Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.14 Lecture 02

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Review of last week

Chapter 1 Crystal structure and crystal growth

Crystal structure

- Basis, primitive cell, unit cell
- Lattice, Bravais lattice
- Reciprocal lattice
- Brillouin zone

Semiconductor materials

- Group IV: C, Si, Ge, Sn, SiC, Si_xGe_{1-x}
- Group III-V: GaAs, InP, AlAs, InAs, GaSb, …
- III-N: GaN, InN, …
- Group II-VI: CdTe, HgTe, …

Crystal growth

Bulk

- Czochralski
- Bridgman
- Floating zone

Thin film

- MOCVD
- MBE

Chapter 2 Energy bands, effective mass approximation

Nearly free electron model, empty lattice approximation

Tight-binding approximation (TBA)

Single atom on single unit cell

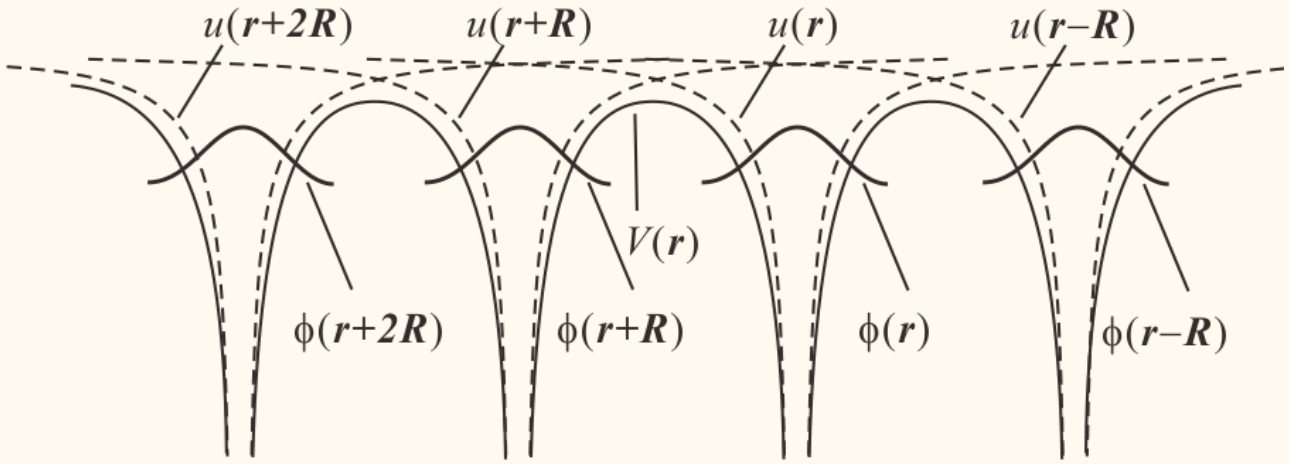
Single atom Hamiltonian: $\mathscr{H}_a = \hat{T} + u$

$\hat{T}$: kinetic energy, u: atomic potential

$$\mathscr{H}_a(R_i) = \hat{T} + u(r - R_i)$$

$$\mathscr{H}_a(R_i)\phi_n(r - R_i) = \epsilon_n \phi_n(r - R_i)$$

ϕ_n: eigenfunctions for $R_i = 0$



$$\psi_{nk}(r) = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} \phi_n(r - R_i)$$

$$= \frac{e^{ikr}}{\sqrt{N}} \left[\sum_i e^{-ik(r-R_i)} \phi_n(r - R_i) \right]$$

Lattice periodic function

: Bloch form

$$\mathscr{H} = [\hat{T}_x + V(x)]\psi(x) = E\psi(x)$$

Tight binding approximation (2)

$$\langle\psi_{nk}|\mathscr{H}|\psi_{nk}\rangle = N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\langle\phi_n(r-R_i)|[\hat{T}_r+V(r)]|\phi_n(r-R_j)\rangle$$

$$= N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}$$

$$\times\langle\phi_n(r-R_i)|[\hat{T}_r+u(r-R_i)+V(r)-u(r-R_i)]|\phi_n(r-R_j)\rangle$$

$$= \epsilon_n + N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\langle\phi_n(r-R_i)|[V(r)-u(r-R_i))]|\phi_n(r-R_j)\rangle$$

$$= \epsilon_n + \sum_{j} e^{ikR_j}\langle\phi_n(r)|[V(r)-u(r))]|\phi_n(r-R_j)\rangle.$$

$$E_n(k) = \epsilon_n + \langle\phi_n(r)|v(r)|\phi_n(r)\rangle - \sum_{R_j\neq 0} e^{ikR_j}t_n(R_j)$$

$\alpha_n \equiv -\langle\phi_n(r)|v(r)|\phi_n(r)\rangle$ Crystal field contribution

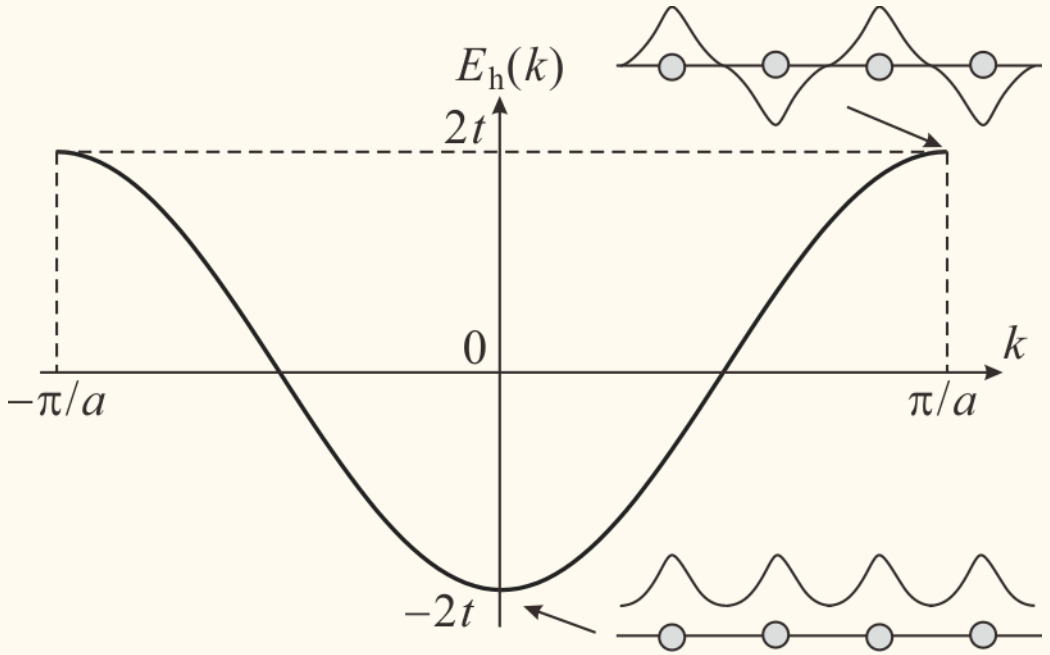
$t_n(R_j) \equiv -\langle\phi_n(r)|v(r)|\phi_n(r-R_j)\rangle$ Hopping integral

Tight binding approximation (3)

t_n nearest neighbor only = t

$$E_n(k) = \epsilon_n - \alpha_n - t(e^{ika} + e^{-ika})$$
$$= \epsilon_n - \alpha_n - 2t\cos ka$$

Cosine band with the width of $4t$.



Methods for obtaining band structure

Experiments

- Hot electron transport
- Optical absorption
- Electroreflectance
- Cyclotron resonance
- Photoemission spectroscopy

Empirical calculation

- Pseudo-potential approximation
- $k \cdot p$ perturbation

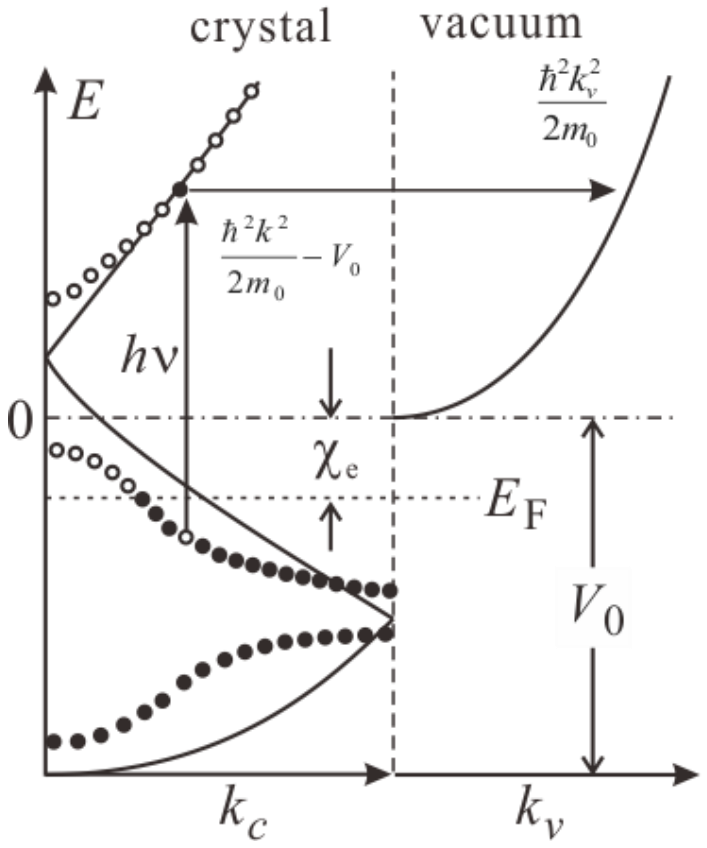
ab-initio calculation

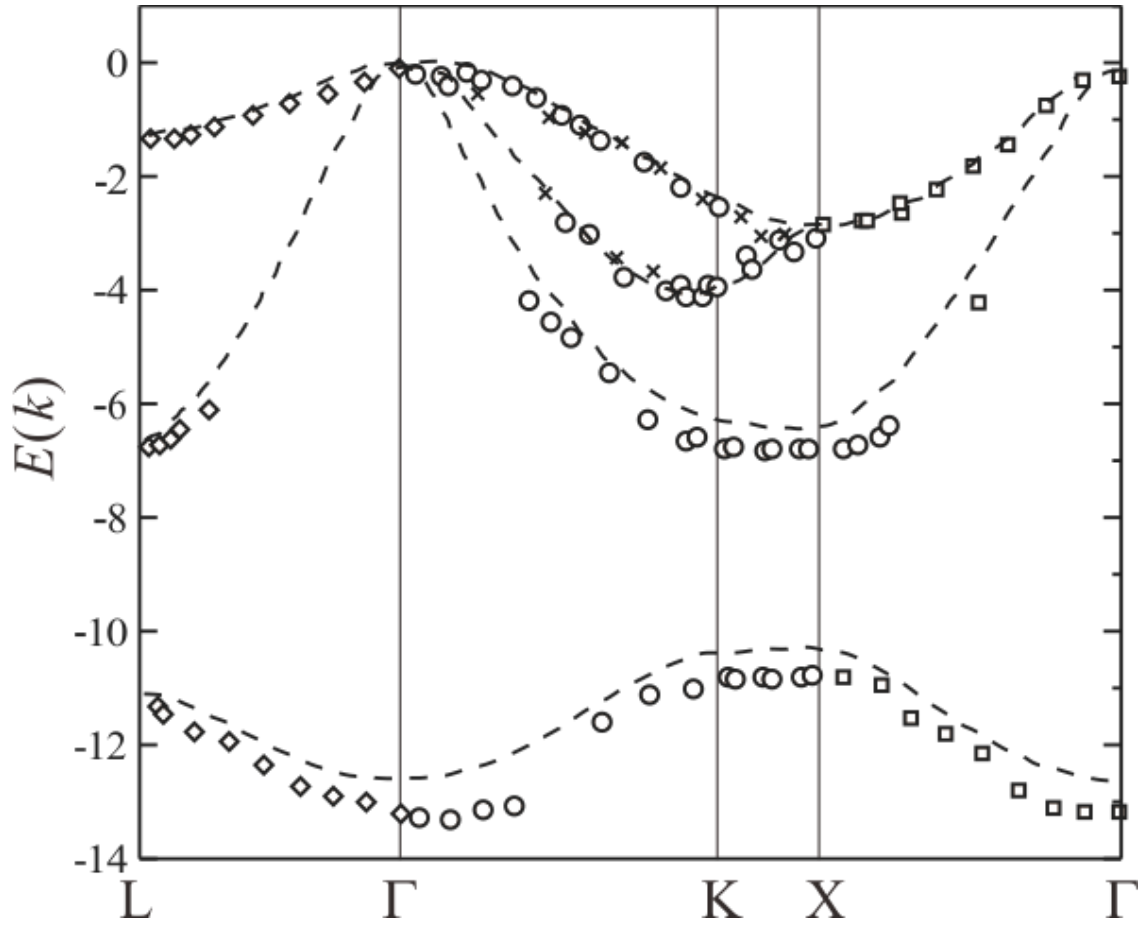
- Local density approximation
- Augmented plane wave
- Generalized gradient approximation

Angle resolved photoemission spectroscopy (ARPES)

$$h\nu = E_c(\boldsymbol{k}_c) - E_v(\boldsymbol{k}_v)$$

$$\hbar k_{\parallel} = \sqrt{2m_0(E_e + h\nu - \chi_e)}\sin\theta,$$
$$\hbar k_{\perp} = \sqrt{2m_0[(E_e + h\nu - \chi_e)\cos^2\theta - V_0]}$$



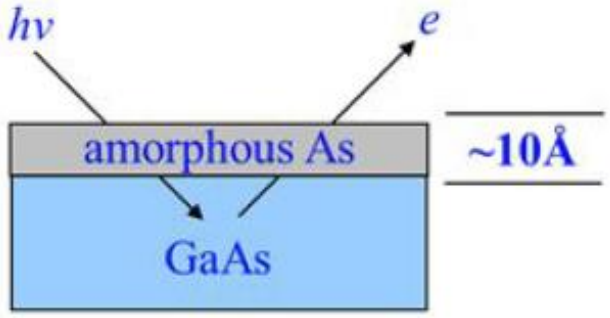


GaAs

T. C. Chang *et al.* Phys. Rev. B**21**, 3513 (1980).

see, e.g. for short review B. Lv, T. Qian, H. Ding, Nature Reviews Physics **1**, 609 (2019).

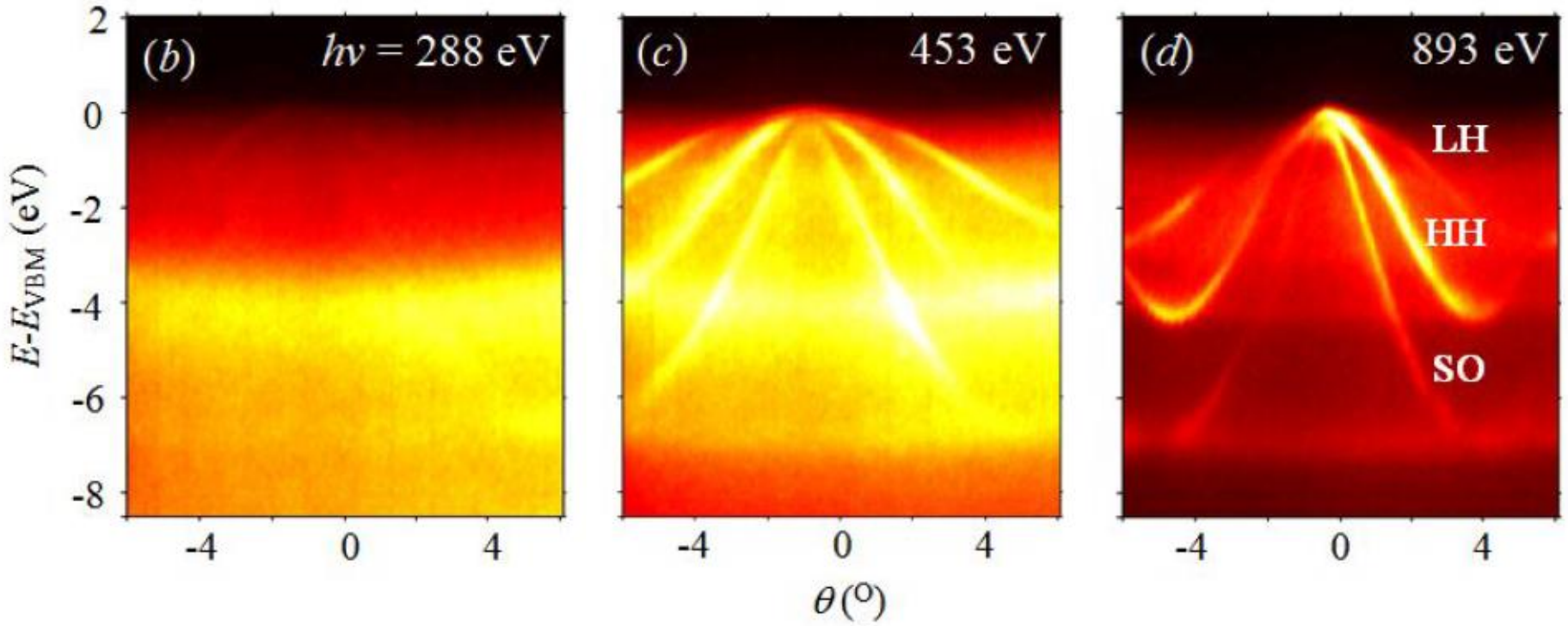
Angle resolved photoemission spectroscopy (ARPES) (2)



Soft-X ray ARPES of GaAs

Bands below Fermi energy can be detected

Strocov *et al.*, J. Electron Spectroscopy and Related Phenomena **236**, 1 (2019).



Plane wave expansion

Crystal Schrodinger equation:

$$\mathscr{H}\psi(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \tag{1}$$

Bloch function (omit band index)

$$\psi(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r}) \tag{2}$$

Fourier expansion
(∵ lattice periodicity)

$$V(\boldsymbol{r}) = \sum_{\boldsymbol{G}} V_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}, \quad u_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} C_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} \tag{3}$$

(2), (3) → (1)

$$\sum_{\boldsymbol{G}}\left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E\right\}C_{\boldsymbol{G}} + \sum_{\boldsymbol{G}'} V_{\boldsymbol{G}-\boldsymbol{G}'}C_{\boldsymbol{G}'}\right]e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}} = 0 \tag{4}$$

Each term in the sum over $\boldsymbol{G}$ is zero in (4)

$$\sum_{\boldsymbol{G}'}\left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E\right\}\delta_{\boldsymbol{G}\boldsymbol{G}'} + V_{\boldsymbol{G}-\boldsymbol{G}'}\right]C_{\boldsymbol{G}'} = 0 \tag{5}$$

For (5) to have non-trivial solution

$$\left|\left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E\right\}\delta_{\boldsymbol{G}\boldsymbol{G}'} + V_{\boldsymbol{G}-\boldsymbol{G}'}\right]_{\boldsymbol{G}\boldsymbol{G}'}\right| = 0$$

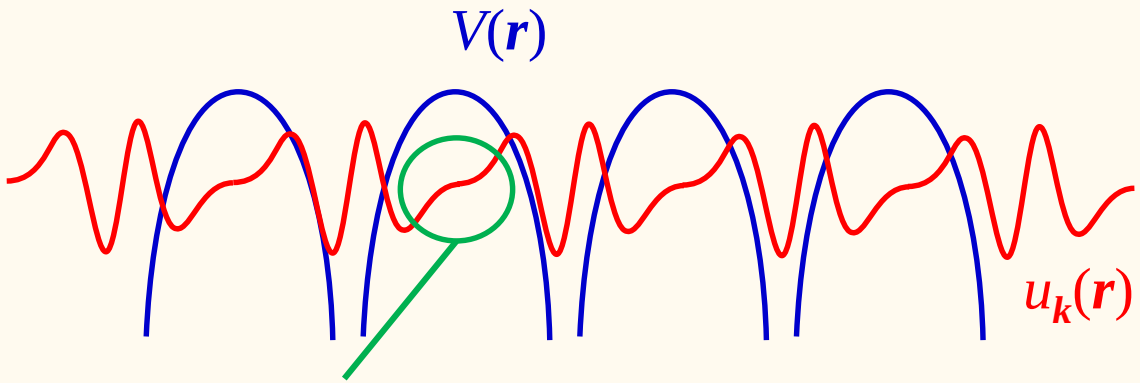
Pseudo-potential calculation method

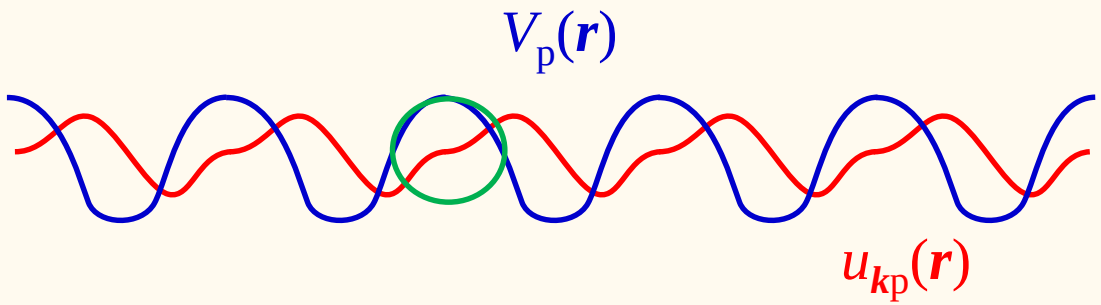
$$\left| \left[\left\{ \frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E \right\} \delta_{\boldsymbol{G}\boldsymbol{G}'} + V_{\boldsymbol{G}-\boldsymbol{G}'} \right]_{\boldsymbol{G}\boldsymbol{G}'} \right| = 0$$

→ We need $V_{\boldsymbol{G}}$

Pseudo potential method:

1. Only consider valence bands and conduction bands around the Fermi level. Effect of core electrons in renormalized into periodic potential.
2. Replace real potential with pseudo potential which gives similar tailing of wavefunction.





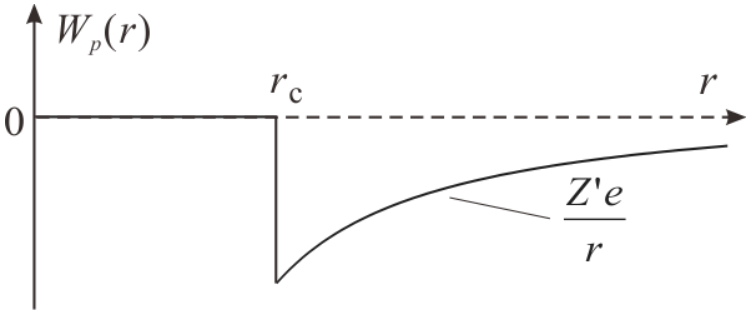
band structure: almost determined in skirt characteristics

Pseudo potential calculation method (2)

Replacement with pseudo potential

$$V(r) = -\frac{Ze}{r} \Rightarrow W_p(r) = \begin{cases} 0 & (r < r_c) \\ -\dfrac{Z'e}{r} & (r \geq r_c) \end{cases}$$

simplest example



Crystal pseudo potential

$$V_p(\boldsymbol{r}) = \sum_{j,\alpha} W_p^{\alpha}(\boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{\tau}_\alpha)$$

$\boldsymbol{\tau}_\alpha$: vectors pointing nuclei in the unit cell

Fourier transform:

$$v_p(\boldsymbol{K}) = \int \sum_{j,\alpha} W_p^{\alpha}(\boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{\tau}_\alpha) e^{-i\boldsymbol{K}\cdot\boldsymbol{r}} \frac{d\boldsymbol{r}}{V}$$

$\boldsymbol{r}' \equiv \boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{\tau}_\alpha$
N: unit cell number
Ω: unit cell volume

$$= \frac{1}{N} \sum_j e^{-i\boldsymbol{K}\cdot\boldsymbol{R}_j} \sum_\alpha e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_\alpha} \frac{1}{\Omega} \int_\Omega W_p^{\alpha}(\boldsymbol{r}') e^{-i\boldsymbol{K}\cdot\boldsymbol{r}'} d\boldsymbol{r}$$

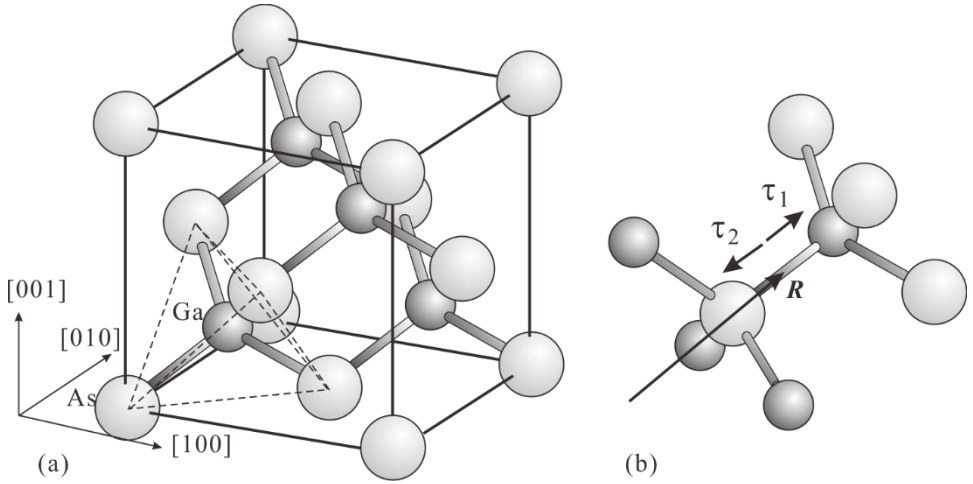
$$= \sum_\alpha e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_\alpha} \frac{1}{\Omega} \int_\Omega W_p^{\alpha}(\boldsymbol{r}') e^{-i\boldsymbol{K}\cdot\boldsymbol{r}'} d\boldsymbol{r}' \quad \because e^{-i\boldsymbol{K}\cdot\boldsymbol{R}_j} = 1$$

$$= \sum_\alpha e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_\alpha} w_p^{\alpha}(\boldsymbol{K})$$

$w_p^{\alpha}(\boldsymbol{K})$: form factor (Fourier transform of $W_p(r)$) depends only on potential form

$e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_\alpha}$: structure factor depends only on internal structure of unit cell

Empirical pseudo potential calculation for fcc semiconductors



ex) GaAs $\quad \mathrm{Ga}: \frac{a}{8}(1,1,1) \quad \mathrm{As}: -\frac{a}{8}(1,1,1)$

$$\boldsymbol{\tau}_1 = \frac{a}{8}(1,1,1) \quad \boldsymbol{\tau}_2 = -\frac{a}{8}(1,1,1)$$

$$\begin{aligned} v_p(\boldsymbol{K}) &= e^{i\boldsymbol{K}\cdot\boldsymbol{\tau}_1} v_p^1(\boldsymbol{K}) + e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_1} v_p^2(\boldsymbol{K}) \\ &= (v_p^1 + v_p^2)\cos\boldsymbol{K}\cdot\boldsymbol{\tau} + (v_p^1 - v_p^2)\sin\boldsymbol{K}\cdot\boldsymbol{\tau} \\ &= v_p^s(\boldsymbol{K})\cos\boldsymbol{K}\cdot\boldsymbol{\tau} + v_p^a(\boldsymbol{K})\sin\boldsymbol{K}\cdot\boldsymbol{\tau} \end{aligned}$$

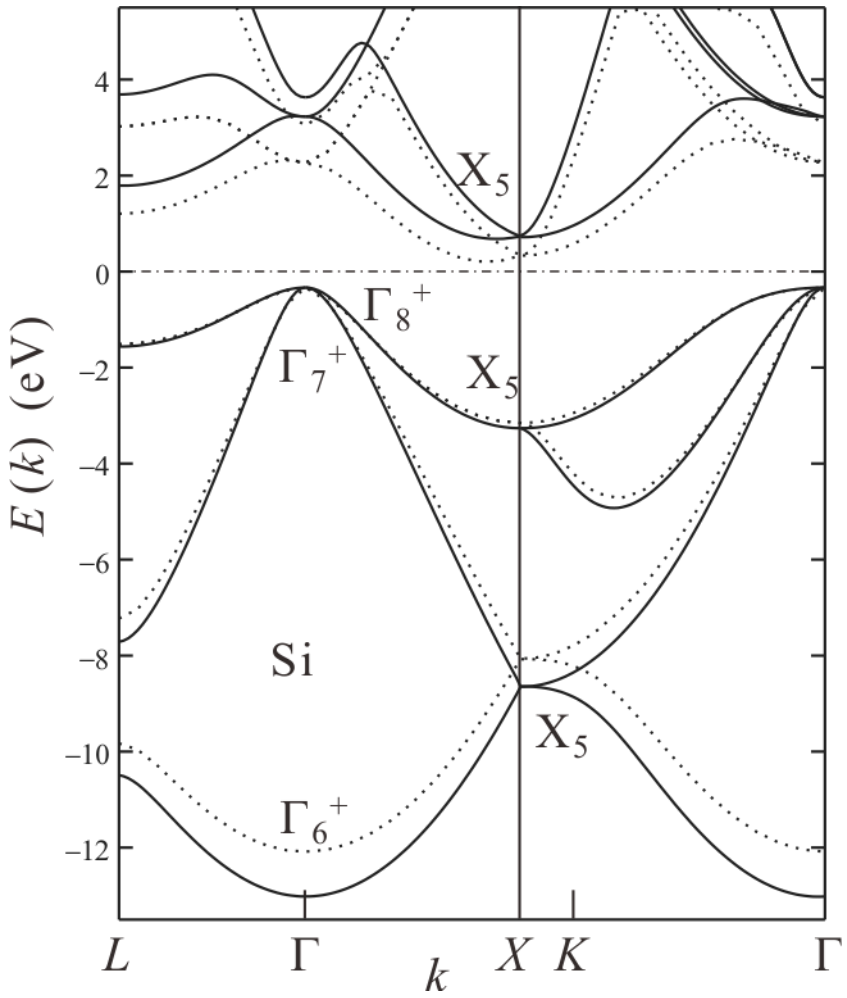
Distance from the origin and number of points in reciprocal lattice

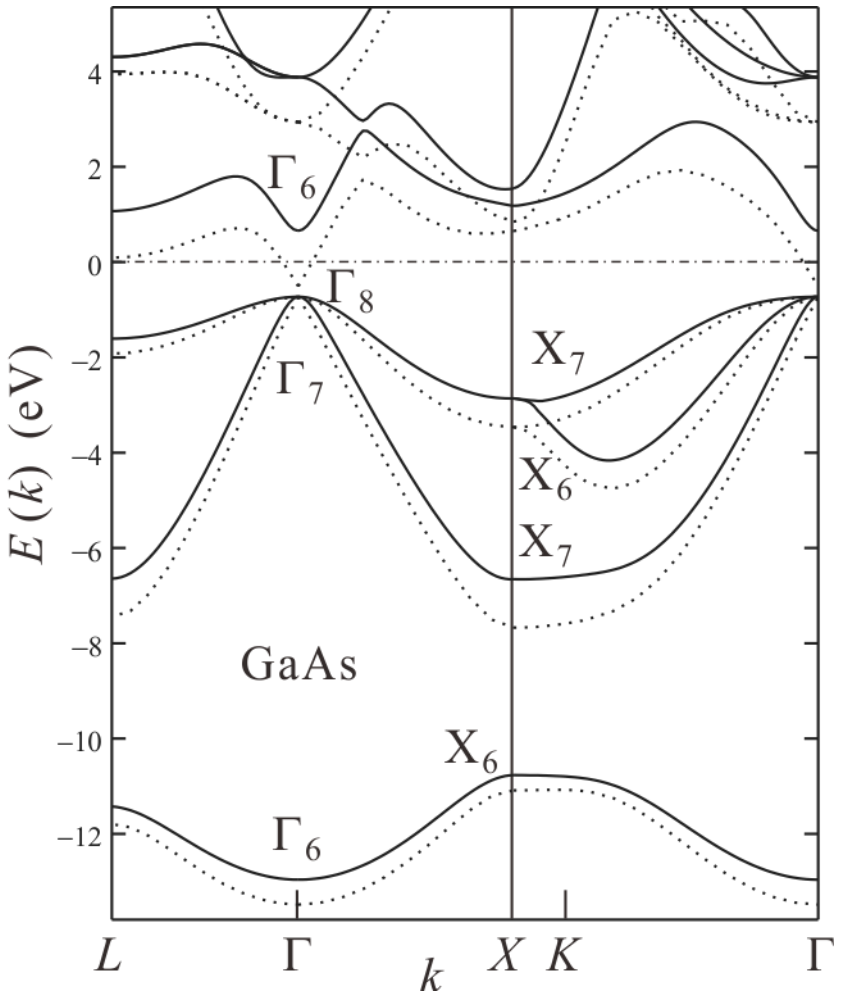
distance	Points	number
0	(0,0,0)	1
$\sqrt{3}$	(1,1,1),…	8
2	(2,0,0),…	6
$\sqrt{8}$	(2,0,2),…	12
$\sqrt{11}$	(3,1,1),…	24

Form factors obtained from fitting to optical experiment

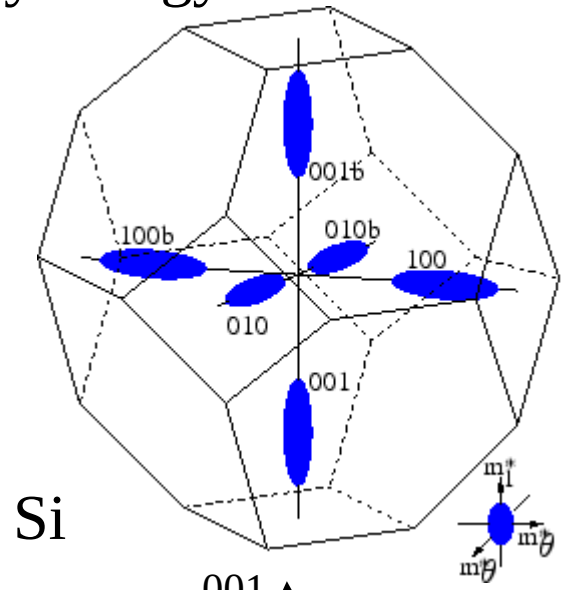
	$v_p^s(111)$	$v_p^s(220)$	$v_p^s(311)$	$v_p^a(111)$	$v_p^a(200)$	$v_p^a(311)$
Si	−2.856	0.544	1.088	0	0	0
Ge	−3.128	0.136	0.816	0	0	0
GaAs	−3.128	0.136	0.816	0.952	0.68	0.136
CdTe	−2.72	0	0.544	2.04	1.224	0.544

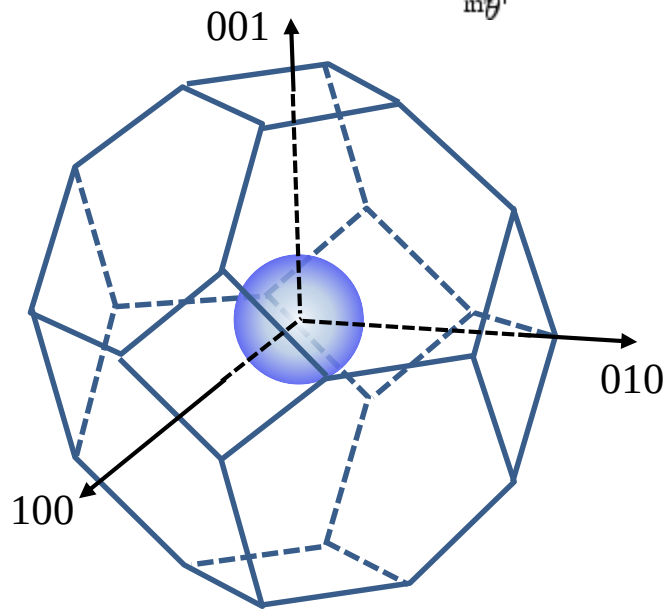
Band structure of Si and GaAs





conduction valley energy surface





spin-orbit interaction is not taken into account

Definition of effective mass

Group velocity of wavefunction with energy eigenvalue $E_n(k)$

$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}} E_n(\boldsymbol{k})$$

Acceleration

$$\frac{d\boldsymbol{v}_n}{dt} = \frac{d\boldsymbol{k}}{\hbar dt}\cdot\nabla_{\boldsymbol{k}}(\nabla_{\boldsymbol{k}} E_n(\boldsymbol{k})) = \frac{\nabla_{\boldsymbol{k}}}{\hbar^2}\sum_{j=x,y,z}\frac{\partial E_n(\boldsymbol{k})}{\partial k_j}F_j$$

With definition

$$\left(\frac{1}{m^*}\right)_{ij} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E(\boldsymbol{k})}{\partial k_i \partial k_j}$$

$$\frac{dv_i(\boldsymbol{k})}{dt} = \sum_j \left(\frac{1}{m^*}\right)_{ij} F_j = \overleftrightarrow{\left(\frac{1}{m^*}\right)}\boldsymbol{F}$$

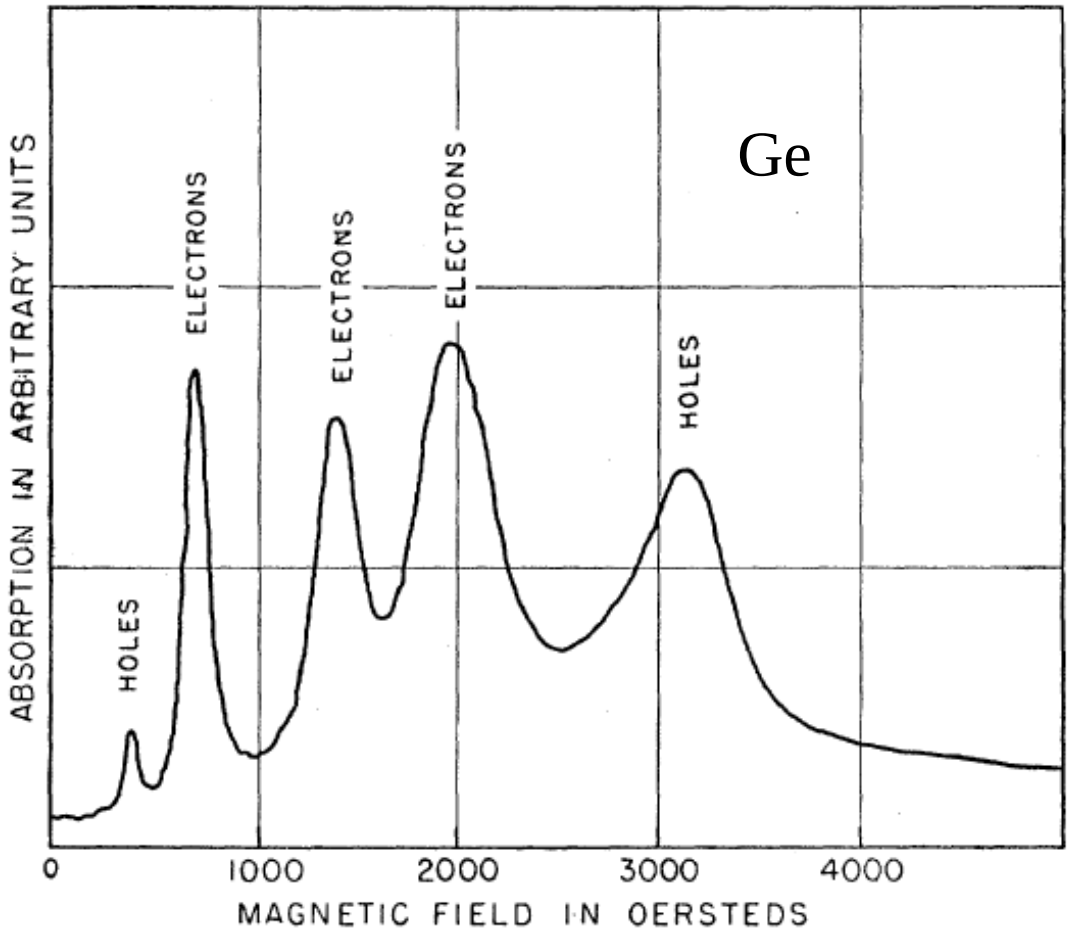
$\frac{1}{m^*}$: inverse effective mass tensor

$\left(\frac{1}{m^*}\right)^{-1}$:effective mass tensor

$$E(\boldsymbol{k}) - E(\boldsymbol{k}_0) \approx \sum_{i,j=x,y,z}\left(\frac{\hbar^2}{2m^*}\right)_{ij}\delta k_i \delta k_j = \sum_{l=1,2,3}\frac{\hbar^2}{2m_l^*}\delta k_l^2$$

Energy surface measurement (cyclotron resonance)

Motion of charged particle in magnetic field: cyclotron motion in the plane perpendicular to the magnetic field

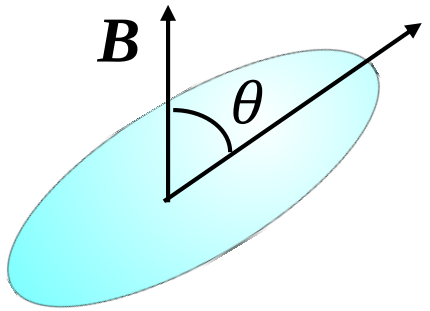


Cyclotron frequency $\omega_c = \frac{qB}{m}$

Landau quantization $E_n = \hbar\omega_c\left(n + \frac{1}{2}\right)$

Optical pumping → microwave absorption

ω_c → cyclotron mass m_c



Energy surface: ellipsoid

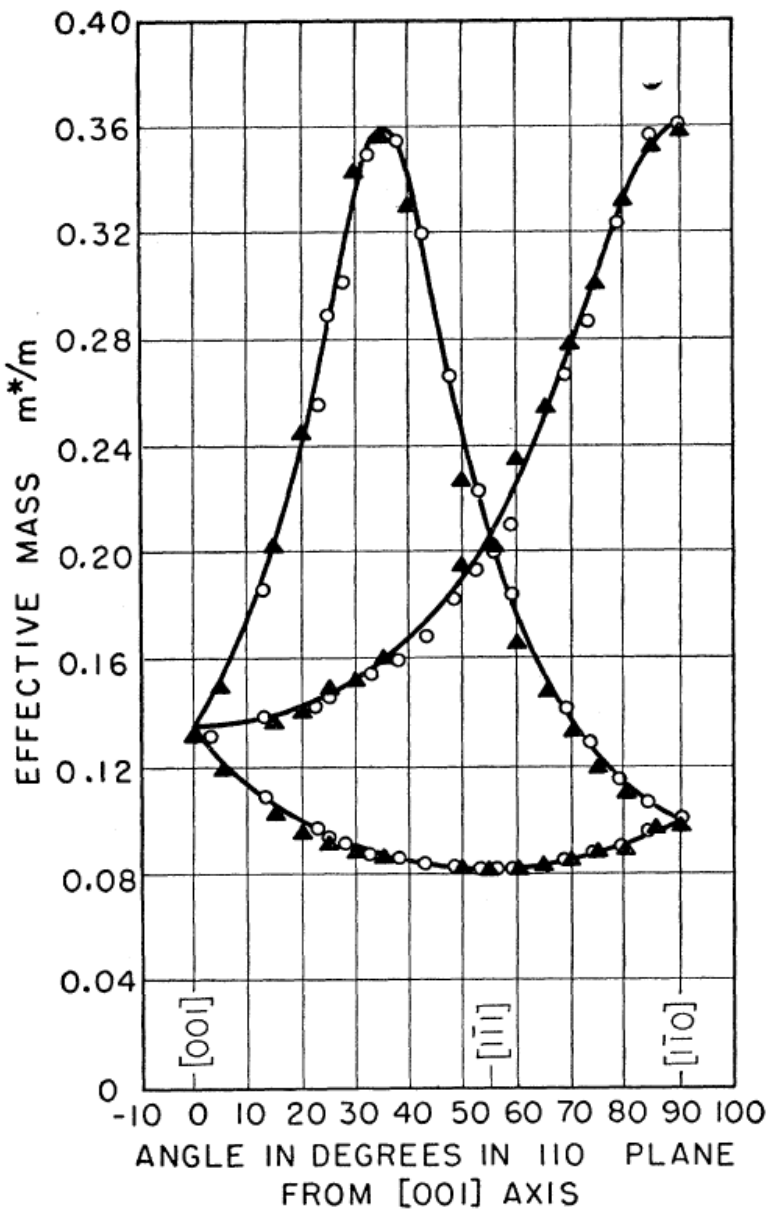
$$\left(\frac{1}{m_c}\right)^2 = \frac{\cos^2\theta}{m_t^2} + \frac{\sin^2\theta}{m_l m_t}$$

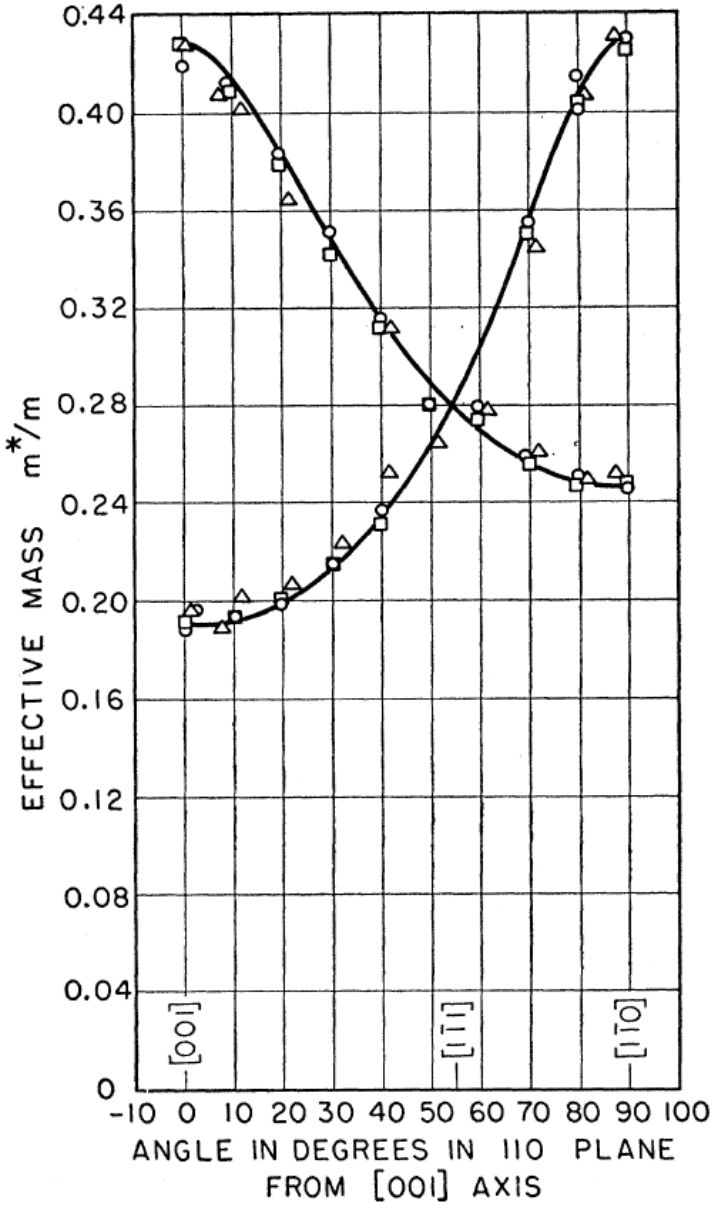
Electron-hole distinction ← circular polarization

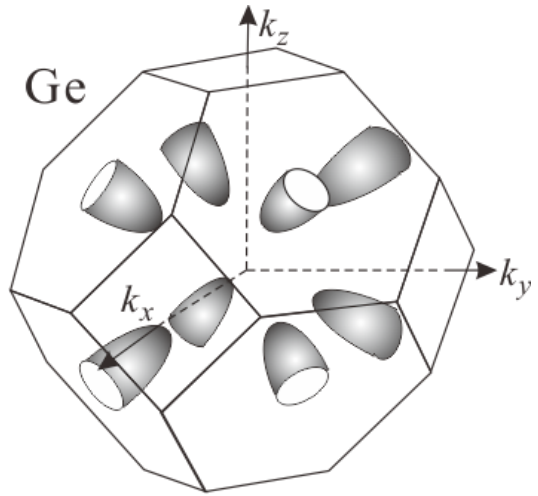
(24 GHz microwave)

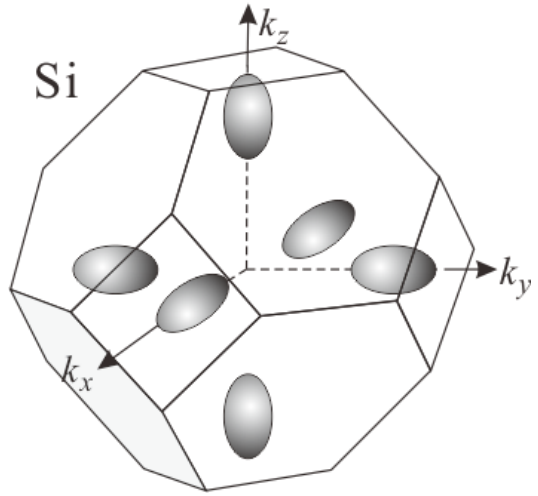
Dresselhaus, Kip, Kittel, Phys. Rev. **98**, 368 (1955).

Cyclotron resonance









k·p perturbation

Crystal Schrodinger equation:

$$\mathscr{H}\psi(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \quad (1)$$

Bloch function

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{n\boldsymbol{k}}(\boldsymbol{r}) \quad (2)$$

Equation for lattice periodic function

$$\left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m_0} + V(\boldsymbol{r}) + \frac{\hbar^2\boldsymbol{k}^2}{2m_0} - i\frac{\hbar^2}{m_0}\boldsymbol{k}\cdot\boldsymbol{\nabla}\right]u_{n\boldsymbol{k}}(\boldsymbol{r}) = E_n u_{n\boldsymbol{k}}(\boldsymbol{r}) \quad (3)$$

Perturbation by $\boldsymbol{k}$-dependent term

$$\mathscr{H}_0 \equiv \mathscr{H}(\boldsymbol{0}) \qquad \mathscr{H}'(\boldsymbol{k}) = \frac{\hbar^2\boldsymbol{k}^2}{2m_0} - i\frac{\hbar^2}{m_0}\boldsymbol{k}\cdot\boldsymbol{\nabla}$$

Good approximation for small k → band edge information

(a) In the case of no degeneracy

$$\begin{cases} u_{i\boldsymbol{k}}(\boldsymbol{r}) = u_{i0}(\boldsymbol{r}) + \sum_{j\neq i}\dfrac{\langle j|\mathscr{H}'|i\rangle}{E_i - E_j}u_{i0}(\boldsymbol{r}) \qquad |i\rangle \equiv |u_{i0}\rangle \\ E_i(\boldsymbol{k}) = E_i(0) + \langle i|\mathscr{H}'|i\rangle + \sum_{j\neq i}\dfrac{|\langle i|\mathscr{H}'|j\rangle|^2}{E_i - E_j} \end{cases}$$

$$E_i(\boldsymbol{k}) = E_i(0) + \frac{\hbar^2\boldsymbol{k}^2}{2m_0} - \frac{\hbar^4}{m_0^2}\sum_{j\neq i}\frac{\langle i|\boldsymbol{k}\cdot\boldsymbol{\nabla}|j\rangle\langle j|\boldsymbol{k}\cdot\boldsymbol{\nabla}|i\rangle}{E_i - E_j}$$

k·p approximation (2)

(b) In the case of *n*-fold degeneracy in $u_{00}(\boldsymbol{r})$

$\{u_{00}^{j}\ (j=i,\cdots,n)\}\ (\equiv\{|0j\rangle\})$ orthogonal

Approximate the perturbed wavefunction

$$|u_{0\boldsymbol{k}}^{i}\rangle=\sum_{j=1}^{n}A_{ij}(\boldsymbol{k})|0j\rangle$$

Substitute to the equation for *u*

$$[\mathscr{H}_0+\mathscr{H}'-E_0(\boldsymbol{k})]|u_{0\boldsymbol{k}}^{j}\rangle=0$$

Taking inner product with $|0i\rangle$

$$\sum_{j=1}^{n}A_{ij}(\boldsymbol{k})[\langle 0i|\mathscr{H}_0|0j\rangle+\langle 0i|\mathscr{H}_0'|0j\rangle-\langle 0i|E_0(\boldsymbol{k})|0j\rangle]$$

$$=\sum_{j=1}^{n}A_{ij}(\boldsymbol{k})[\langle 0i|\mathscr{H}'|0j\rangle+(E_0-E_0(\boldsymbol{k}))\delta_{ij}]=0 \qquad (4)$$

For eq.(4) to have non-trivial solution

$$|\langle 0i|\mathscr{H}'|0j\rangle+(E_0-E_0(\boldsymbol{k}))\delta_{ij}|=0$$

Spin-orbit interaction

Spin-orbit Hamiltonian $\mathscr{H}_{\rm so} = -\dfrac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot\boldsymbol{p}\times(\nabla V)$

spin-operator $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ $\quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

From identity

$|\boldsymbol{a}\ \boldsymbol{b}\ \boldsymbol{c}| = \boldsymbol{a}\cdot(\boldsymbol{b}\times\boldsymbol{c})$
$= -\boldsymbol{b}\cdot(\boldsymbol{c}\times\boldsymbol{a})$

$$\left[\frac{p^2}{2m_0} + V + \frac{\hbar^2k^2}{2m_0} + \frac{\hbar}{m_0}\boldsymbol{k}\cdot\boldsymbol{\pi} + \frac{\hbar}{4m_0^2c^2}\boldsymbol{p}\cdot\boldsymbol{\sigma}\times\nabla V\right]|n\boldsymbol{k}\rangle = E_n(\boldsymbol{k})|n\boldsymbol{k}\rangle,$$

$$\boldsymbol{\pi} \equiv \boldsymbol{p} + \frac{\hbar}{4mc^2}\boldsymbol{\sigma}\times\nabla V$$

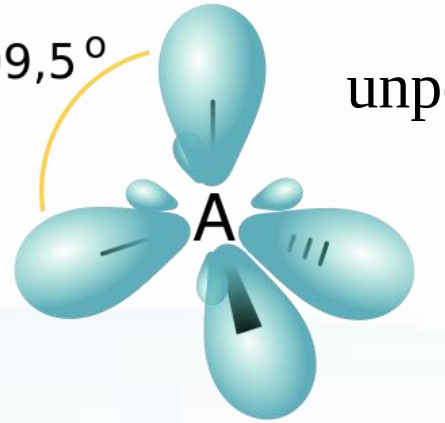
$$|\nu,\sigma\rangle \equiv |\nu 0\rangle\otimes|\sigma\rangle \qquad |n\boldsymbol{k}\rangle = \sum_{\nu',\sigma'} c_{n,\nu\sigma}|\nu',\sigma'\rangle$$

eigenequation

$$\sum_{\nu',\sigma'}\left\{\left[E_{\nu'}(0) + \frac{\hbar^2k^2}{2m}\right]\delta_{\nu\nu'}\delta_{\sigma\sigma'} + \frac{\hbar}{m}\boldsymbol{k}\cdot\boldsymbol{P}^{\nu\nu'}_{\sigma\sigma'} + \Delta^{\nu\nu'}_{\sigma\sigma'}\right\}c_{n\nu'\sigma'} = E_n(\boldsymbol{k})c_{n\nu\sigma}$$

$$\boldsymbol{P}^{\nu\nu'}_{\sigma\sigma'} \equiv \langle\nu\sigma|\boldsymbol{\pi}|\nu'\sigma'\rangle, \quad \Delta^{\nu\nu'}_{\sigma\sigma'} \equiv \frac{\hbar^2}{4m^2c^2}\langle\nu\sigma|[\boldsymbol{p}\cdot\sigma\times(\nabla V)]|\nu'\sigma'\rangle$$

Γ-band edges of diamond and zinc-blende semiconductors



unperturbed equation: $\mathscr{H}_0|\zeta\rangle = \left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m_0} + V(\boldsymbol{r})\right]|\zeta\rangle = E_b|\zeta\rangle$

Diamond, zinc-blende: formed from sp^3 orbitals

$$|\zeta\rangle : \ |S\rangle,\ |X\rangle,\ |Y\rangle,\ |Z\rangle$$
$$(|s\rangle,\ |p_x\rangle,\ |p_y\rangle,\ |p_z\rangle)$$

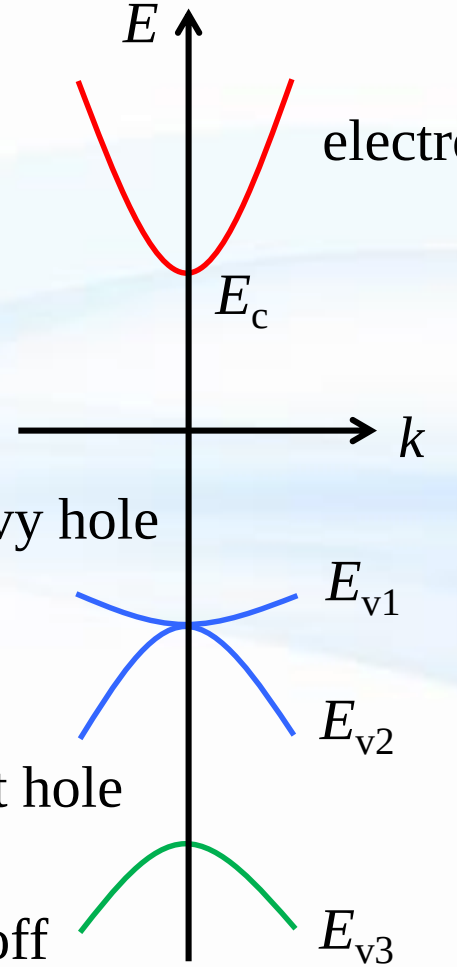
perturbation $\mathscr{H}' + \mathscr{H}_{\mathrm{SO}} = -i\frac{\hbar^2}{m_0}\boldsymbol{k}\cdot\boldsymbol{\nabla} - \frac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{p}\times\nabla V)$

$$\{|S\rangle, |X\rangle, |Y\rangle, |Z\rangle\} \to \{|S\rangle, |\pm\rangle \equiv (|X\rangle \pm i|Y\rangle)/\sqrt{2}, |Z\rangle\}$$

non-zero element $P \equiv \frac{\hbar}{m_0}\langle S|p_x|X\rangle = \frac{\hbar}{m_0}\langle S|p_y|Y\rangle = \frac{\hbar}{m_0}\langle S|p_z|Z\rangle,$

$\Delta \equiv -\frac{3i\hbar}{4m_0^2c^2}\langle X|[\nabla V\times\boldsymbol{p}]_y|Z\rangle$ xyz cycling

$$\langle\pm\uparrow|\mathscr{H}_{\mathrm{SO}}|\pm\uparrow\rangle = -\langle\pm\downarrow|\mathscr{H}_{\mathrm{SO}}|\pm\downarrow\rangle = \pm\Delta/3,$$
$$\langle\pm\alpha|\mathscr{H}_{\mathrm{SO}}|Z\alpha'\rangle = (1-\delta_{\alpha\alpha'})\sqrt{2}\Delta/3$$



α: spin coordinate

Γ-band edges of diamond and zinc-blende semiconductors (2)

$$\langle S\alpha|\mathscr{H}_0|S\alpha'\rangle = \delta_{\alpha\alpha'}E_c, \quad \langle\{+,Z,-\}\alpha|\mathscr{H}_0|\{+,Z,-\}\alpha'\rangle = \delta_{\alpha\alpha'}E_v$$

Hamiltonian $\mathscr{H}$ expression

	$\lvert S\uparrow\rangle$	$\lvert S\downarrow\rangle$	$\lvert +\uparrow\rangle$	$\lvert +\downarrow\rangle$	$\lvert -\uparrow\rangle$	$\lvert -\downarrow\rangle$	$\lvert Z\uparrow\rangle$	$\lvert Z\downarrow\rangle$
$\lvert S\uparrow\rangle$	E_c	0	$-\frac{Pk_+}{\sqrt{2}}$	0	$\frac{Pk_-}{\sqrt{2}}$	0	Pk_z	0
$\lvert S\downarrow\rangle$	0	E_c	0	$-\frac{Pk_+}{\sqrt{2}}$	0	$\frac{Pk_-}{\sqrt{2}}$	0	Pk_z
$\lvert +\uparrow\rangle$	$-\frac{P^*k_-}{\sqrt{2}}$	0	$E_v+\frac{\Delta}{3}$	0	0	0	0	0
$\lvert +\downarrow\rangle$	0	$-\frac{P^*k_-}{\sqrt{2}}$	0	$E_v-\frac{\Delta}{3}$	0	0	$\frac{\sqrt{2}\Delta}{3}$	0
$\lvert -\uparrow\rangle$	$\frac{P^*k_+}{\sqrt{2}}$	0	0	0	$E_v-\frac{\Delta}{3}$	0	0	$\frac{\sqrt{2}\Delta}{3}$
$\lvert -\downarrow\rangle$	0	$\frac{P^*k_+}{\sqrt{2}}$	0	0	0	$E_v+\frac{\Delta}{3}$	0	0
$\lvert Z\uparrow\rangle$	P^*k_z	0	0	$\frac{\sqrt{2}\Delta}{3}$	0	0	E_v	0
$\lvert Z\downarrow\rangle$	0	P^*k_z	0	0	$\frac{\sqrt{2}\Delta}{3}$	0	0	E_v

Γ-band edges of diamond and zinc-blende semiconductors (3)

Eigenvalue equation

$$\lambda = E_v + \frac{\Delta}{3},$$

$$(\lambda - E_c)\left(\lambda - E_v + \frac{2\Delta}{3}\right)\left(\lambda - E_v - \frac{\Delta}{3}\right) - |P|^2 k^2 \left(\lambda - E_v + \frac{\Delta}{3}\right) = 0.$$

Ignoring the term $|P|^2 k^2$ we finally obtain:

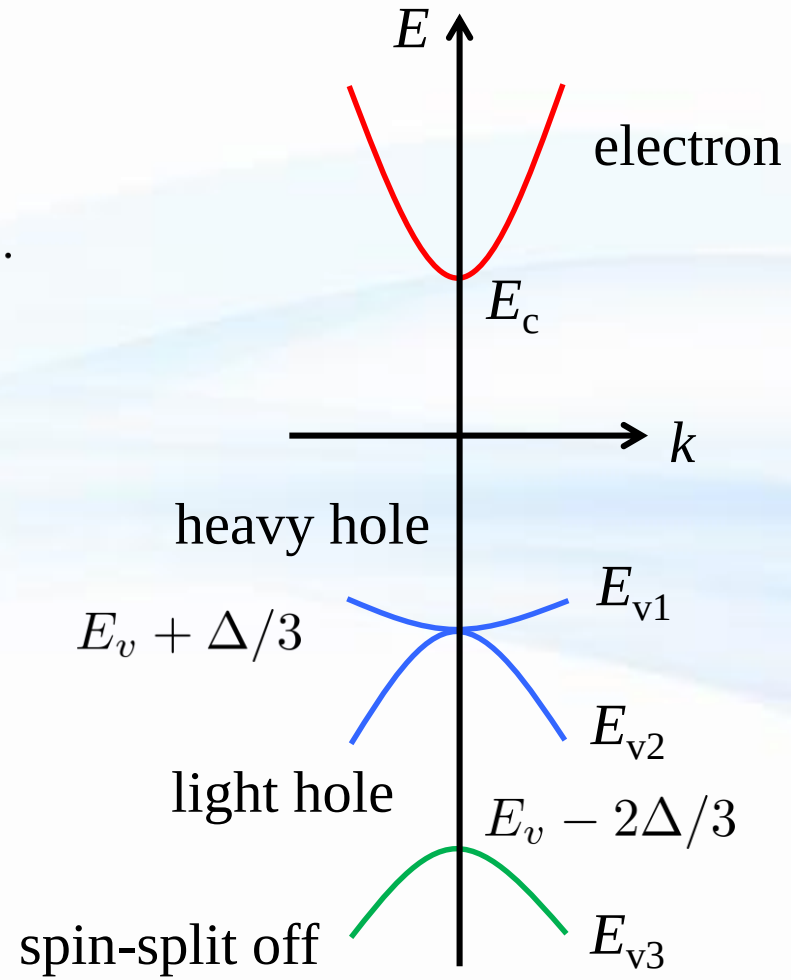
$$E_c(\boldsymbol{k}) = E_c + \frac{\hbar^2 k^2}{2m_0} + \frac{|P|^2 k^2}{3}\left[\frac{2}{E_g} + \frac{1}{E_g + \Delta}\right],$$

$$E_{v1}(\boldsymbol{k}) = E_v + \frac{\Delta}{3} + \frac{\hbar^2 k^2}{2m_0},$$

$$E_{v2}(\boldsymbol{k}) = E_v + \frac{\Delta}{3} + \frac{\hbar^2 k^2}{2m_0} - \frac{2|P|^2 k^2}{3E_g},$$

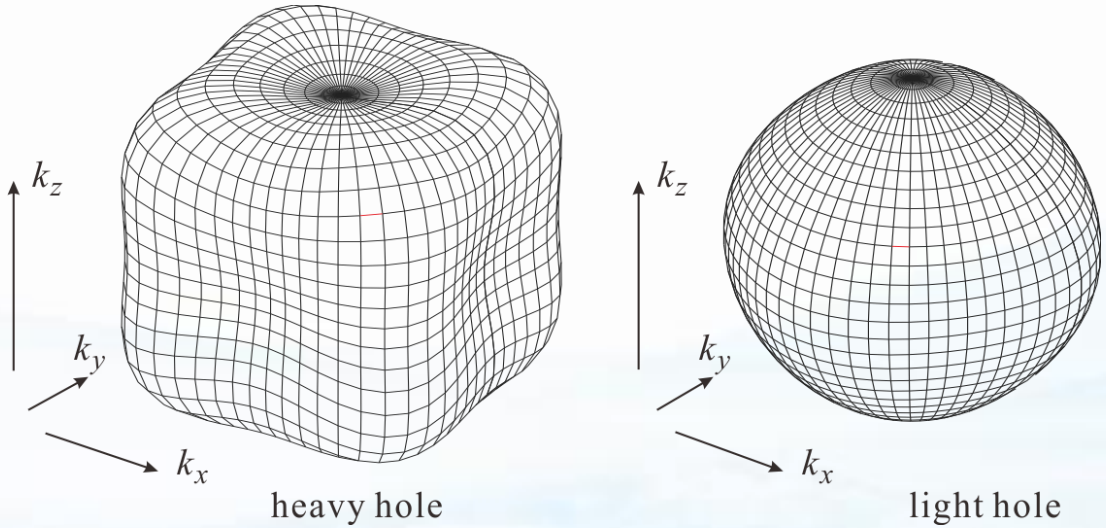
$$E_{v3}(\boldsymbol{k}) = E_v - \frac{2\Delta}{3} + \frac{\hbar^2 k^2}{2m_0} - \frac{|P|^2 k^2}{3(E_g + \Delta)}$$

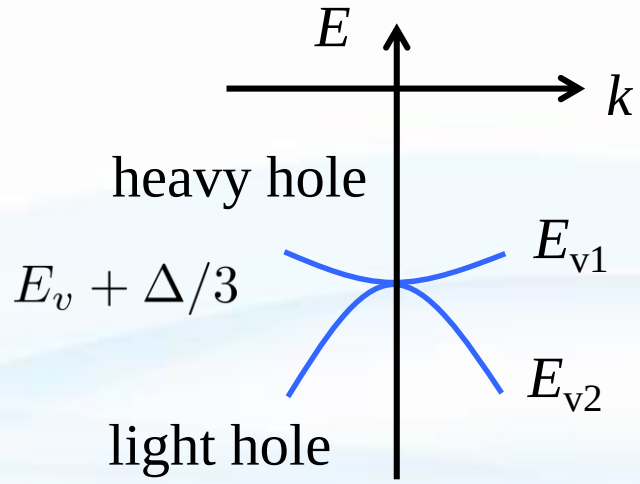
$$E_g = E_c - E_v - \Delta/3$$



Band warping, a conventional way to get band parameters

constant-energy surface





Summary of $k \cdot p$ second order perturbation

$$E_v(\boldsymbol{k}) = E_v + \frac{\Delta}{3} + Ak^2 \mp \sqrt{B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)}$$

$$E_{vsp}(\boldsymbol{k}) = E_v - \frac{2\Delta}{3} + Ak^2$$

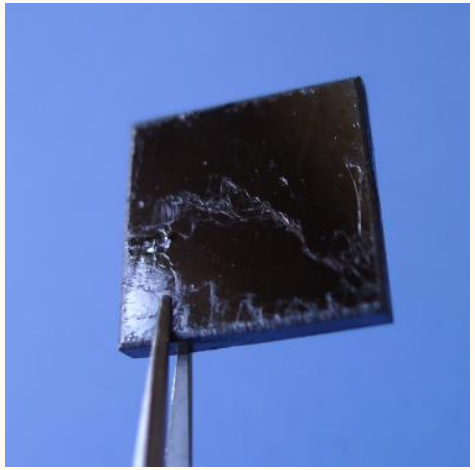
Table of band parameters

	E_r (eV)	E_L (eV)	E_Δ (eV)	E_{so} (eV)	m_t^* (m_0)	m^* (m_0)	m_t^* (m_0)	$\|A\|$ (eV^{-1})	$\|B\|$	$\|C\|$
C	11.67	12.67	5.45	0.006	1.4	-	0.36	3.61	0.18	3.76
Si	4.08	1.87	1.13	0.044	0.98	-	0.19	4.22	0.78	4.8
Ge	0.89	0.76	0.96	0.29	1.64	-	0.082	13.35	8.5	13.11
AlAs	2.95	2.67	2.16	0.28	2	-	-	4.04	1.56	4.71
GaP	2.7	2.7	2.2	0.08	1.12	-	0.22	4.2	1.96	4.65
GaAs	1.42	1.71	1.9	0.34	-	0.067	-	7.65	4.82	7.71
GaSb	0.67	1.07	1.3	0.77	-	0.045	-	11.8	8.06	11.71
InP	1.26	2	2.3	0.13	-	0.08	-	6.28	4.16	6.35
InAs	0.35	1.45	2.14	0.38	-	0.023	-	19.67	16.74	13.96
InSb	0.23	0.98	0.73	0.81	-	0.014	-	35.08	31.28	22.27
CdTe	1.8	3.4	4.32	0.91	-	0.096	-	5.29	3.78	5.46

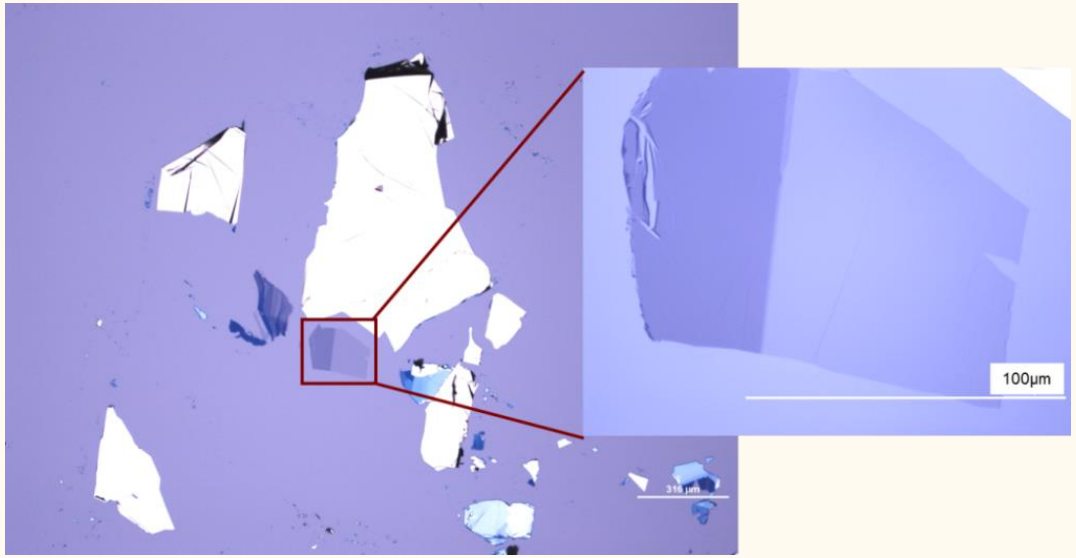
Lundstrom “Fundamentals of Carrier Transport” (Cambridge, 2000).

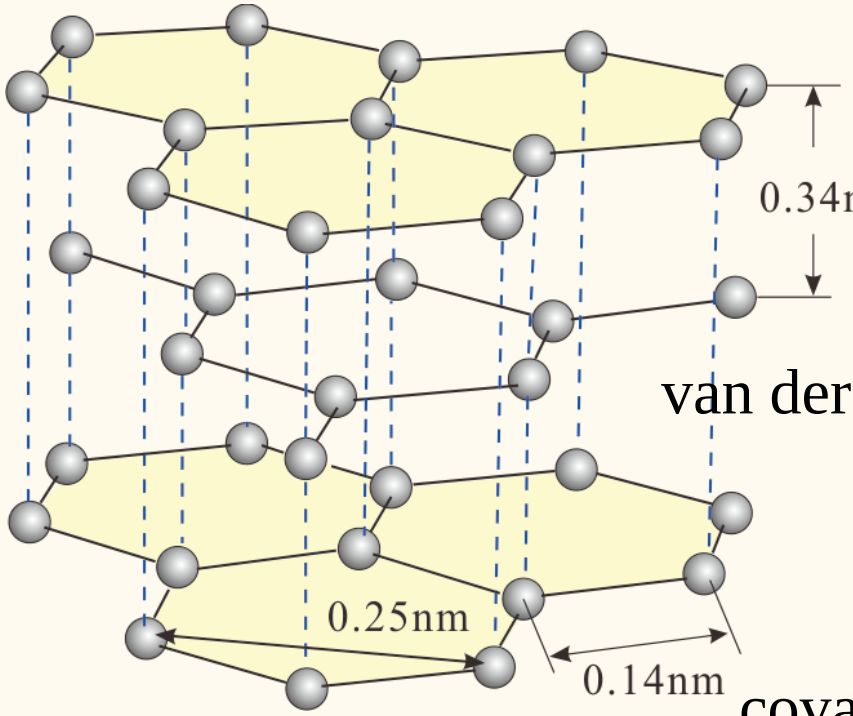
Graphene: A two-dimensional material (another example of TBA)

Graphite



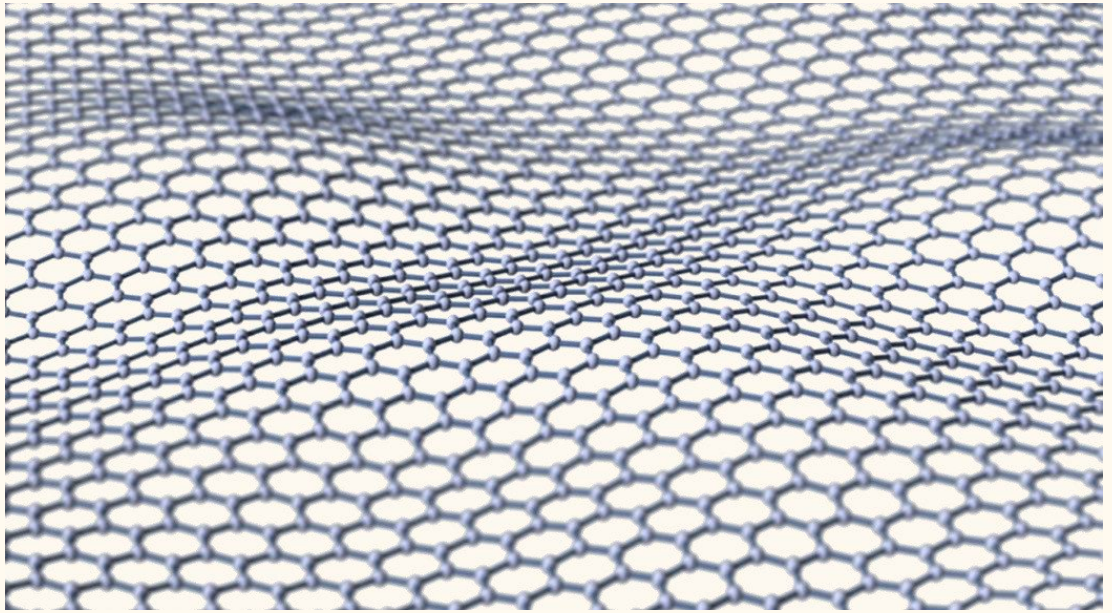
Graphene





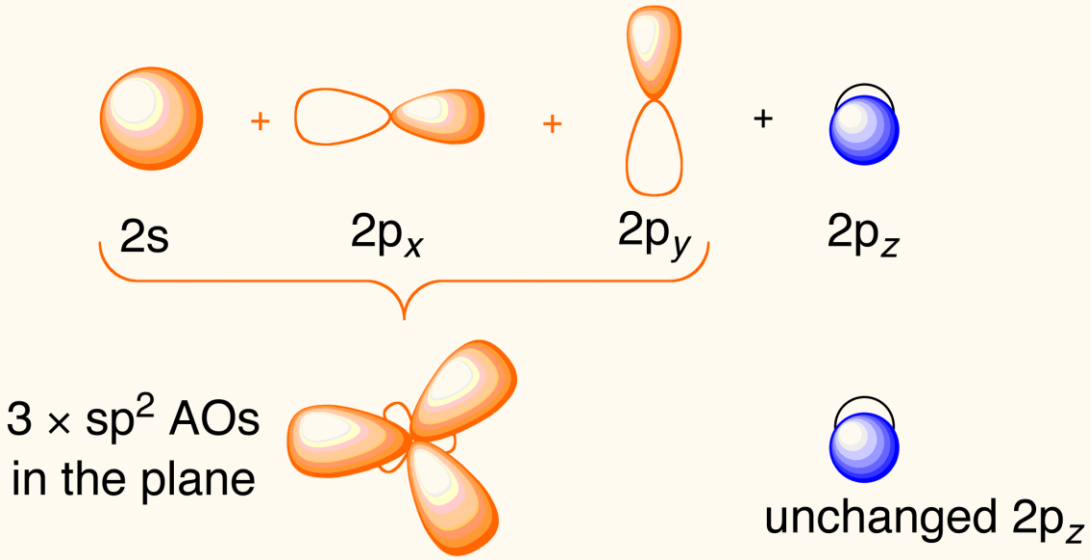
van der Waals

covalent

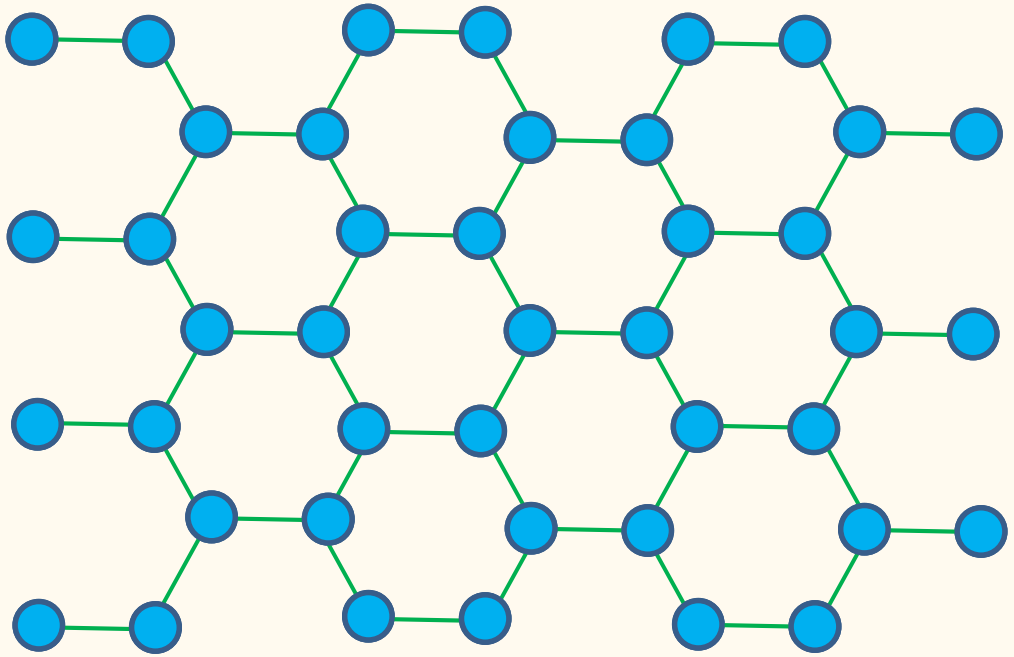


Graphene lattice/reciprocal lattice structure

Atomic orbitals

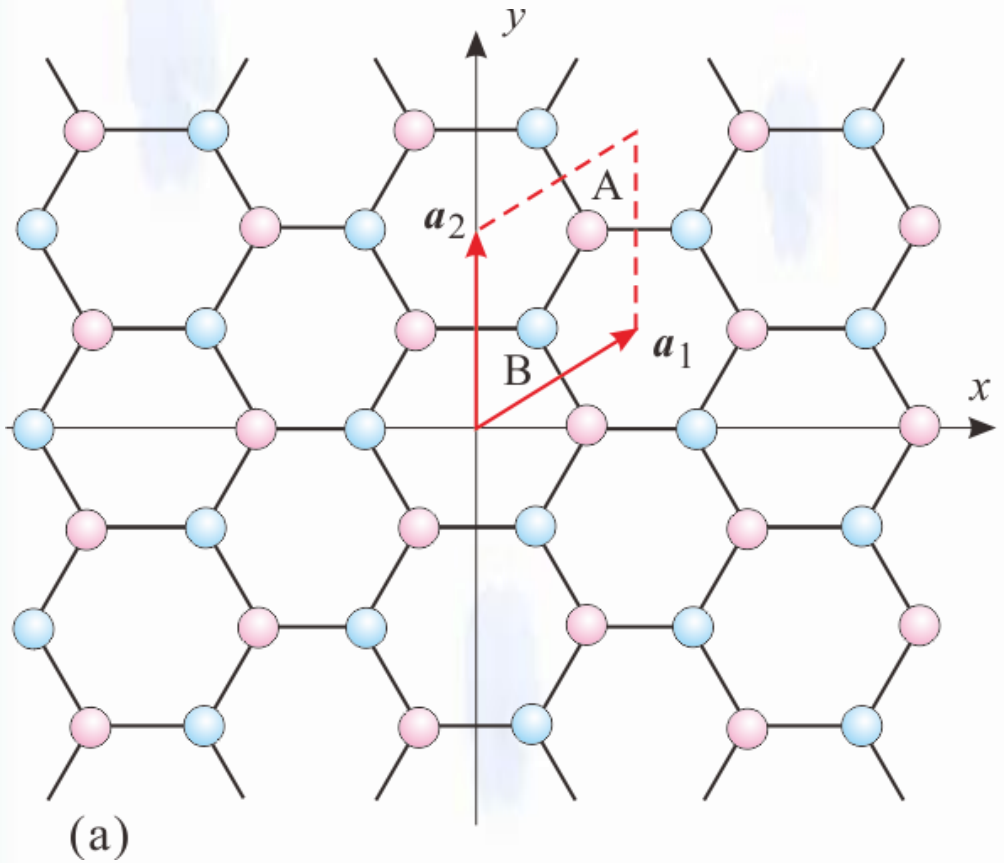


Honeycomb lattice

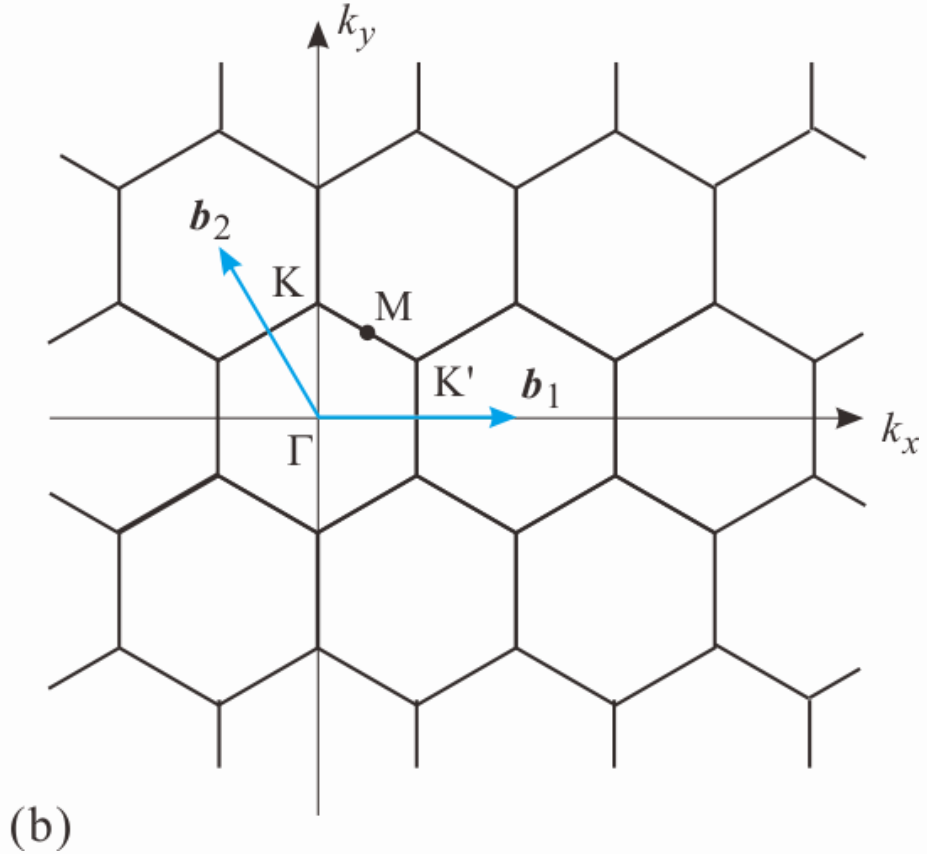


Graphene lattice/reciprocal lattice structure

Lattice: unit cell



Reciprocal lattice



$$\boldsymbol{a}_1 = \begin{pmatrix} \sqrt{3}a/2 \\ a/2 \end{pmatrix}, \quad \boldsymbol{a}_2 = \begin{pmatrix} 0 \\ a \end{pmatrix}$$

$$\boldsymbol{b}_1 = \begin{pmatrix} 4\pi/\sqrt{3}a \\ 0 \end{pmatrix}, \quad \boldsymbol{b}_2 = \begin{pmatrix} -2\pi/\sqrt{3}a \\ 2\pi/a \end{pmatrix}$$

Tight binding model

Sublattice wavefunction

$$\psi_{\mathrm{A}} = \sum_{j\in A} \exp(i\boldsymbol{k}\boldsymbol{r}_j)\phi(\boldsymbol{r}-\boldsymbol{r}_j), \quad \psi_{\mathrm{B}} = \sum_{j\in B} \exp(i\boldsymbol{k}\boldsymbol{r}_j)\phi(\boldsymbol{r}-\boldsymbol{r}_j)$$

tight-binding

$$\langle\psi_\alpha|\psi_\beta\rangle = N\delta_{\alpha\beta} \quad (\alpha,\beta = \mathrm{A},\mathrm{B})$$

Linear combination

$$\psi = \zeta_{\mathrm{A}}\psi_{\mathrm{A}} + \zeta_{\mathrm{B}}\psi_{\mathrm{B}} = \begin{pmatrix}\zeta_{\mathrm{A}}\\ \zeta_{\mathrm{B}}\end{pmatrix}$$

tight-binding
Hamiltonian equation

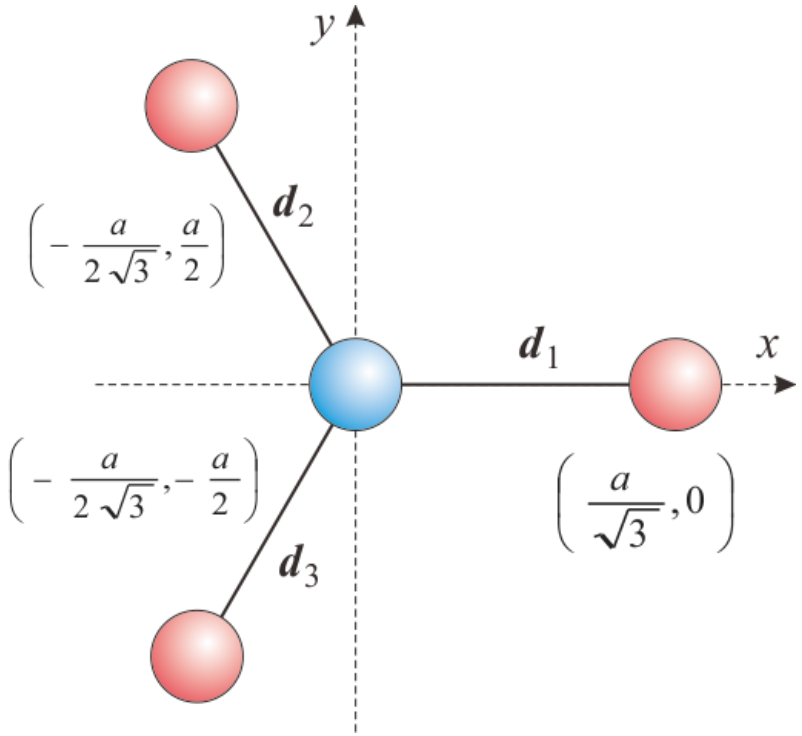
$$H_{\mathrm{AA}} = \langle\psi_{\mathrm{A}}|\mathscr{H}|\psi_{\mathrm{A}}\rangle, \quad H_{\mathrm{BB}} = \langle\psi_{\mathrm{B}}|\mathscr{H}|\psi_{\mathrm{B}}\rangle,$$
$$H_{\mathrm{AB}} = H^*_{\mathrm{BA}} = \langle\psi_{\mathrm{A}}|\mathscr{H}|\psi_{\mathrm{B}}\rangle$$

$$\mathscr{H}\psi = \begin{pmatrix}H_{\mathrm{AA}} & H_{\mathrm{AB}}\\ H_{\mathrm{BA}} & H_{\mathrm{BB}}\end{pmatrix}\begin{pmatrix}\zeta_{\mathrm{A}}\\ \zeta_{\mathrm{B}}\end{pmatrix} = NE\psi = NE\begin{pmatrix}\zeta_{\mathrm{A}}\\ \zeta_{\mathrm{B}}\end{pmatrix}$$

Eigenvalues:

$$E = \frac{1}{2N}\left(H_{\mathrm{AA}} + H_{\mathrm{BB}} \pm \sqrt{(H_{\mathrm{AA}} - H_{\mathrm{BB}})^2 + 4|H_{\mathrm{AB}}|^2}\right)$$
$$= \frac{H_{\mathrm{AA}}}{N} \pm \frac{|H_{\mathrm{AB}}|}{N} \equiv h_{\mathrm{AA}} \pm |h_{\mathrm{AB}}|$$

Sublattice transition term



$$H_{\mathrm{AB}} = \sum_{l\in \mathrm{A}, j\in \mathrm{B}} \exp\left[i\boldsymbol{k}(\boldsymbol{r}_j - \boldsymbol{r}_l)\right] \left\langle \phi(\boldsymbol{r}-\boldsymbol{r}_l)\middle|\mathscr{H}\middle|\phi(\boldsymbol{r}-\boldsymbol{r}_j)\right\rangle_{\boldsymbol{r}}$$

Take the nearest neighbor approximation:

$$\boldsymbol{k}\cdot\boldsymbol{d}_1 = \frac{k_x a}{\sqrt{3}},\ \boldsymbol{k}\cdot\boldsymbol{d}_2 = \left(-\frac{k_x}{2\sqrt{3}} + \frac{k_y}{2}\right) a,$$

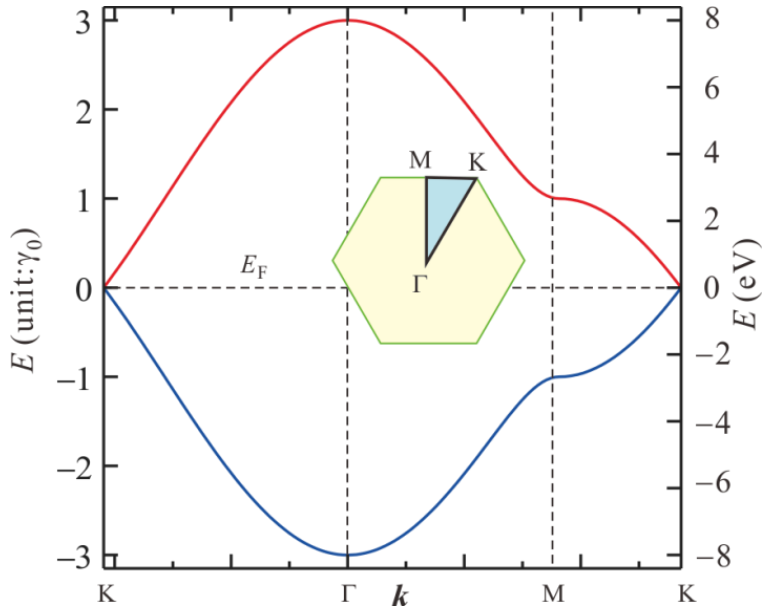
$$\boldsymbol{k}\cdot\boldsymbol{d}_3 = \left(-\frac{k_x}{2\sqrt{3}} - \frac{k_y}{2}\right) a$$

$$\left\langle \phi(\boldsymbol{r}-\boldsymbol{r}_l)\middle|\mathscr{H}\middle|\phi(\boldsymbol{r}-\boldsymbol{r}_j)\right\rangle_{\boldsymbol{r}} = \xi \quad \text{:constant}$$

$$|h_{\mathrm{AB}}|^2 = \left|\sum_{j=1}^{3} \exp(i\boldsymbol{k}\cdot\boldsymbol{d}_j)\right|^2 \xi^2$$

$$= \left(1 + 4\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2} + 4\cos^2\frac{k_y a}{2}\right)\xi^2$$

Dirac points in $\boldsymbol{k}$ -space

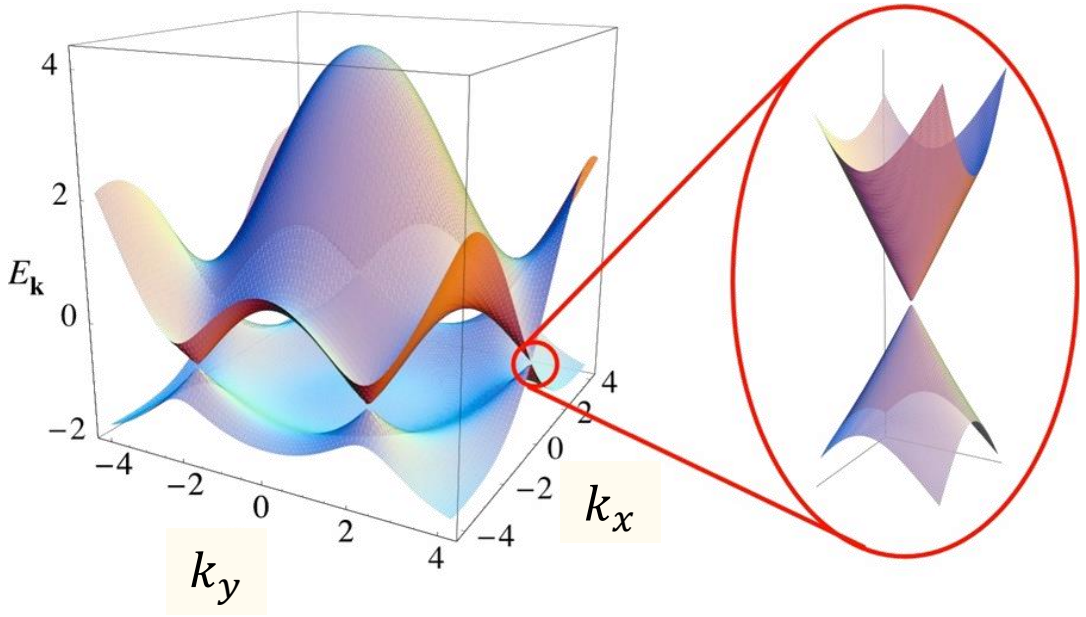


$$E = h_{\mathrm{AA}} \pm \xi \sqrt{1 + 4\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2} + 4\cos^2\frac{k_y a}{2}}$$

$$k_x = 0$$

$$E = h_{\mathrm{AA}} \pm \xi \left| 1 + 2\cos\frac{k_y a}{2} \right|$$

$$E\left(k_x, \frac{4\pi}{3a}\right) \approx h_{\mathrm{AA}} + \frac{\sqrt{3}\xi a}{2}|k_x|$$



A Dirac point