
-0.3
-0.4
-0.5
E_Fermi
Γ
X
W
L
Γ
K
X
LDA band Structure
Energy / a.u.
0
-0.1
-0.2
-0.3
-0.4
-0.5
E_Fermi
MgO
B3LYP band structure
Energy / a.u.
0.7
0.5
0.3
0.1
-0.1
-0.3
E_Fermi
LDA band structure
Energy / a.u.
0.0
10.0
20.0
Γ
X
W
K
Γ
L

k·p Theory

How do we calculate realistic band diagrams?

- Tight-binding
- Pseudopotentials
- k·p theory

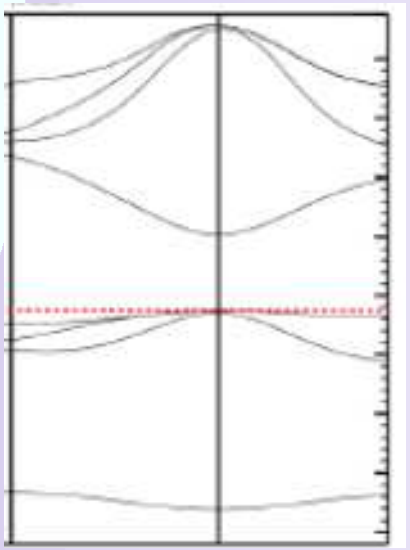
$$\hat{H} = \left(\frac{\vec{p}^2}{2m} + V_c(\vec{r}) \right) \qquad \Psi_k(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_k(\vec{r})$$

$$e^{-i\vec{k}\vec{r}}\, \hat{H}\, \Psi_k(\vec{r}) = \varepsilon_k\, e^{-i\vec{k}\vec{r}}\, \Psi_k(\vec{r})$$

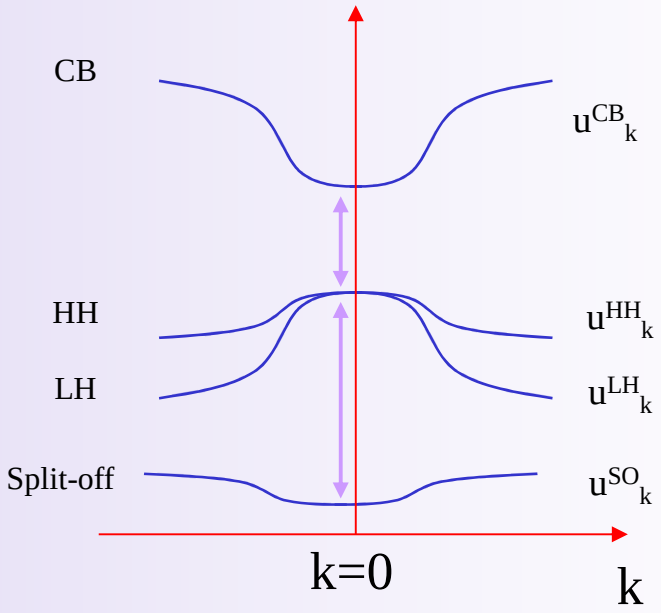
$$\left(\frac{\vec{p}^2}{2m} + V_c(\vec{r}) + \frac{\hbar^2 k^2}{2m} + \hbar \frac{\vec{k}\cdot\vec{p}}{m} \right) u_k(\vec{r}) = \varepsilon_k\, u_k(\vec{r})$$

The k·p Hamiltonian

MgO



k=Γ



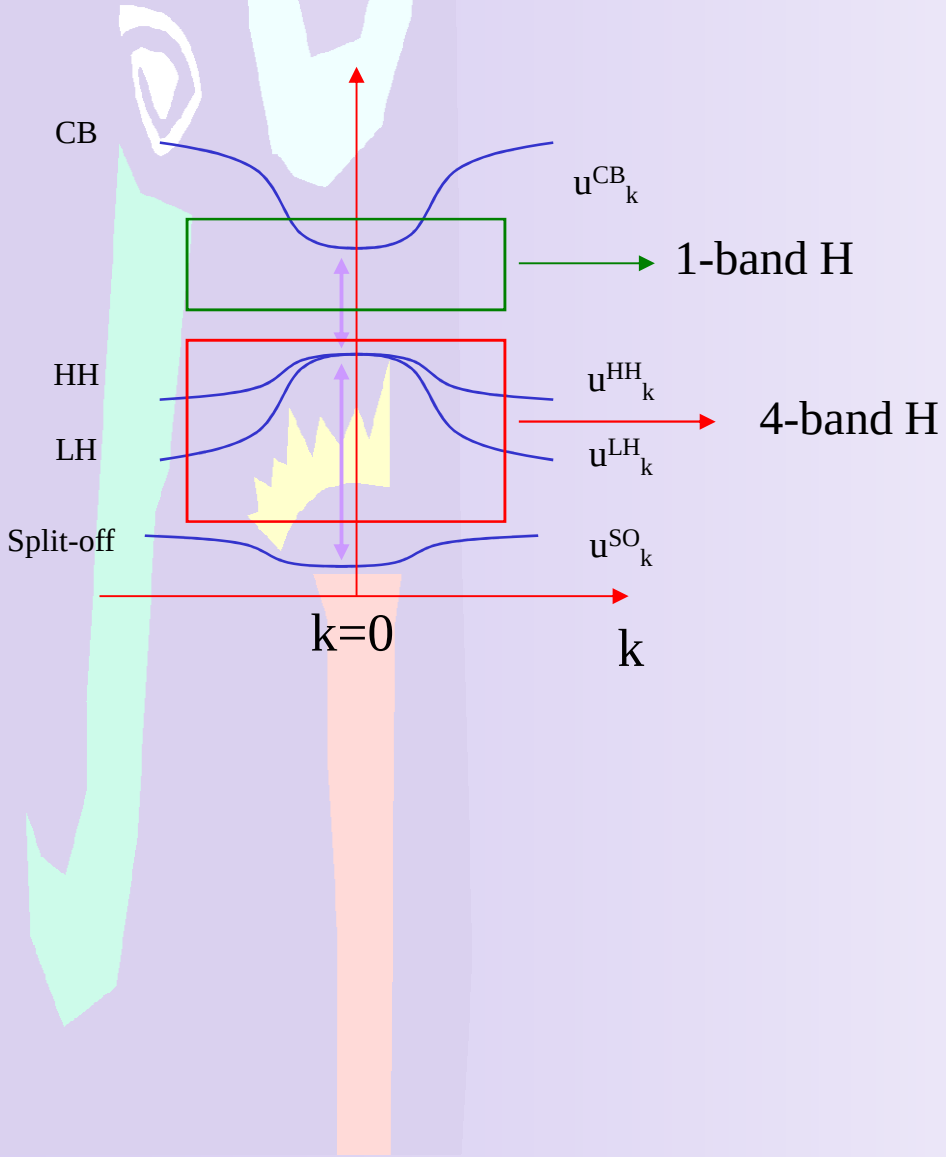
$$\left(\frac{\vec{p}^2}{2m}+V_c(\vec{r})+\frac{\hbar^2 k^2}{2m}+\hbar\frac{\vec{k}\cdot\vec{p}}{m}\right)u_k^n(\vec{r})=\varepsilon_k^n u_k^n(\vec{r})$$

$$u_k^n(\vec{r})=\sum_{n'}^{\infty}c_{n'k}\,u_0^{n'}(\vec{r})$$

$$\left\langle u_0^n\left|\hat{H}_{kp}\right|u_0^{n'}\right\rangle=\left(\varepsilon_0^n+\frac{\hbar^2|\vec{k}|^2}{2m}\right)\delta_{n,n'}+\hbar\frac{\vec{k}}{m}\left\langle u_0^n\left|\vec{p}\right|u_0^{n'}\right\rangle$$

Kane parameter

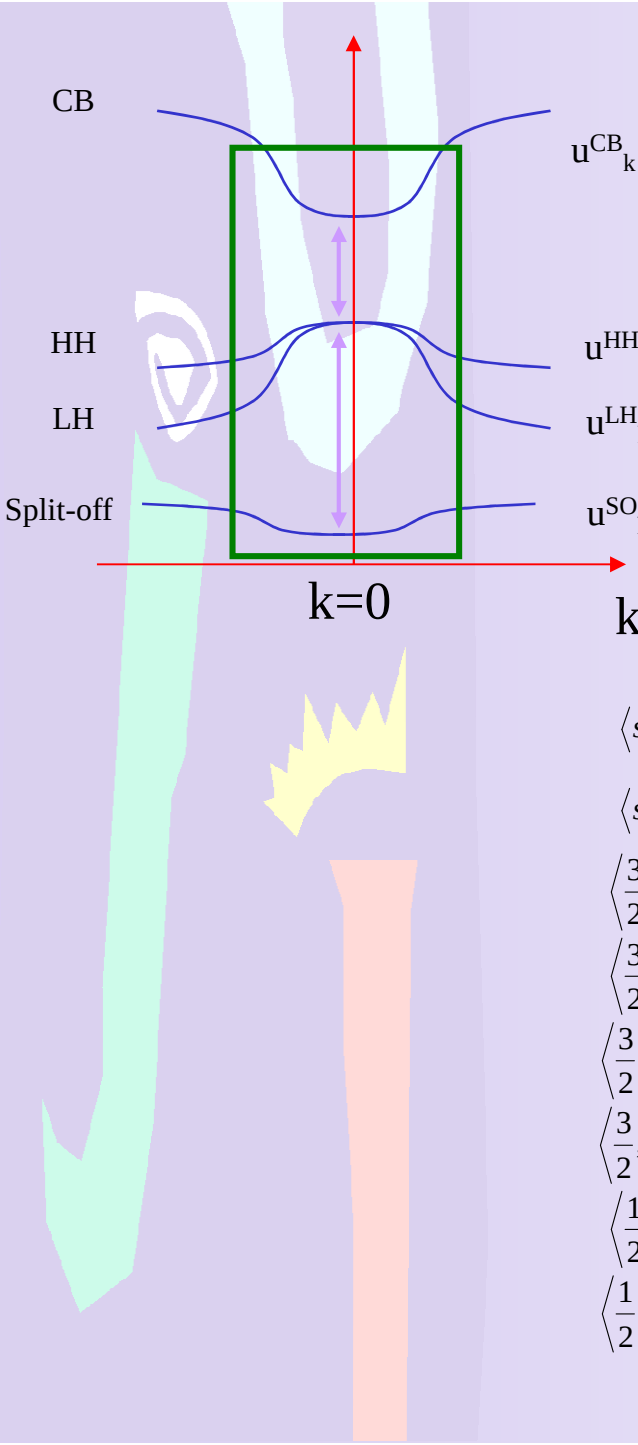
$$\left\langle u_0^n \left| \hat{H}_{kp} \right| u_0^{n'} \right\rangle = \left(\varepsilon_0^n + \frac{\hbar^2 |\vec{k}|^2}{2m} \right) \delta_{n,n'} + \hbar \frac{\vec{k}}{m} \left\langle u_0^n \left| \vec{p} \right| u_0^{n'} \right\rangle$$



$$u_k^n(\vec{r}) = \sum_n^{\infty} c_{nk}\, u_0^n(\vec{r})$$

1-band H

	$\lvert s\uparrow\rangle$	$\lvert s\downarrow\rangle$
$\lvert s\uparrow\rangle$	$\frac{k^2}{2m}$	0
$\lvert s\downarrow\rangle$	0	$\frac{k^2}{2m}$



8-band H

	$\left\|s\uparrow\right\rangle$	$\left\|s\downarrow\right\rangle$	$\left\|\frac{3}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{3}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{3}{2},\frac{-1}{2}\right\rangle$	$\left\|\frac{3}{2},\frac{-3}{2}\right\rangle$	$\left\|\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{1}{2},\frac{-1}{2}\right\rangle$
$\left\langle s\uparrow\right\|$	$\frac{k^2}{2m}$	0	Pk_+	$-\sqrt{\frac{2}{3}}Pk_z$	$-\sqrt{\frac{1}{3}}Pk_-$	0	$\sqrt{\frac{1}{3}}Pk_z$	$-\sqrt{\frac{2}{3}}Pk_-$
$\left\langle s\downarrow\right\|$	0	$\frac{k^2}{2m}$	0	$\sqrt{\frac{1}{3}}Pk_-$	$-\sqrt{\frac{2}{3}}Pk_z$	Pk_-	$\sqrt{\frac{2}{3}}Pk_-$	$\sqrt{\frac{1}{3}}Pk_z$
$\left\langle\frac{3}{2},\frac{3}{2}\right\|$	Pk_+	0	$-\varepsilon_0+\frac{k^2}{2m}$	0	0	0	0	0
$\left\langle\frac{3}{2},\frac{1}{2}\right\|$	$-\sqrt{\frac{2}{3}}Pk_z$	$\sqrt{\frac{1}{3}}Pk_-$	0	$-\varepsilon_0+\frac{k^2}{2m}$	0	0	0	0
$\left\langle\frac{3}{2},\frac{-1}{2}\right\|$	$-\sqrt{\frac{1}{3}}Pk_-$	$-\sqrt{\frac{2}{3}}Pk_z$	0	0	$-\varepsilon_0+\frac{k^2}{2m}$	0	0	0
$\left\langle\frac{3}{2},\frac{-3}{2}\right\|$	0	Pk_-	0	0	0	$-\varepsilon_0+\frac{k^2}{2m}$	0	0
$\left\langle\frac{1}{2},\frac{1}{2}\right\|$	$\sqrt{\frac{1}{3}}Pk_z$	$\sqrt{\frac{2}{3}}Pk_-$	0	0	0	0	$-\varepsilon_0-\Delta+\frac{k^2}{2m}$	0
$\left\langle\frac{1}{2},\frac{-1}{2}\right\|$	$-\sqrt{\frac{2}{3}}Pk_-$	$\sqrt{\frac{1}{3}}Pk_z$	0	0	0	0	0	$-\varepsilon_0-\Delta+\frac{k^2}{2m}$

One-band Hamiltonian for the conduction band

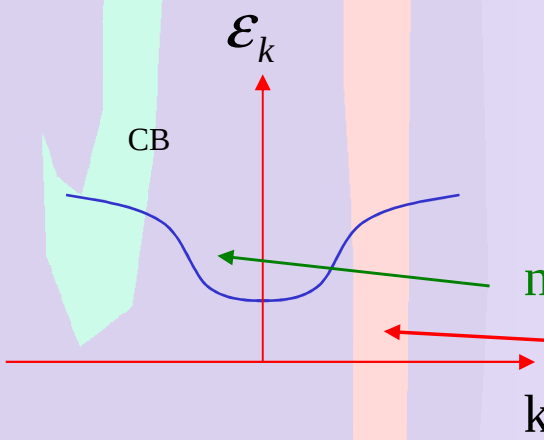
$$\left\langle u_0^n \left| \hat{H}_{kp} \right| u_0^{n'} \right\rangle = \left(\varepsilon_0^n + \frac{\hbar^2 |\vec{k}|^2}{2m} \right) \delta_{n,n'} + \hbar \frac{\vec{k}}{m} \left\langle u_0^n \left| \vec{p} \right| u_0^{n'} \right\rangle$$

$$\varepsilon_k^{cb} = \varepsilon_0^{cb} + \frac{\hbar^2 |\vec{k}|^2}{2m}$$

This is a crude approximation... Let's include remote bands perturbationally

$$\varepsilon_k^{cb} = \varepsilon_0^{cb} + \sum_{\alpha=x,y,z} \frac{\hbar^2 |k_\alpha|^2}{2m} + \frac{\hbar^2}{m^2} |k_\alpha|^2 \sum_{n \neq cb} \frac{\left| \left\langle u_0^{cb} \left| p_\alpha \right| u_0^n \right\rangle \right|^2}{\varepsilon_0^{cb} - \varepsilon_0^n}$$

1/m*



Free electron m=1 a.u.

InAs m*=0.025 a.u.

negative mass?

Effective mass

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial \varepsilon_k^{cb}}{\partial k^2}$$

$$\varepsilon_k^{cb} = \varepsilon_0^{cb} + \frac{\hbar^2 k_\alpha^2}{2m_\alpha^*}$$

Theory of invariants

1. Perturbation theory becomes more complex for many-band models

2. Nobody calculate the huge amount of integrals involved

$\Rightarrow$ grup them and **fit to experiment**

Alternative (**simpler and deeper**) to perturbation theory:

Determine the Hamiltonian H by **symmetry** considerations

Theory of invariants (basic ideas)

1. Second order perturbation: H second order in k: $H = \sum_{i \geq j}^{3} M_{ij} k_i k_j$

2. H must be an invariant under point symmetry (T_d ZnBl, D_{6h} wurtzite)

A·B is invariant (A_1 symmetry) if A and B are of the same symmetry

e.g. (x, y, z) basis of T_2 of T_d: $x \cdot x + y \cdot y + z \cdot z = r^2$ basis of A_1 of T_d

Theory of invariants (machinery)

1. **k** basis of T_2

2. $k_i\, k_j$ basis of $T_2 \otimes T_2 = A_1 \oplus E \oplus T_2 \oplus [T_1]$

3. Character Table:

$$A_1 \rightarrow k_x^2 + k_y^2 + k_z^2$$
$$E \rightarrow \left\{2k_z^2 - k_x^2 - k_y^2, k_x^2 - k_y^2\right\}$$
$$T_2 \rightarrow \left\{k_x k_y, k_x k_z, k_y k_z\right\}$$
$$T_1 \rightarrow NO\ (k_i k_j\ \textit{symmetric tensor})$$

notation: elements of these basis: k_i^{Γ} .

4. Invariant: sum of invariants: $H = \sum_i^{\dim(\Gamma)} \sum_{\Gamma} a_{\Gamma} N_i^{\Gamma} k_i^{\Gamma}$

irrep

basis element

fitting parameter

(not determined by symmetry)

Machinery (cont.)

How can we determine the N_i^Γ matrices?

$$(J_x, J_y, J_z) \ basis\ of\ T_1, \quad and \quad T_2 \otimes T_2 = T_1 \otimes T_1$$

→ **we can use symmetry-adapted J_iJ_j products**

<u>Example</u>: 4-th band model: $\{|3/2,3/2>,|3/2,1/2>,|3/2,-1/2>,|3/2,-3/2>\}$

$$\mathbb{J}_x = \begin{bmatrix} 0 & \sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \end{bmatrix}$$

$$\mathbb{J}_z = \begin{bmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{bmatrix}$$

$$\mathbb{J}_y = \begin{bmatrix} 0 & -i\sqrt{3}/2 & 0 & 0 \\ i\sqrt{3}/2 & 0 & -i & 0 \\ 0 & i & 0 & -i\sqrt{3}/2 \\ 0 & 0 & i\sqrt{3}/2 & 0 \end{bmatrix}$$

$$\mathbb{J}^2 = \tfrac{3}{2}(\tfrac{3}{2}+1)\mathbb{I}_{4x4} = \tfrac{15}{4}\mathbb{I}_{4x4}$$

$$\{\mathbb{J}_x, \mathbb{J}_y\} = \tfrac{1}{2}(\mathbb{J}_x\mathbb{J}_y + \mathbb{J}_y\mathbb{J}_x)$$

$\mathbb{J}_x^2$ $\mathbb{J}_y^2$ $\mathbb{J}_z^2$

Machinery (cont.)

We form the following invariants

$$A_1: \quad X_{A_1} = \mathbb{I} \cdot (k_x^2 + k_y^2 + k_z^2) = k^2 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} k^2 & 0 & 0 & 0 \\ 0 & k^2 & 0 & 0 \\ 0 & 0 & k^2 & 0 \\ 0 & 0 & 0 & k^2 \end{bmatrix}$$

$$E: \quad X_E = \frac{1}{\sqrt{6}}(2\mathbb{J}_z^2 - \mathbb{J}_y^2 - \mathbb{J}_x^2)\frac{1}{\sqrt{6}}(2k_z^2 - k_y^2 - k_x^2) + \frac{1}{\sqrt{2}}(\mathbb{J}_x^2 - \mathbb{J}_y^2)\frac{1}{\sqrt{2}}(k_x^2 - k_y^2)$$

$$T_2: \quad X_{T_2} = \frac{1}{2}(\mathbb{J}_x\mathbb{J}_y + \mathbb{J}_y\mathbb{J}_x)k_xk_y + \frac{1}{2}(\mathbb{J}_y\mathbb{J}_z + \mathbb{J}_z\mathbb{J}_y)k_yk_z + \frac{1}{2}(\mathbb{J}_z\mathbb{J}_x + \mathbb{J}_x\mathbb{J}_z)k_zk_x$$

Finally we build the Hamiltonian

$$\mathbb{H} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1 + \frac{5}{2}\gamma_2)X_{A_1} - 2\gamma_2 X_E + 4\gamma_3 X_{T_2}\right]$$

Luttinger parameters: determined by fitting

Four band Hamiltonian:

$$\mathbb{H} = -\frac{\hbar^2}{2m_0}\begin{bmatrix} \gamma_1 k^2 + \gamma_2(k_x^2 + k_y^2 - 2k_z^2) & -2\sqrt{3}\gamma_3 k_z(k_x - i\,k_y) & -\sqrt{3}\gamma_2(k_x^2 - k_y^2) + 2\,i\,\sqrt{3}\,\gamma_3\,k_x k_y & 0 \\ -2\sqrt{3}\gamma_3 k_z(k_x + i\,k_y) & \gamma_1 k^2 - \gamma_2(k_x^2 + k_y^2 - 2k_z^2) & 0 & -\sqrt{3}\gamma_2(k_x^2 - k_y^2) + 2\,i\,\sqrt{3}\,\gamma_3\,k_x k_y \\ -\sqrt{3}\gamma_2(k_x^2 - k_y^2) - 2\,i\,\sqrt{3}\,\gamma_3\,k_x k_y & 0 & \gamma_1 k^2 - \gamma_2(k_x^2 + k_y^2 - 2k_z^2) & 2\sqrt{3}\gamma_3 k_z(k_x - i\,k_y) \\ 0 & -\sqrt{3}\gamma_2(k_x^2 - k_y^2) - 2\,i\,\sqrt{3}\,\gamma_3\,k_x k_y & 2\sqrt{3}\gamma_3 k_z(k_x + i\,k_y) & \gamma_1 k^2 + \gamma_2(k_x^2 + k_y^2 - 2k_z^2) \end{bmatrix}$$

Exercise: Show that the 2-bands {|1/2,1/2>,|1/2,-1/2>} conduction band k·p Hamiltonian reads H= $a\,k^2\,\mathbf{I}$, where **I** is the 2x2 unit matrix, k the modulus of the linear momentum and *a* is a fitting parameter (that we cannot fix by symmetry considerations)

Hints: 1. $T_2 \otimes T_2 = T_1 \otimes T_1 = A_1 \oplus E \oplus T_2 \oplus [T_1]$

2. Angular momentum components in the ±1/2 basis: S_i=1/2 σ_i, with

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

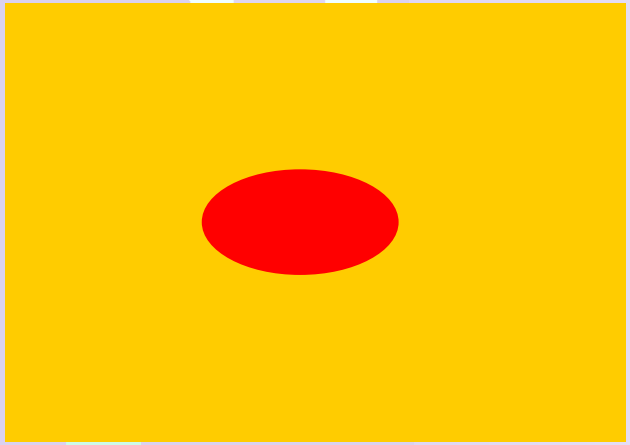
3. Character tables and basis of irreps

Character table for T_d point group

	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear, rotations	quadratic
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2-x^2-y^2, x^2-y^2)$
T_1	3	0	-1	1	-1	(L_x, L_y, L_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

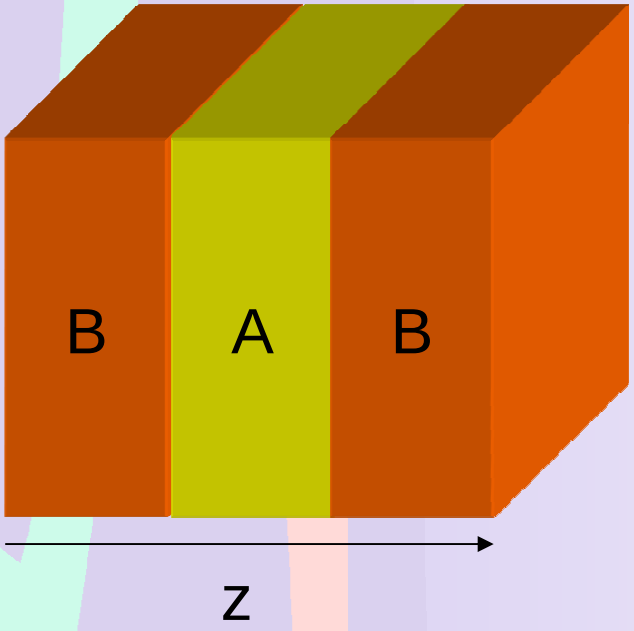
$$A_1 \rightarrow k_x^2 + k_y^2 + k_z^2$$
$$E \rightarrow \left\{2k_z^2 - k_x^2 - k_y^2, k_x^2 - k_y^2\right\}$$
$$T_2 \rightarrow \left\{k_x k_y + k_y k_x, k_x k_z + k_z k_x, k_y k_z + k_z k_y\right\}$$
$$T_1 \rightarrow \left\{k_x k'_y - k_y k'_x, k_x k'_z - k_z k'_x, k_y k'_z - k_z k'_y\right\}$$

Heterostructures

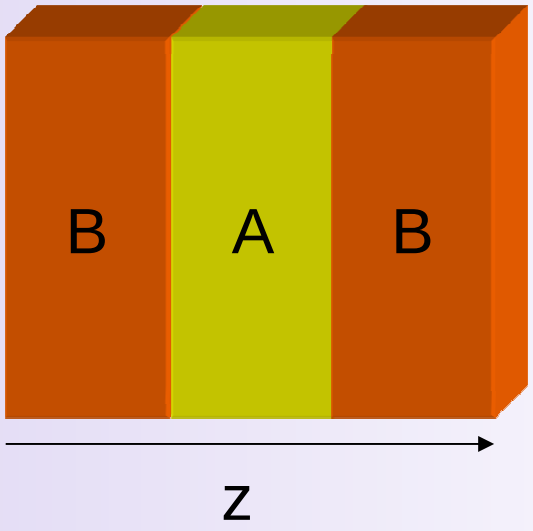


Brocken translational symmetry

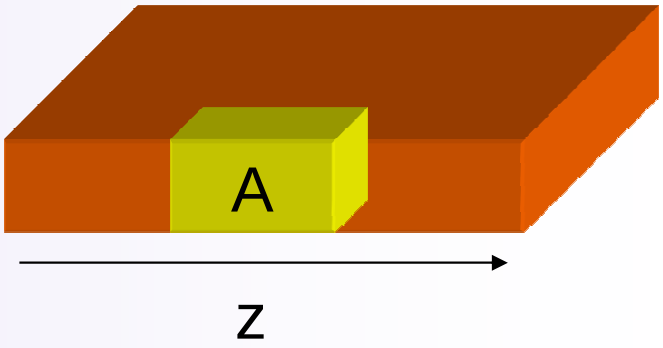
How do we study this?



quantum well

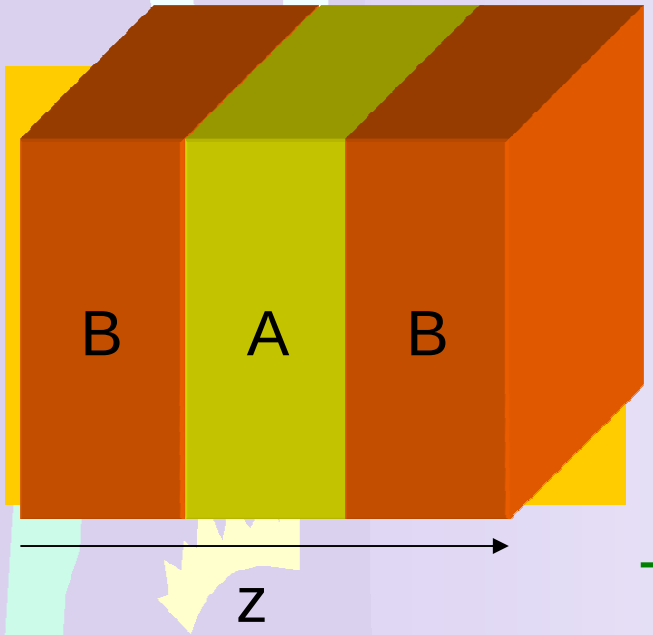


quantum wire



quantum dot

Heterostructures



How do we study this?

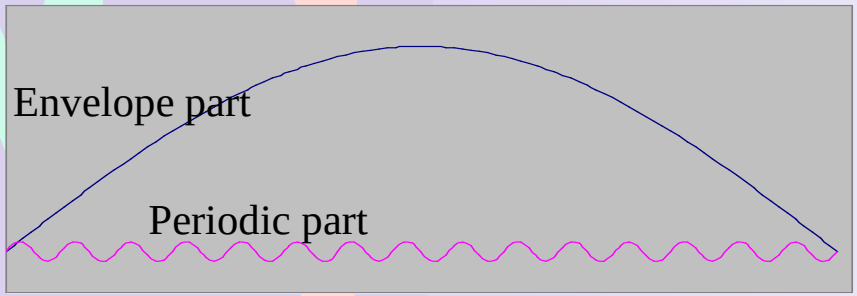
If A and B have:
- the same crystal structure
- similar lattice constants
- no interface defects

...we use the “envelope function approach”

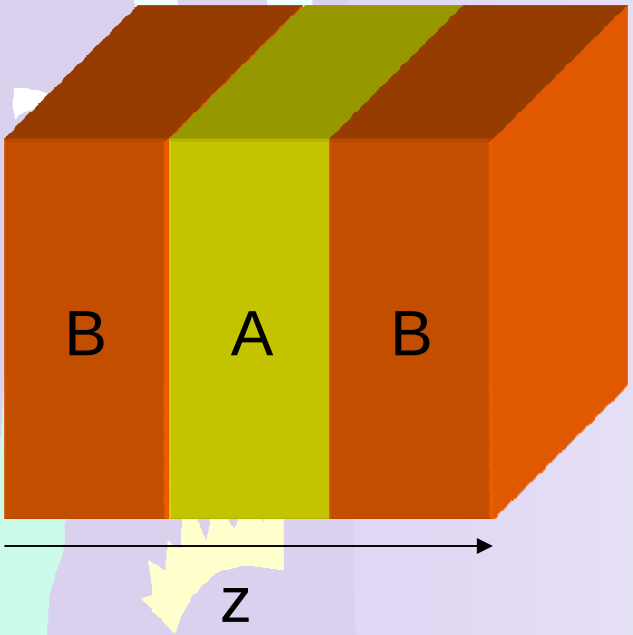
$$\Psi_k(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_k(\vec{r}) \rightarrow \Psi_k(\vec{r}) = e^{i\vec{k}_\perp \vec{r}_\perp}\, \chi(z)\, u_k(\vec{r})$$

Project H_{kp} onto $\{\Psi_{nk}\}$, considering that:

$$\int_\Omega f(r)\, u_{nk}(r)\, dr \approx \frac{1}{\Omega} \int_{unit\,cell} u_{nk}(r)\, dr \cdot \int_\Omega f(r)\, dr \cdot$$

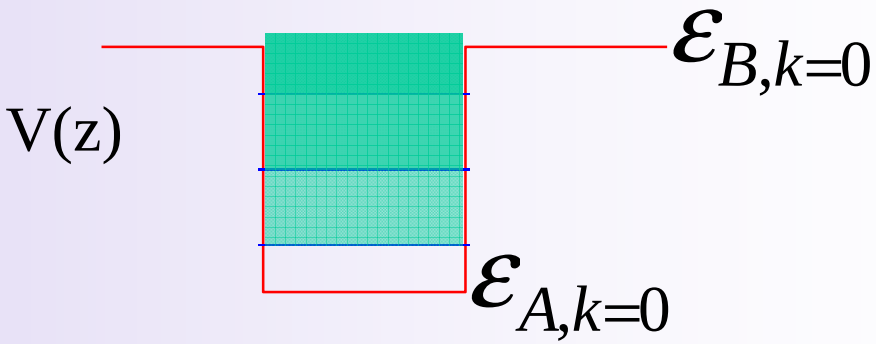


Heterostructures



In a one-band model we finally obtain:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V(z)+\frac{\hbar^2 k_\perp^2}{2m}\right)\chi(z)=\varepsilon\,\chi(z)$$



1D potential well: particle-in-the-box problem

Quantum well

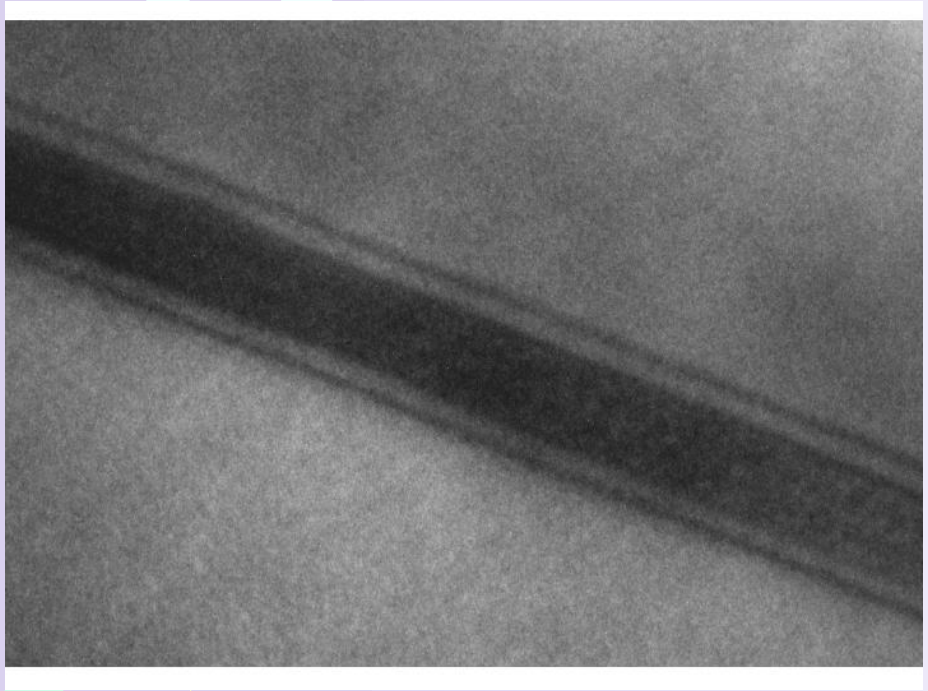


Image: CNRS France

Most prominent applications:

- Laser diodes
- LEDs
- Infrared photodetectors

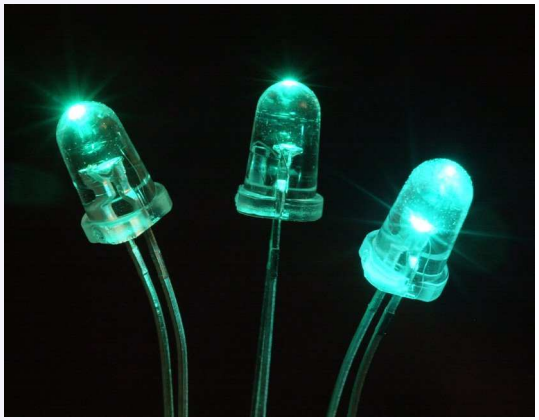
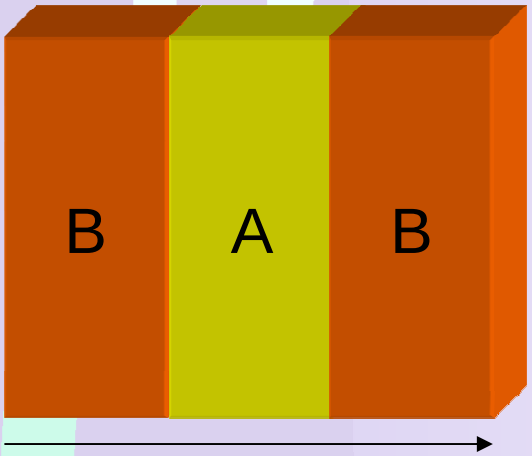


Image: C. Humphrey, Cambridge

Quantum well



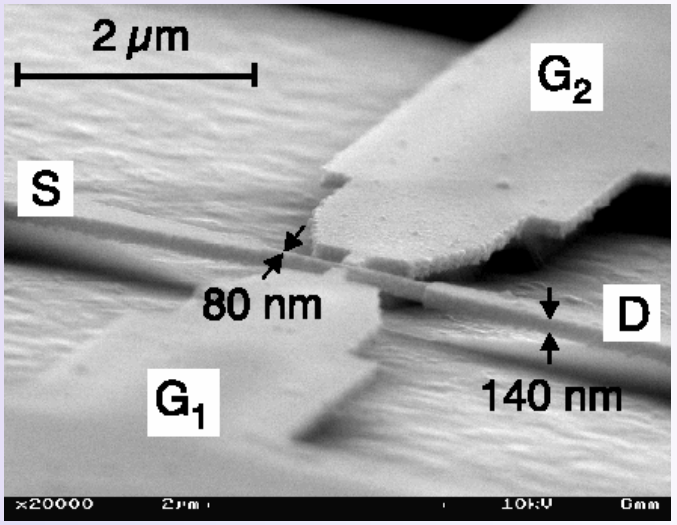
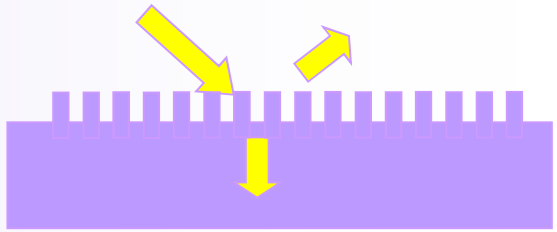
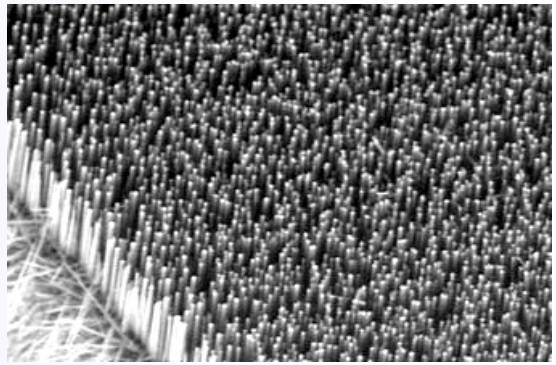


Image: U. Muenchen

$$\left(-\frac{\hbar^2}{2m}(\nabla_y^2+\nabla_z^2)+V(y,z)+\frac{\hbar^2 k_x^2}{2m}\right)\chi(y,z)=\varepsilon\,\chi(y,z)$$

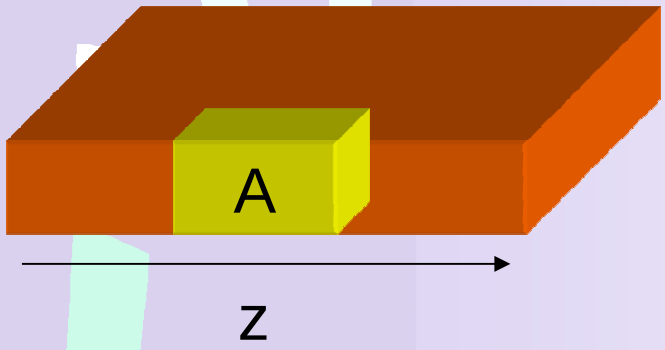


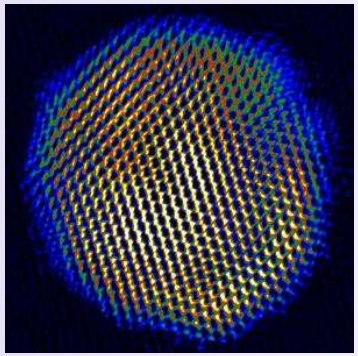


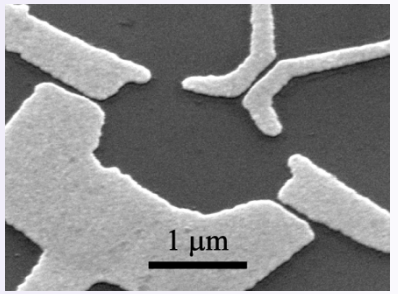
Most prominent applications:

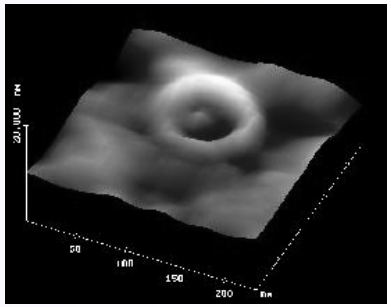
- Transport
- Photovoltaic devices

Quantum wire

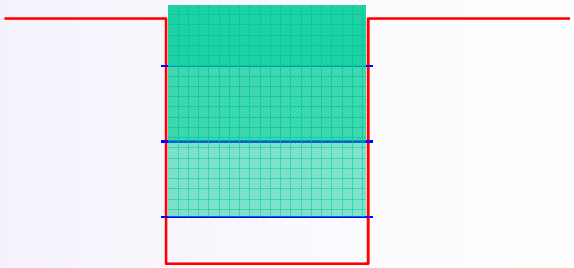








$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right)\chi(x,y,z) = \varepsilon\,\chi(x,y,z)$$



Most prominent applications:

- Single electron transistor
- In-vivo imaging
- Photovoltaics
- LEDs
- Cancer therapy
- Memory devices
- Qubits?

Quantum dot

SUMMARY (keywords)

Lattice → **Wigner-Seitz unit cell**

Periodicity → **Translation group** → **wave-function in Block form**

Reciprocal lattice → **k-labels within the 1rst Brillouin zone**

Schrodinger equation → **BCs depending on k; bands E(k); gaps**

Gaps → **metal, isolators and semiconductors**

Machinery: kp Theory → effective mass **J character table**

Theory of invariants: $\Gamma \otimes \Gamma \ni A_1$; $H = \sum N_i^{\Gamma} k_i^{\Gamma}$

Heterostructures: EFA

$$k \rightarrow \hat{p} = -i\nabla$$

$$confinement \rightarrow V_c = band\ \ offset$$

QWell QWire QDot