Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.7 Lecture 01

Institute for Solid State Physics, University of Tokyo

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How the lecture will go on?

- Powerpoint (converted to pdf) file will be uploaded in the corresponding ITC-LMS site, (https://itc-lms.ecc.u-tokyo.ac.jp/lms/course?idnumber=202135603-00290F01) by the day before the lecture.
- The lecture notes (in Japanese, English) will be uploaded in the site https://kats.issp.u-tokyo.ac.jp/kats/semicon4/ by the end of the lecture week.
- Small amount of problems for your exercise at home will be given in the last of the lecture in every two weeks. Submission deadline of the solutions is two weeks later. I hope I can collect them through LTC-LMS but if that is difficult I will prepare my own web script.
- In the very last of the lecture in July, the problems for your report will be given. The deadline for the submission of the report will be notified then.
- The lecture is recorded on the cloud. I hope I can upload the video for one or two weeks.
- I hope I can find some ways to get questions from you (via chat, etc.?)

Lecture Plan

Related site: https://kats.issp.u-tokyo.ac.jp/kats/semicon4/

1) Crystal structure and crystal growth
2) Energy band, effective mass approximation
3) Carrier statistics and chemical doping
4) Optical properties
5) Semi-classical treatment of charier transport
6) Homo/hetero junctions, semiconductor devices (optical, electrical)
7) Quantum structures (quantum wells, wires, dots) by nanofabrication techniques
8) Basics of quantum transport
9) Galvanomagnetic effects, Quantum Hall effects
10) Spin-related phenomena (spintronics)
11) Topological effects

１）結晶構造と結晶成長
２）エネルギーバンド，有効質量モデル
３）半導体キャリア統計とドーピング
４）光学的性質
５）電気伝導の半古典論
６）ホモ・ヘテロ接合，半導体デバイス（光，電子）
７）微細構造技術による量子構造（量子井戸，細線，ドット）
８）量子輸送の基礎
９）電流磁気効果，量子ホール効果
１０）スピン物性 (スピントロニクス)
１１）トポロジカル効果

Characteristics of semiconductors

- Not metal
- Middle range band gap
- Weak divergence of resistivity with lowering temperature

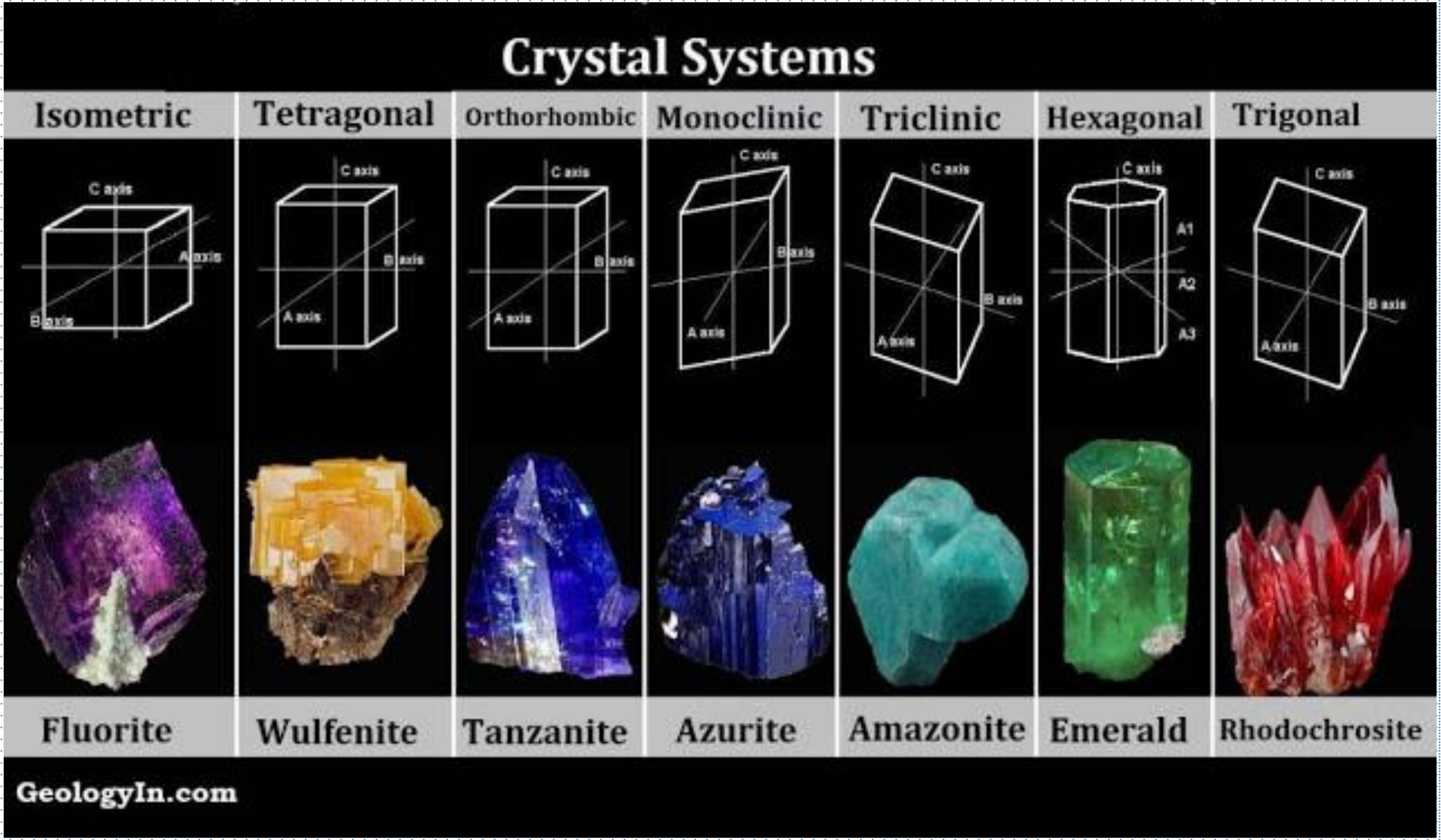
Structure sensitive (conduction) properties

- Drastic changes in electric conduction with ultra-small amount of impurities
- Changes in electronic and optical properties with quantum confinement structures like quantum wells, wires, and dots

A SEMI-CONDUCTOR

Yu & Cardona, "Fundamentals of Semiconductors"

Chapter 1 Crystal structures and crystal growths



http://www.geologyin.com/2014/11/crystal-structure-and-crystal-system.html

Crystal structure

Uniform solids
- crystals
  - poly
  - single
- amorphous

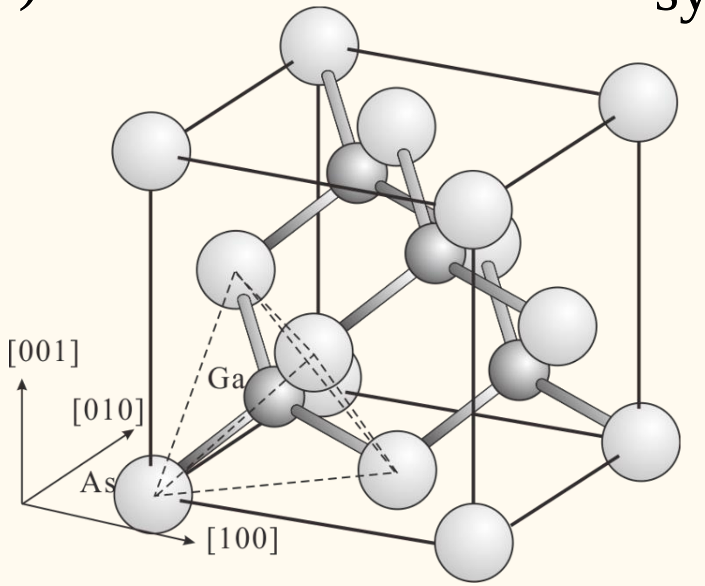
Crystals: Spatially periodic structures

Unit of spatial repetition

Primitive cell: unit of spatial repetition with smallest number of atoms

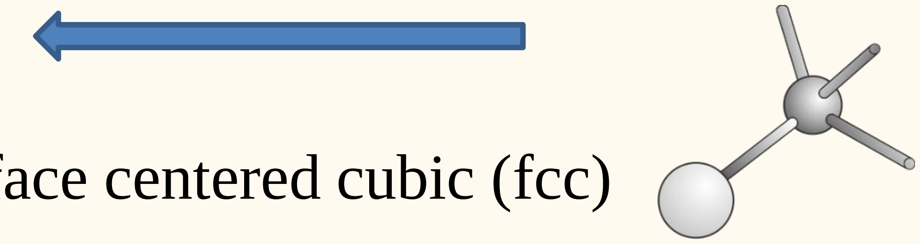
Unit cell: unit of spatial repetition taken as for human to find symmetry of the crystal

ex) GaAs



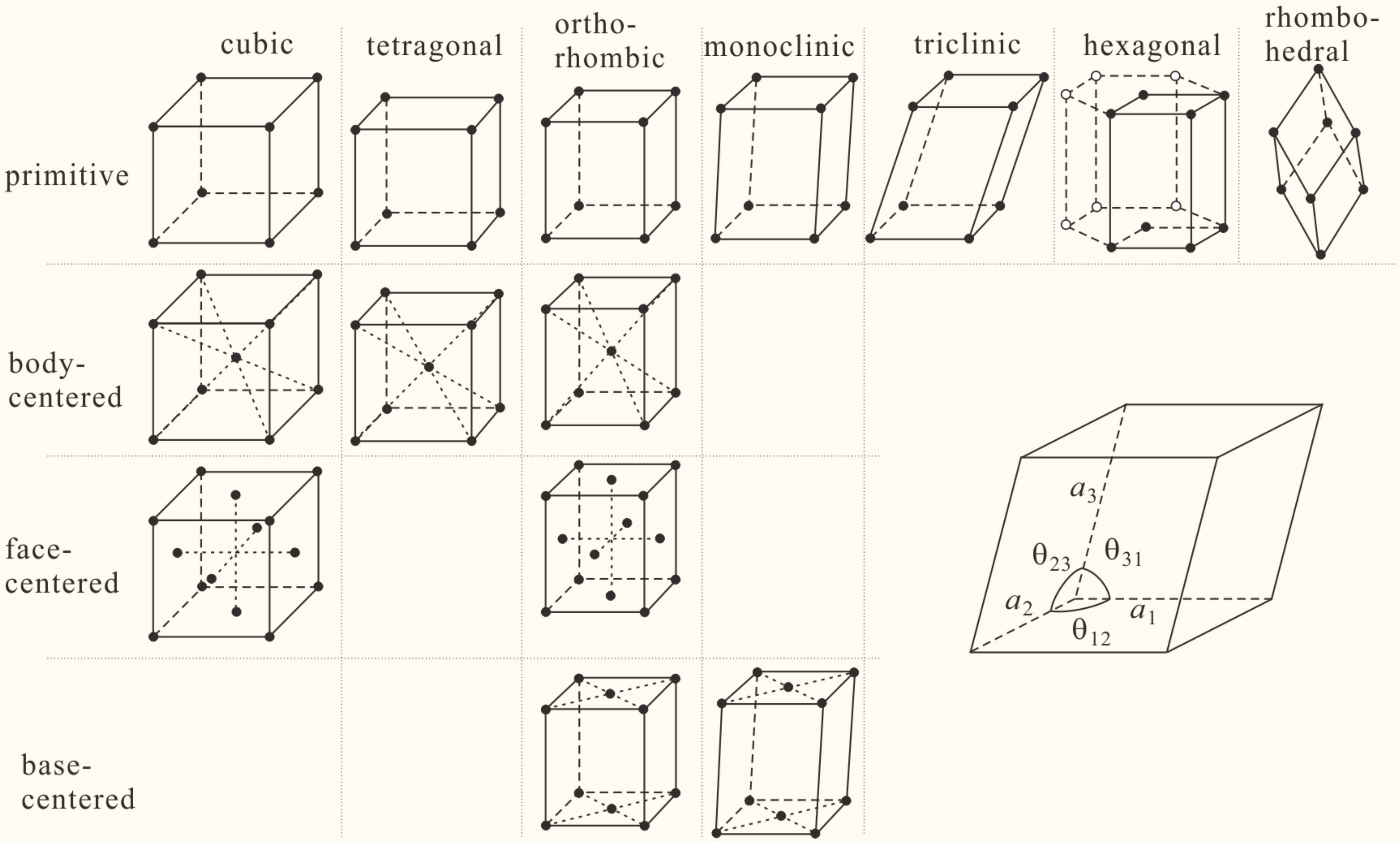
Unit cell

face centered cubic (fcc)



Primitive cell

Bravais lattices



Lattice: spatial repetition of the unit structure.

$$\boldsymbol{r}' = \boldsymbol{r} + \sum_{i=1,2,3} l_i \boldsymbol{a}_i = \boldsymbol{r} + \boldsymbol{R}$$

l_i: integers, $\boldsymbol{a}_i$: primitive (translation) vector

$\boldsymbol{R}$: lattice vector

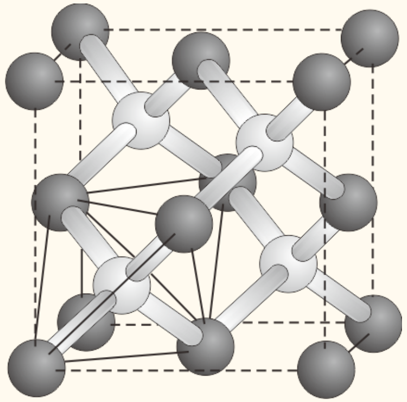
Lattice potential $U(\boldsymbol{r})$ $\quad U(\boldsymbol{r}) = \sum_{\boldsymbol{G}} U_{\boldsymbol{G}} e^{i\boldsymbol{G}\boldsymbol{r}}$

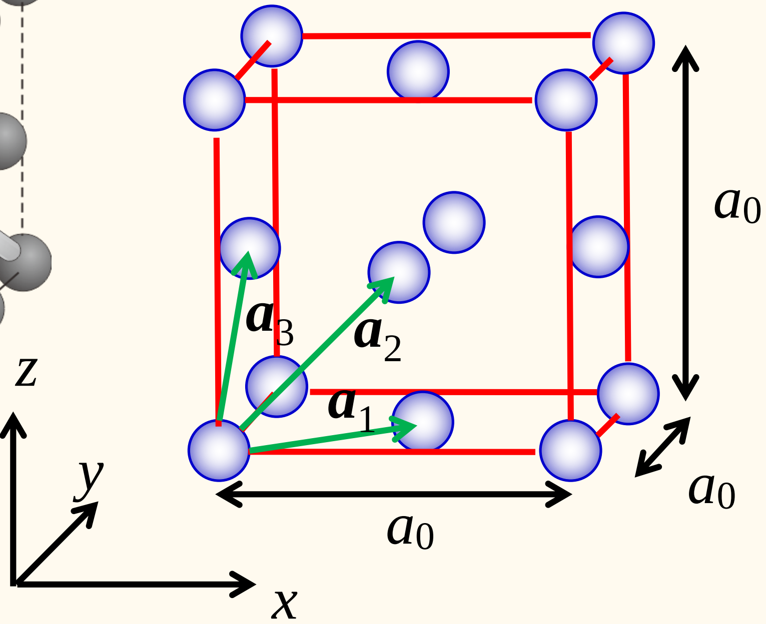
$$U(\boldsymbol{r} + \boldsymbol{R}) = U(\boldsymbol{r})$$

$$\boldsymbol{G} \cdot \boldsymbol{R} = 2\pi n \quad (n : \text{integer}), \quad \therefore e^{i\boldsymbol{G}\cdot\boldsymbol{R}} = 1$$

$\boldsymbol{G}$: reciprocal lattice vector

ex) diamond structure (fcc)





$$\boldsymbol{a}_1 = \frac{a_0}{2}(\boldsymbol{e}_x + \boldsymbol{e}_y), \quad \boldsymbol{a}_2 = \frac{a_0}{2}(\boldsymbol{e}_y + \boldsymbol{e}_z),$$
$$\boldsymbol{a}_3 = \frac{a_0}{2}(\boldsymbol{e}_z + \boldsymbol{e}_x)$$

Lattice, reciprocal lattice (2)

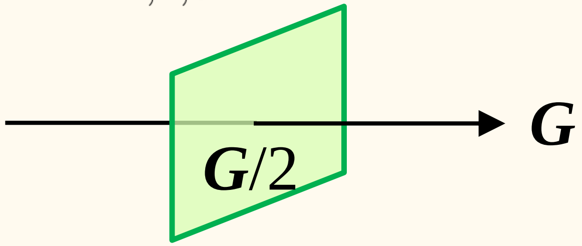
$$|A| \equiv \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$$

$$\boldsymbol{b}_1 = \frac{2\pi \boldsymbol{a}_2 \times \boldsymbol{a}_3}{|A|}, \quad \boldsymbol{b}_2 = \frac{2\pi \boldsymbol{a}_3 \times \boldsymbol{a}_1}{|A|},$$

$$\boldsymbol{b}_3 = \frac{2\pi \boldsymbol{a}_1 \times \boldsymbol{a}_2}{|A|}$$

primitive reciprocal vectors

$$\boldsymbol{G} = \sum_{i=1,2,3} h_i \boldsymbol{b}_1, \quad (h_i\text{: integer})$$



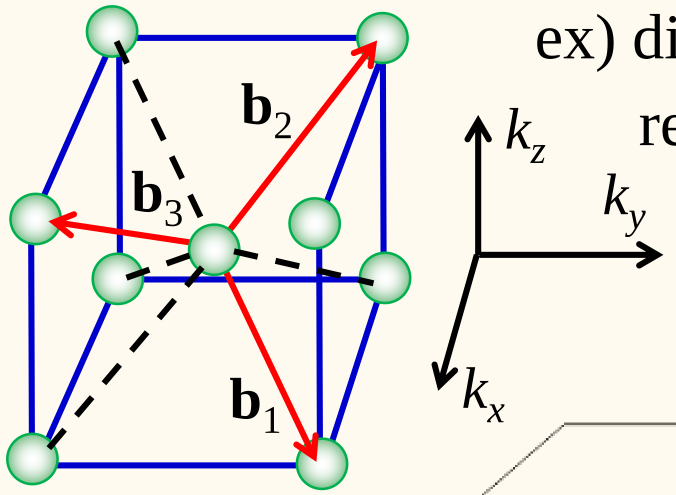
Plane that cuts ***G*** at ***G***/2 vertically

→ unit cell in the reciprocal lattice:

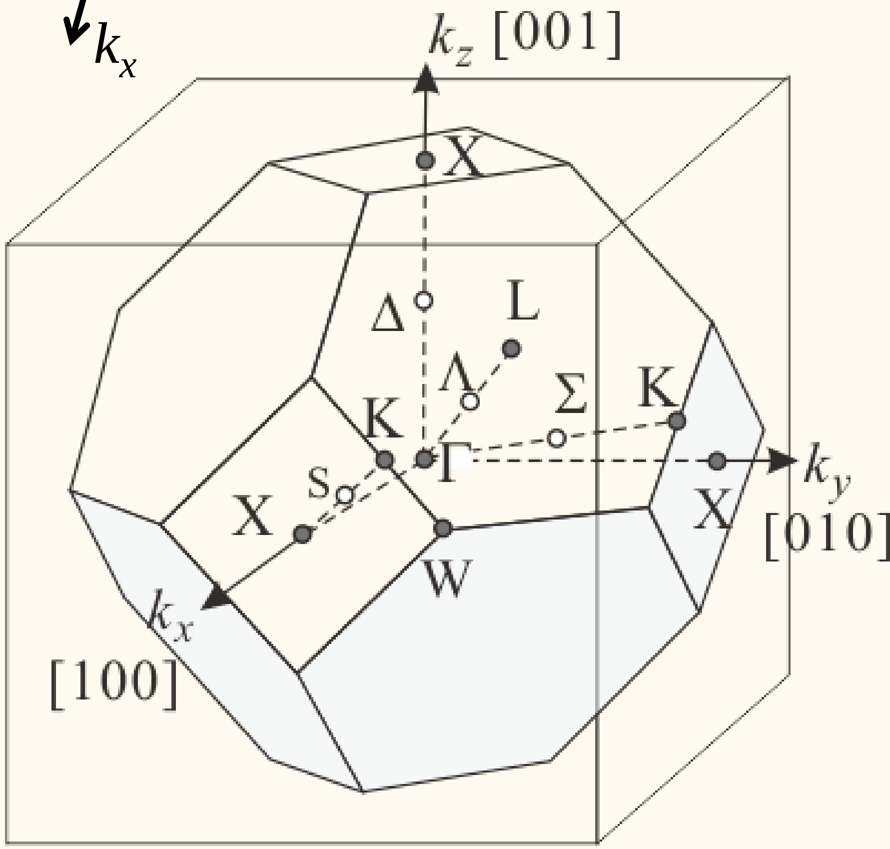
Brillouin zone

ex) diamond structure (fcc)

reciprocal lattice: bcc



First Brillouin zone

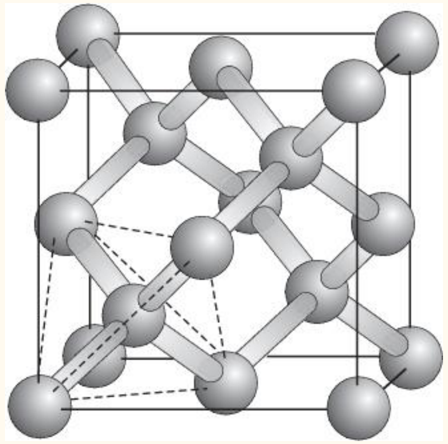


Points with high symmetries:

Γ, X, L, W

Inorganic crystals often used as semiconductors: Group IV

Diamond structure (fcc)



silicon

II	III	IV	V	VI
4 Be ベリリウム 9.012182	5 B ホウ素 10.811	6 C 炭素 12.0107	7 N 窒素 14.0067	8 O 酸素 15.9994
12 Mg マグネシウム 24.305	13 Al アルミニウム 26.98153...	14 Si ケイ素 28.0855	15 P リン 30.973762	16 S 硫黄 32.065
30 Zn 亜鉛 65.38	31 Ga ガリウム 69.723	32 Ge ゲルマニウム 72.63	33 As ヒ素 74.9216	34 Se セレン 78.96
48 Cd カドミウム 112.411	49 In インジウム 114.818	50 Sn スズ 118.71	51 Sb アンチモン 121.76	52 Te テルル 127.6

(α-Sn)

diamond

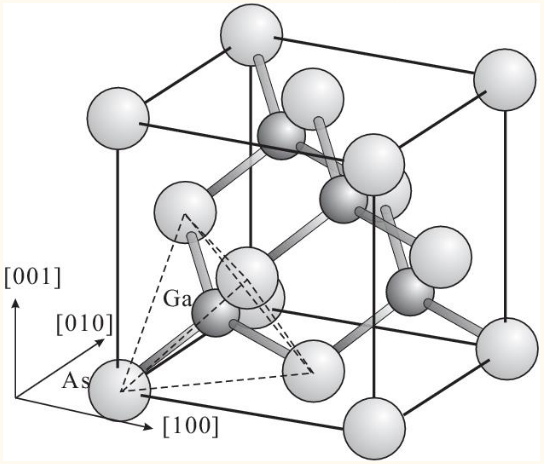
germanium

SiC

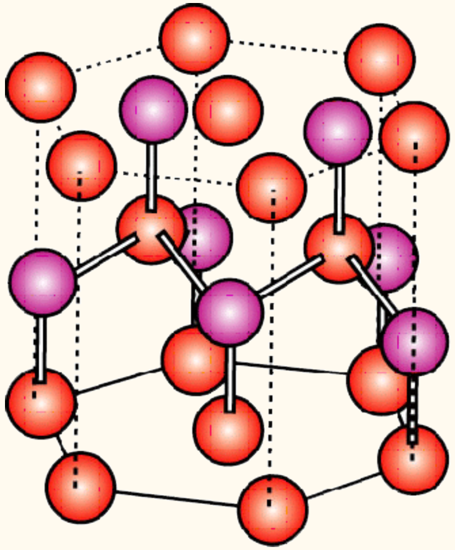
Si_xGe_{1-x}

Inorganic crystals often used as semiconductors: Group III-V

Zinc-blende (fcc)



Wurzeit (hexagonal)

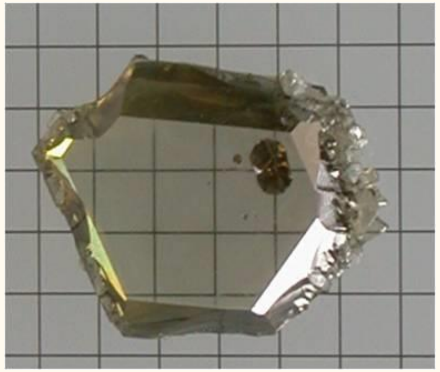


GaAs

(ZB)

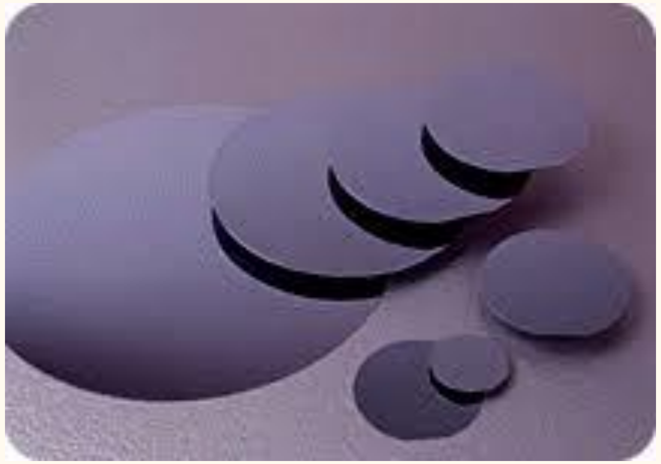
GaN

(WZ)

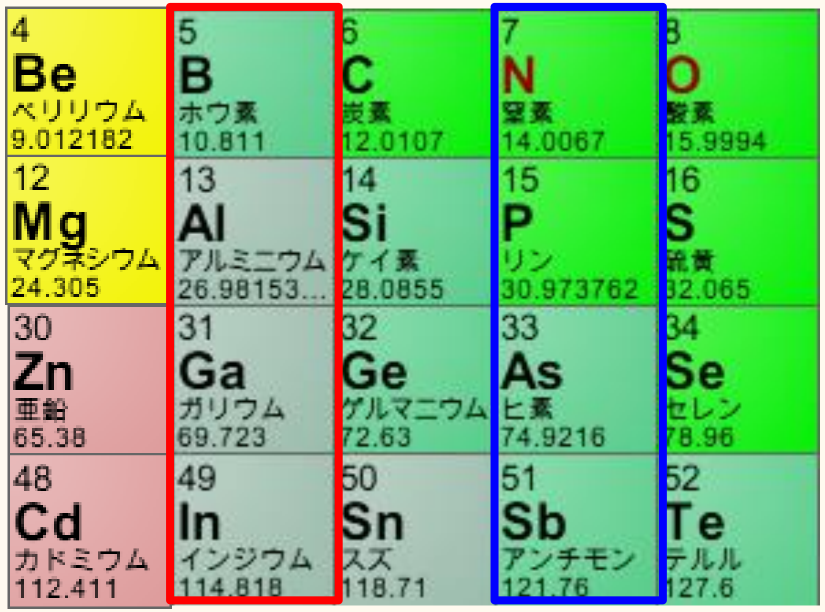


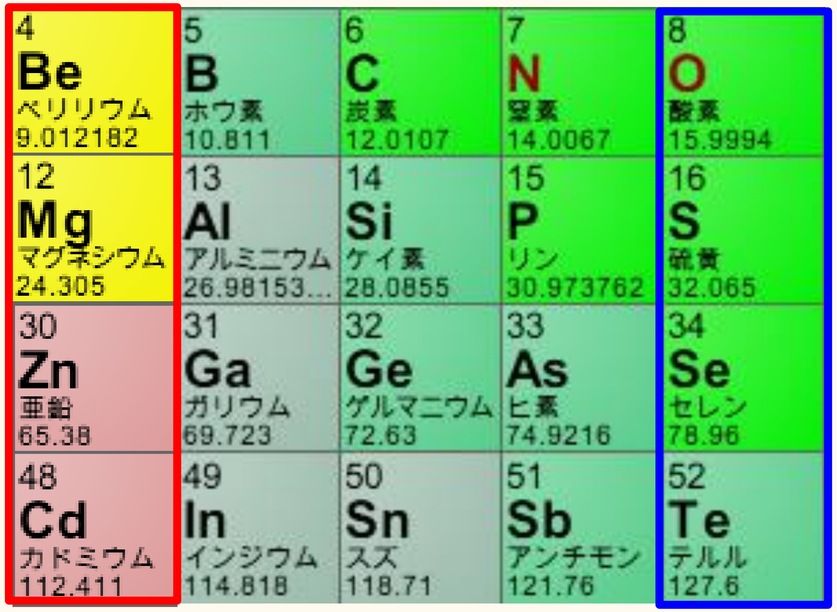
CdTe

(ZB)

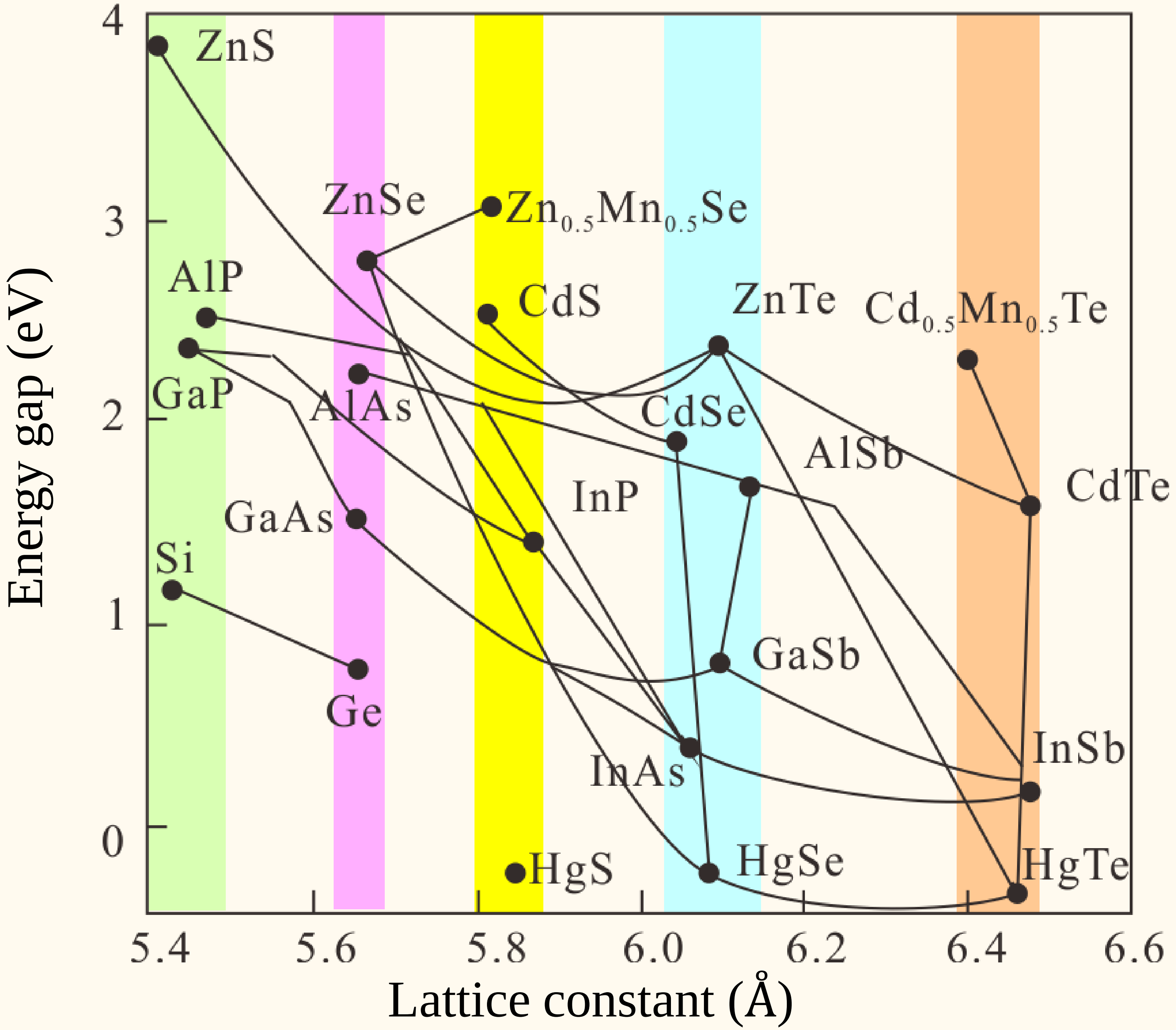


II III IV V VI





Energy gaps and lattice constants of representative (cubic) semiconductors



Room temperature

Colored stripes:

Lattice matching groups

→ Heterojunctions are available

Lines: Mixed crystals

GaN (Wurzeit)

a = 3.19 Å, c = 5.19 Å

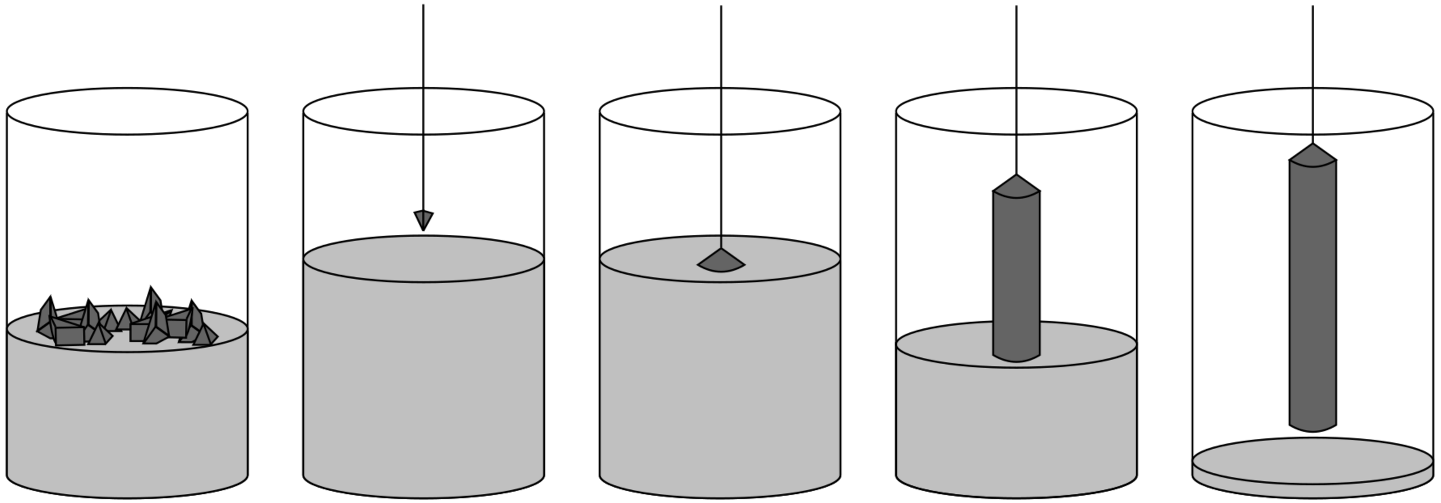
3.4 eV (RT)

Various methods for semiconductor crystal growth

- Bulk growth
  - Vertical
    - Czochralski
    - Bridgman
    - Floating zone melting
  - Horizontal
    - Horizontal Bridgman
    - Zone melting
- Thin film growth
  - Chemical Vapor Deposition (Vapor Phase Epitaxy)
    - Thermal decomposition
      - chloride
      - organic
    - Plasma
    - metal
  - Liquid Phase Epitaxy
  - Molecular Beam Epitaxy
  - Atomic Layer Deposition
  - Laser ablation

“Tree-like” classification is actually difficult.

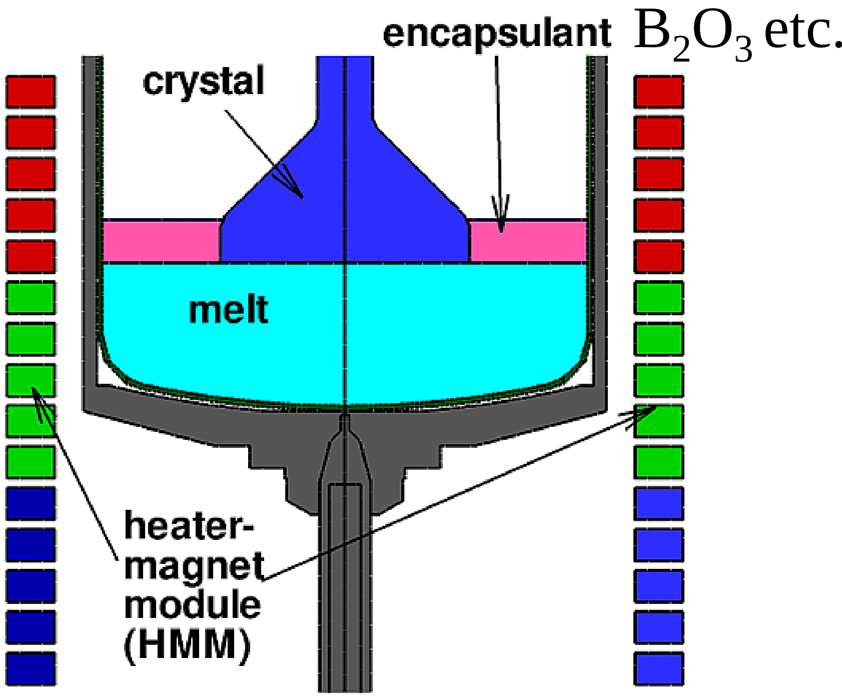
Crystal growth: Czochralski method



Melting of polysilicon, doping | Introduction of the seed crystal | Beginning of the crystal growth | Crystal pulling | Formed crystal with a residue of melted silicon

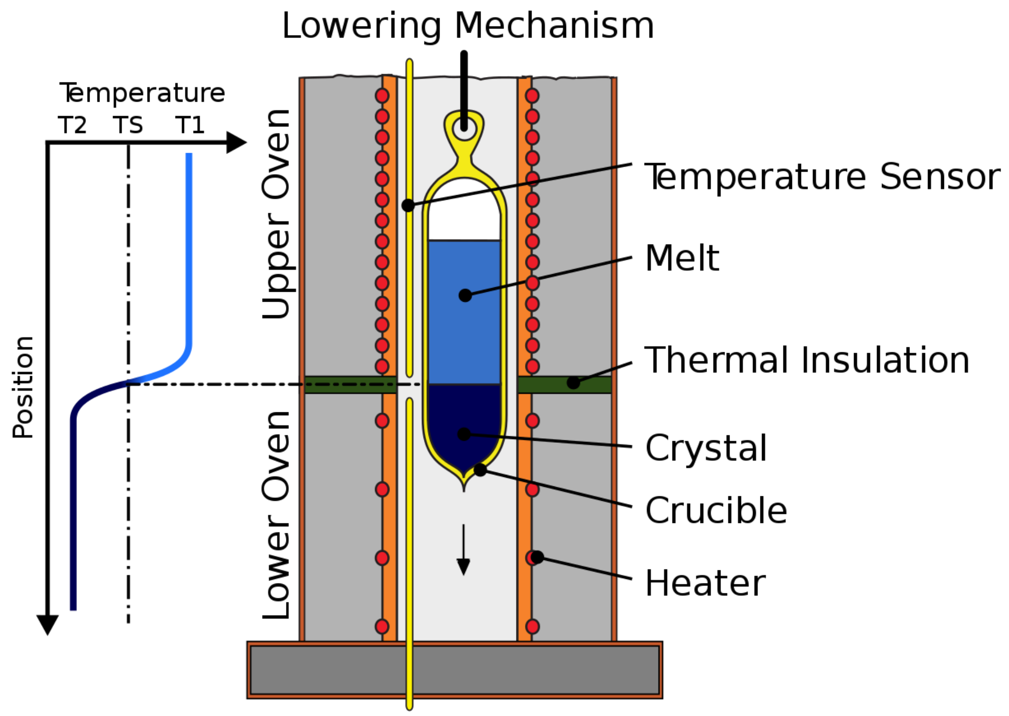
Czochralski method for silicon (Wikipedia)

Liquid encapsulated Czochralski (LEC)
(GaAs, InP, etc. high vapor pressure materials)



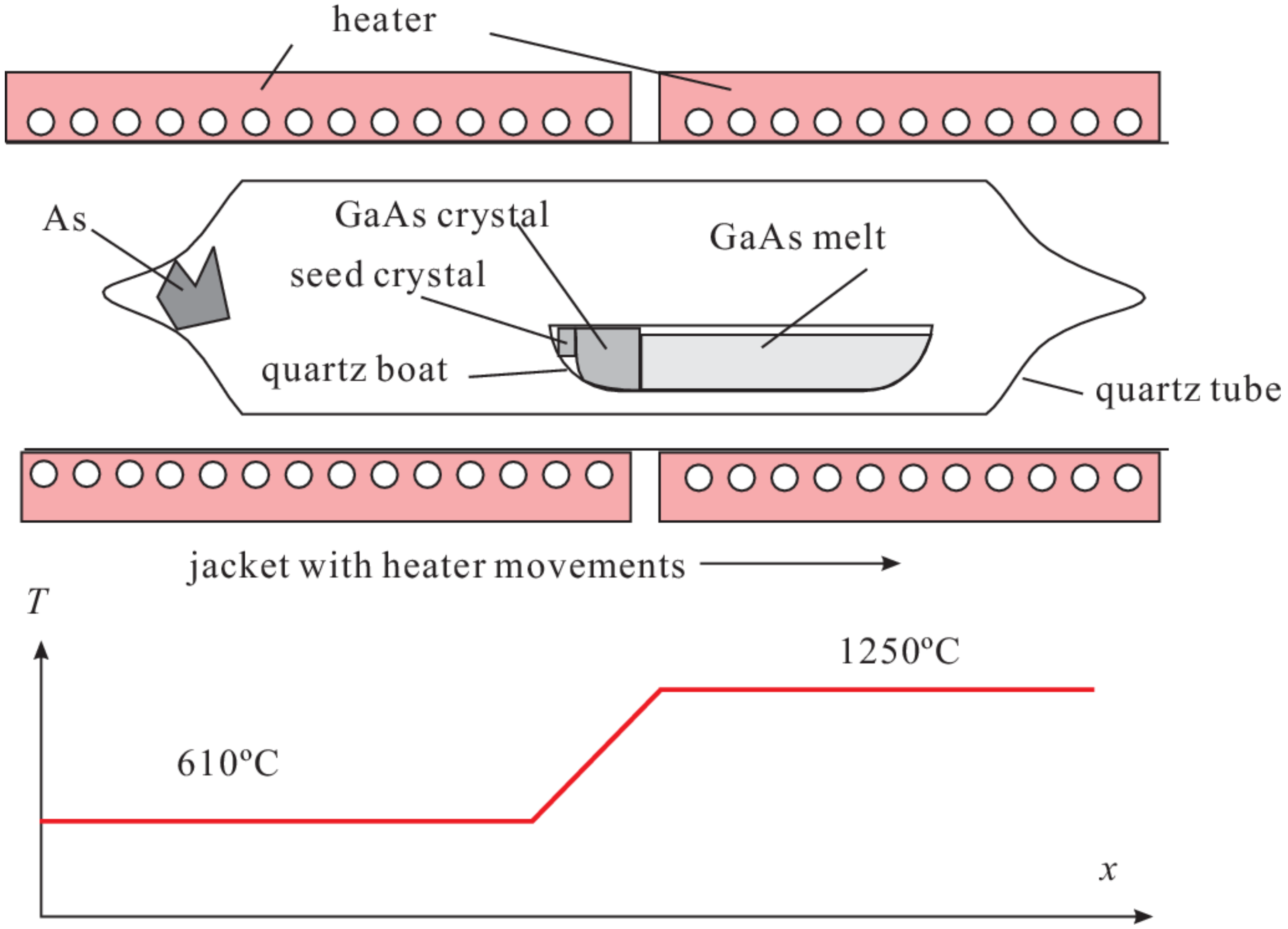
Bridgman methods

Bridgman-Stockbarger method



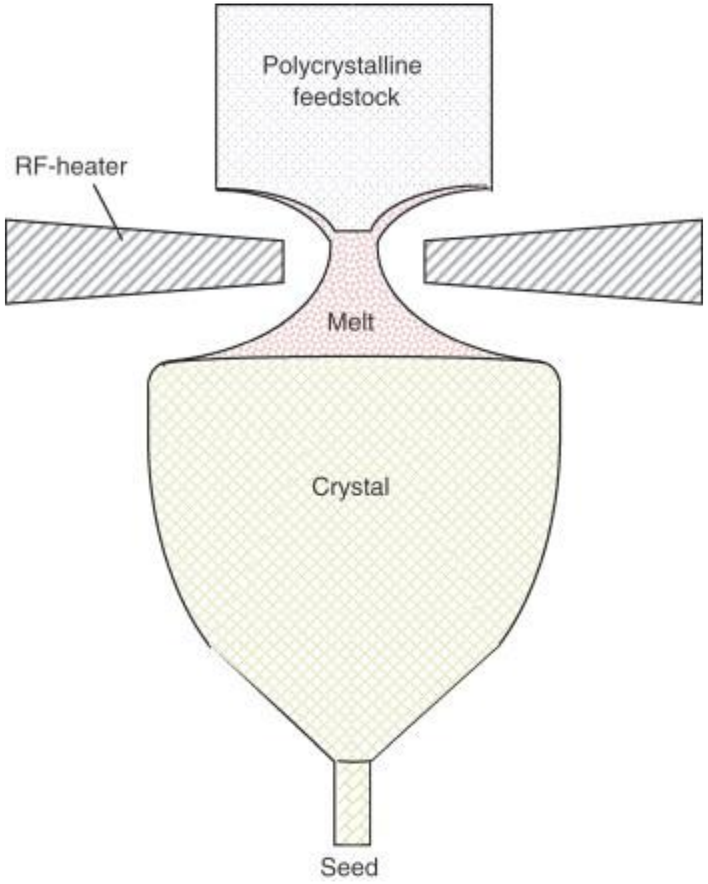
From Wikipedia

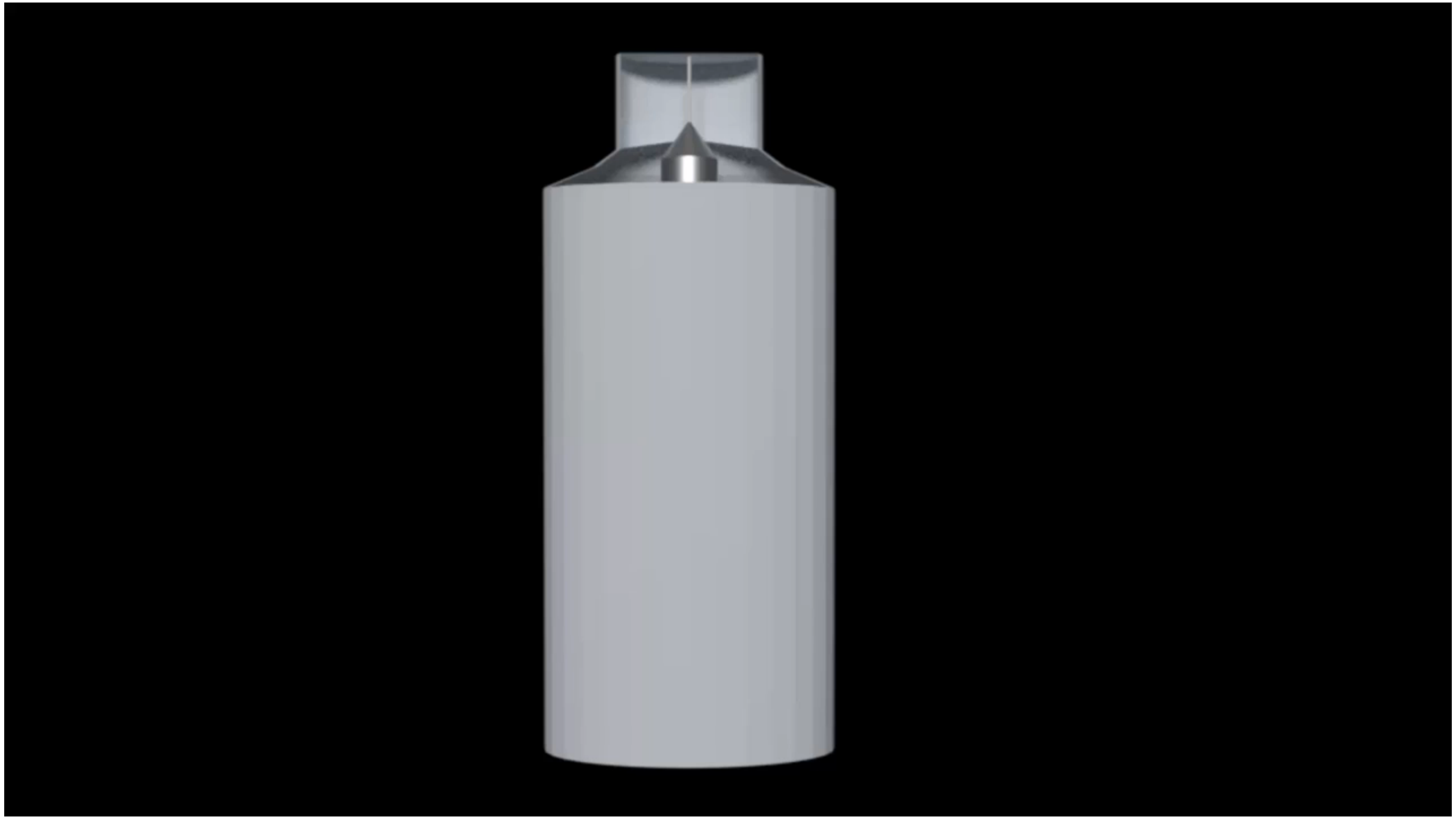
Horizontal Bridgeman (HB) process



temperature gradient freezing method

Floating zone method

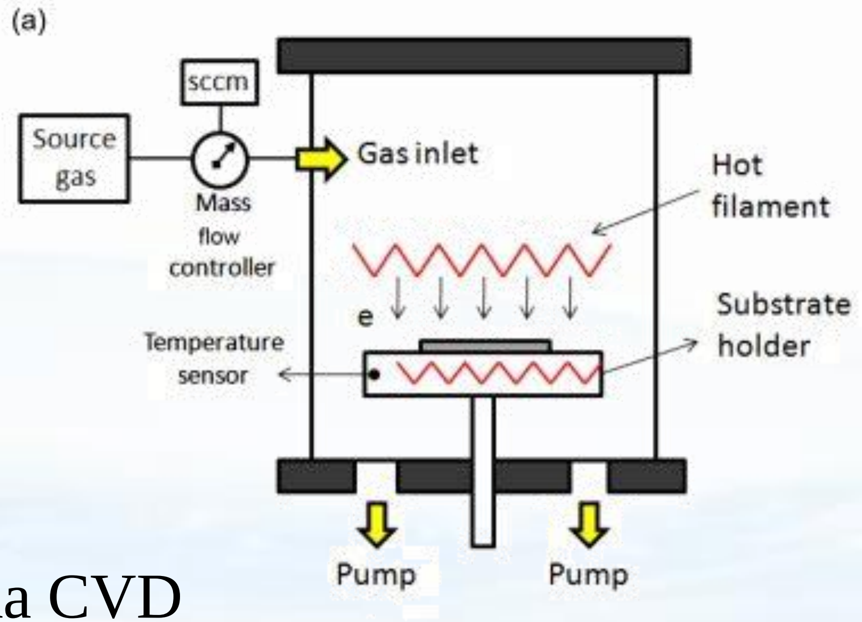




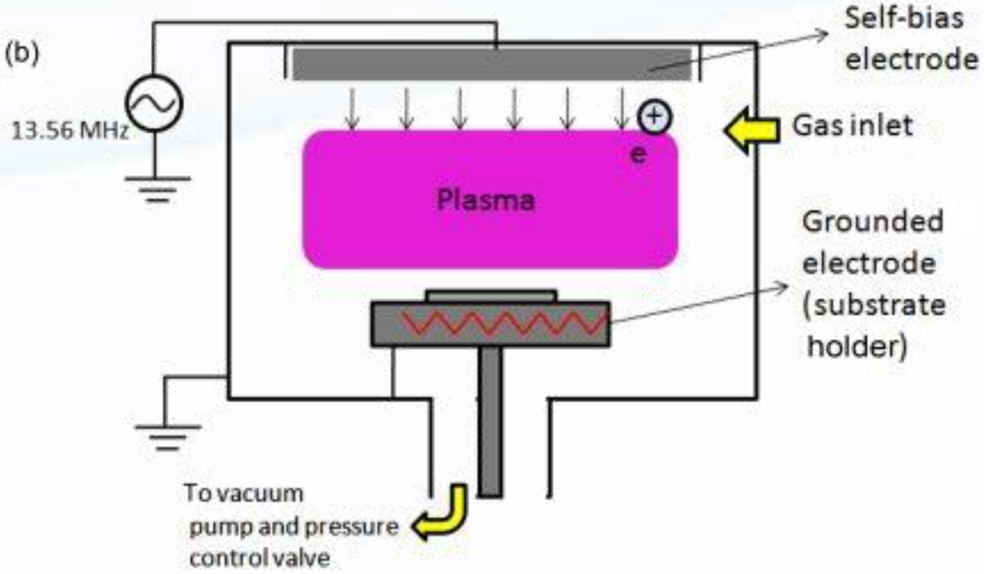
https://www.youtube.com/watch?v=jPijg8NIamo

Chemical vapor deposition (CVD), metal-organic CVD (MOCVD)

Thermal decomposition

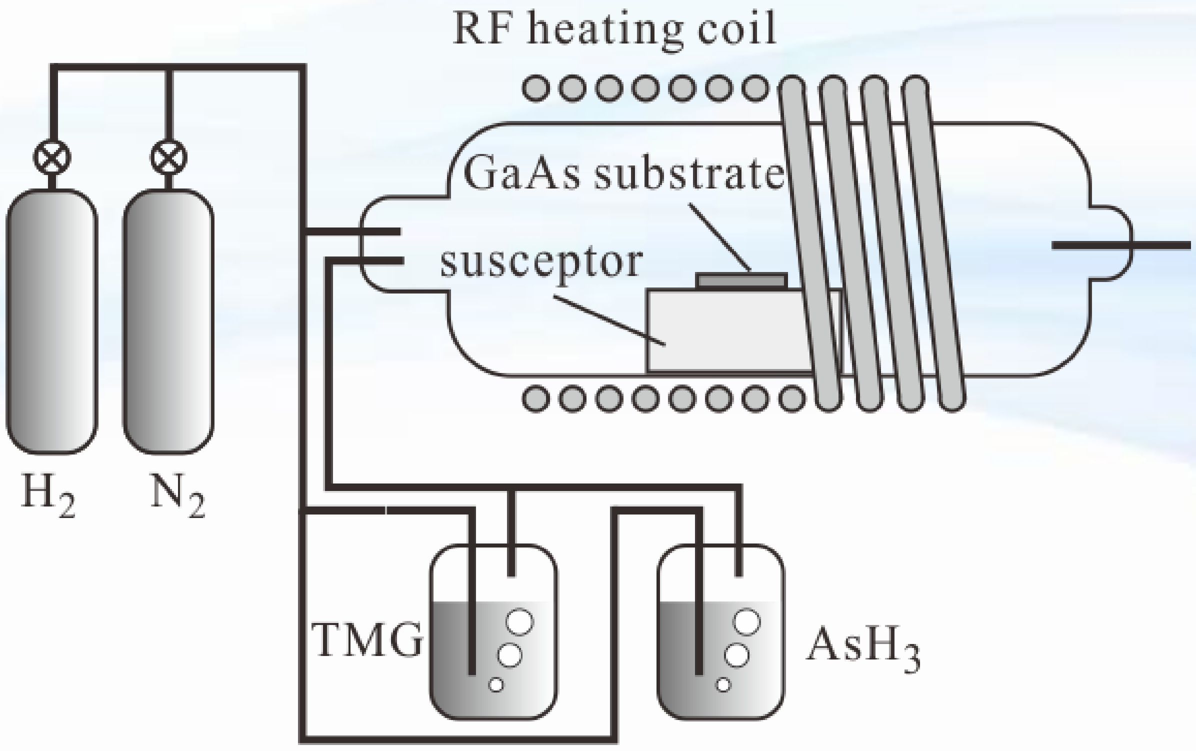


Plasma CVD



MOCVD

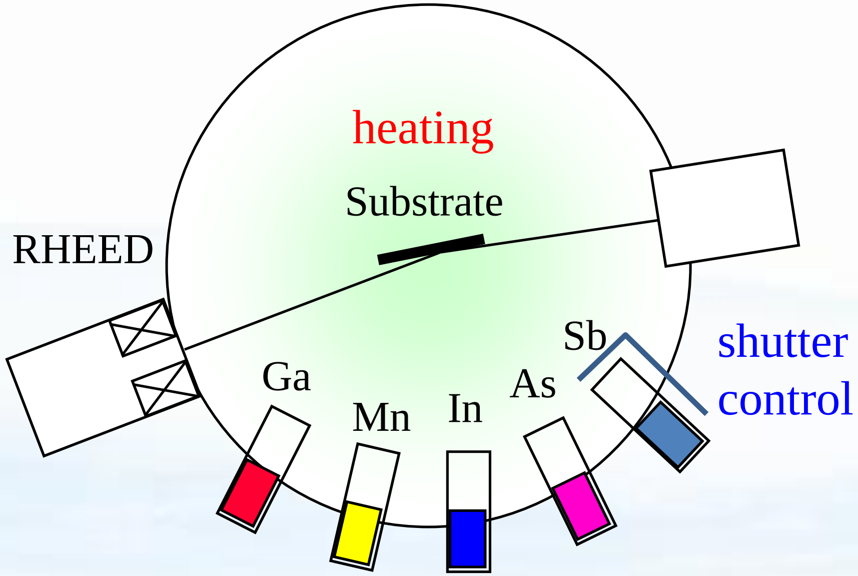
(organometallic vapor phase epitaxy, OMVPE)



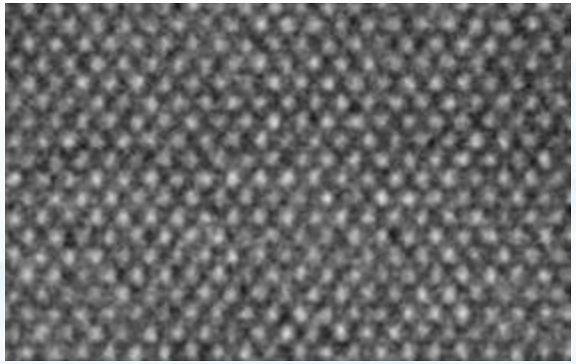
Organic metal gases

Molecular Beam Epitaxy (MBE)

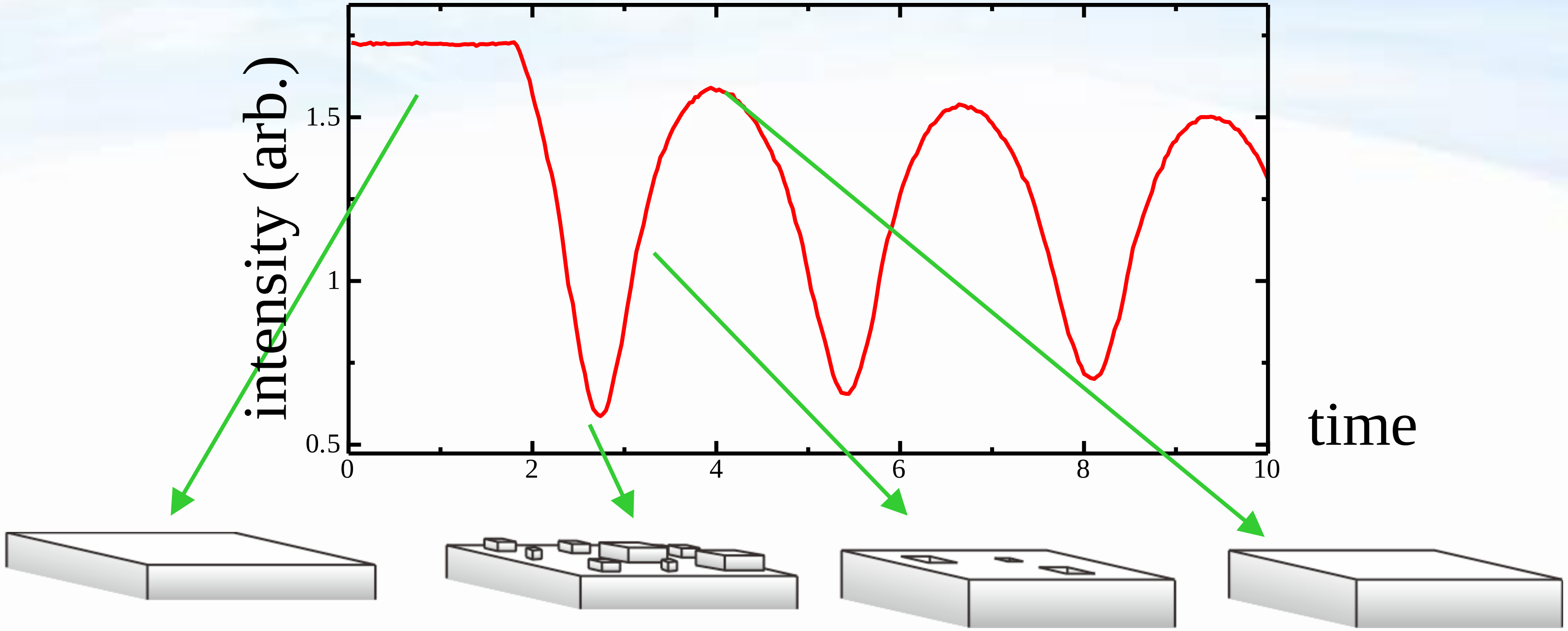
Ultra-high vacuum evaporation



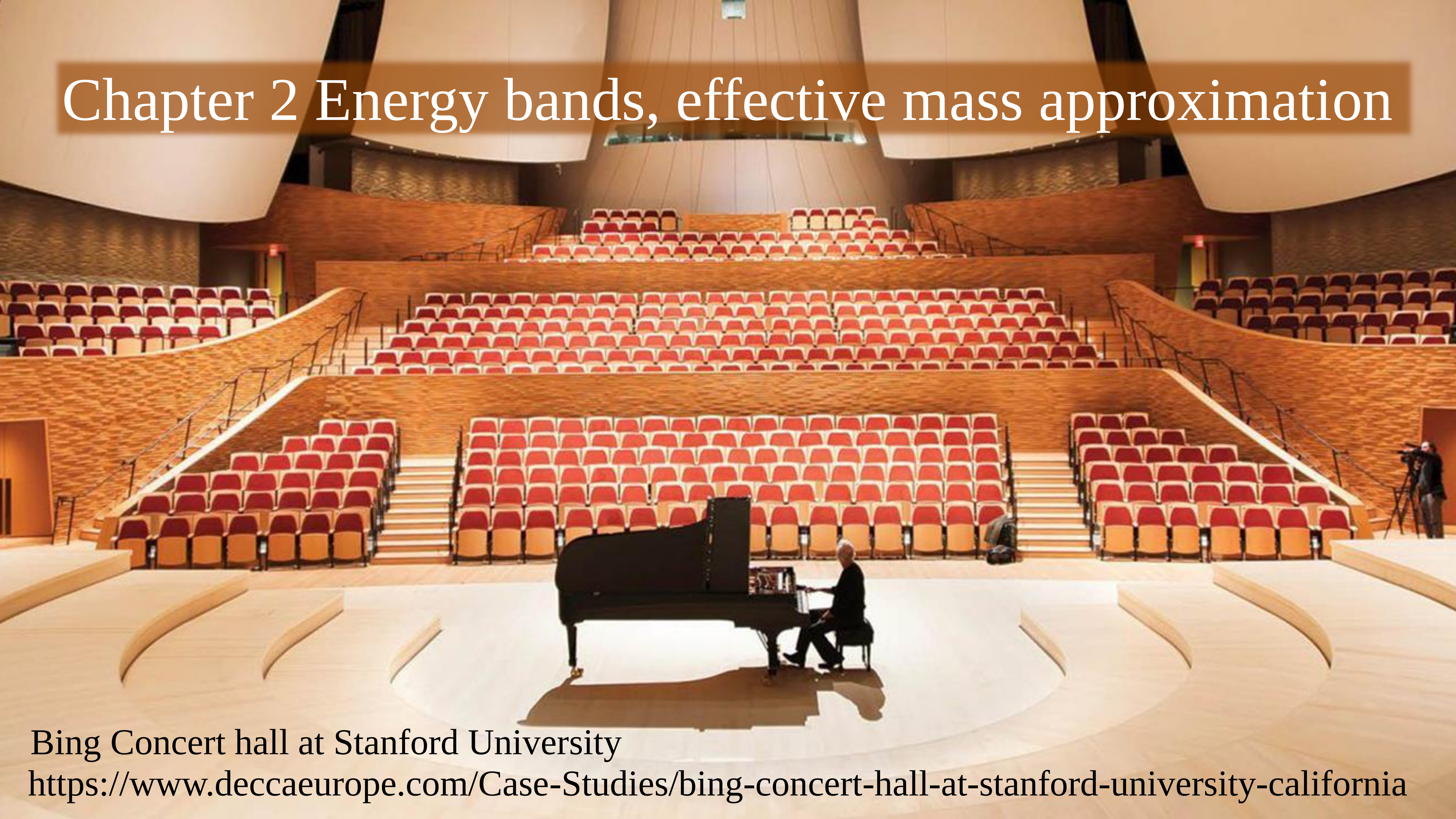
Refractive high energy electron diffraction (RHEED)



HRTEM



Chapter 2 Energy bands, effective mass approximation



Bing Concert hall at Stanford University
https://www.deccaeurope.com/Case-Studies/bing-concert-hall-at-stanford-university-california

Bloch theorem and nearly free electron model

Bloch theorem

Eigenstates in lattice potential:

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r})\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}) = u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$\boldsymbol{R}$: Lattice translation vector
n: band index

One-dimensional system with a weak periodic potential

$V(x) = 2V_0\cos(k_\mathrm{w}x)$ ($k_\mathrm{w} = 2\pi/a$, a: lattice const.)

$\langle k'|V|k\rangle = V_0\langle k'|(e^{ik_\mathrm{w}x}+e^{-ik_\mathrm{w}x})|k\rangle = V_0(\delta_{k'k+k_\mathrm{w}}+\delta_{k'k-k_\mathrm{w}})$ Perturbation is important from $k \pm k_w$

Energy crossing between $|k\rangle$ and $|k-k_w\rangle$ occurs around $k = k_w/2$

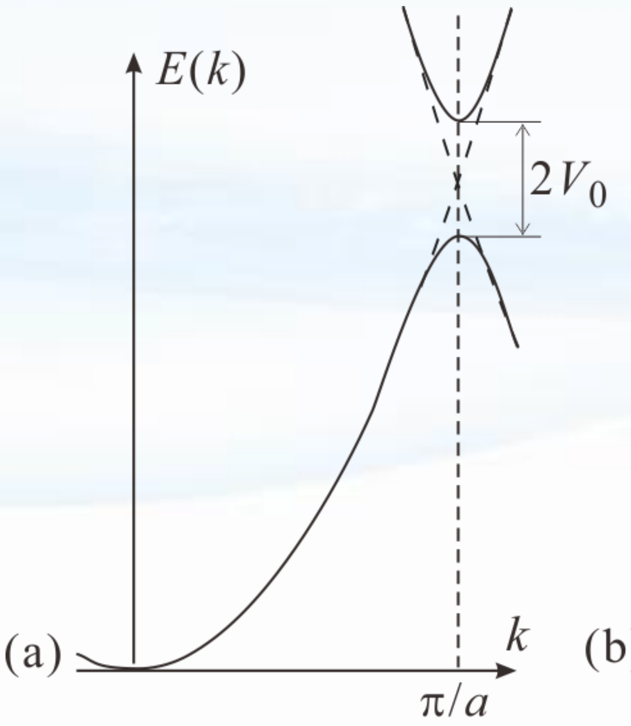
Hamiltonian around $k = k_w/2$ in the space formed with $|k\rangle$ and $|k-k_w\rangle$

$$\mathscr{H} = \begin{bmatrix} \frac{\hbar^2k^2}{2m_0} & V_0 \\ V_0 & \frac{\hbar^2(k-k_\mathrm{w})^2}{2m_0} \end{bmatrix} \approx \begin{bmatrix} \epsilon_\mathrm{z} - \frac{\hbar^2 k_\mathrm{w}\Delta k}{2m_0} & V_0 \\ V_0 & \epsilon_\mathrm{z} + \frac{\hbar^2 k_\mathrm{w}\Delta k}{2m_0} \end{bmatrix} \qquad k = k_\mathrm{w}/2 - \Delta k$$

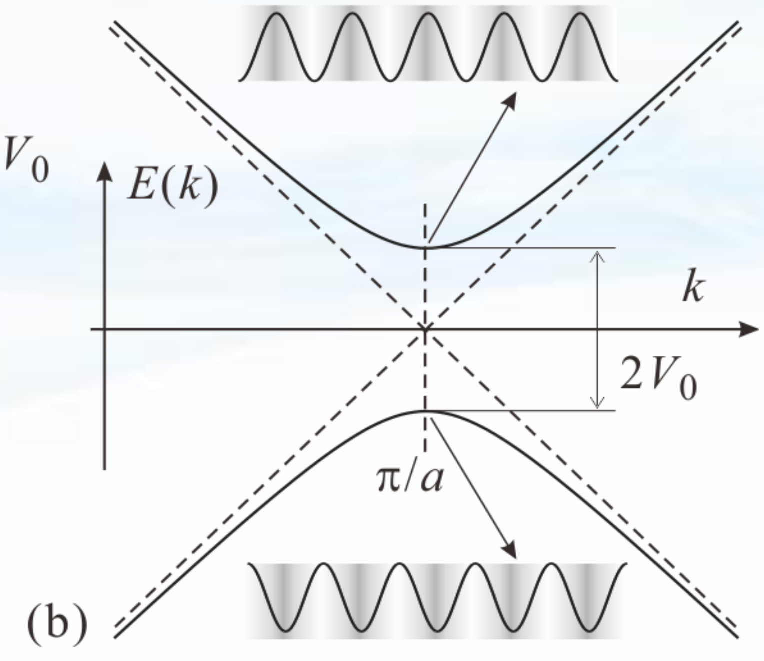
Nearly free electron model (2)

$$E_{\pm} = \epsilon_{\mathrm{z}} \pm \sqrt{\epsilon_{\mathrm{z}} \frac{\hbar^2 (\Delta k)^2}{2m_0} + V_0^2} \qquad \epsilon_{\mathrm{z}} = \frac{\hbar^2 k_{\mathrm{w}}^2}{8m_0}$$

Energy gap: $\Delta k = 0 \rightarrow 2V_0$



Overall dispersion



Energy gap due to the phases of standing waves

Bloch theorem

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r}) \exp(i\boldsymbol{k} \cdot \boldsymbol{r})$$

Standing wave

$$e^{ik_{\mathrm{w}}x/2} \pm e^{-ik_{\mathrm{w}}x/2} = (1 \pm e^{-k_{\mathrm{w}}x}) e^{ik_{\mathrm{w}}x/2}$$
$$= \underline{(e^{k_{\mathrm{w}}x} \pm 1)} e^{-ik_{\mathrm{w}}x/2}$$

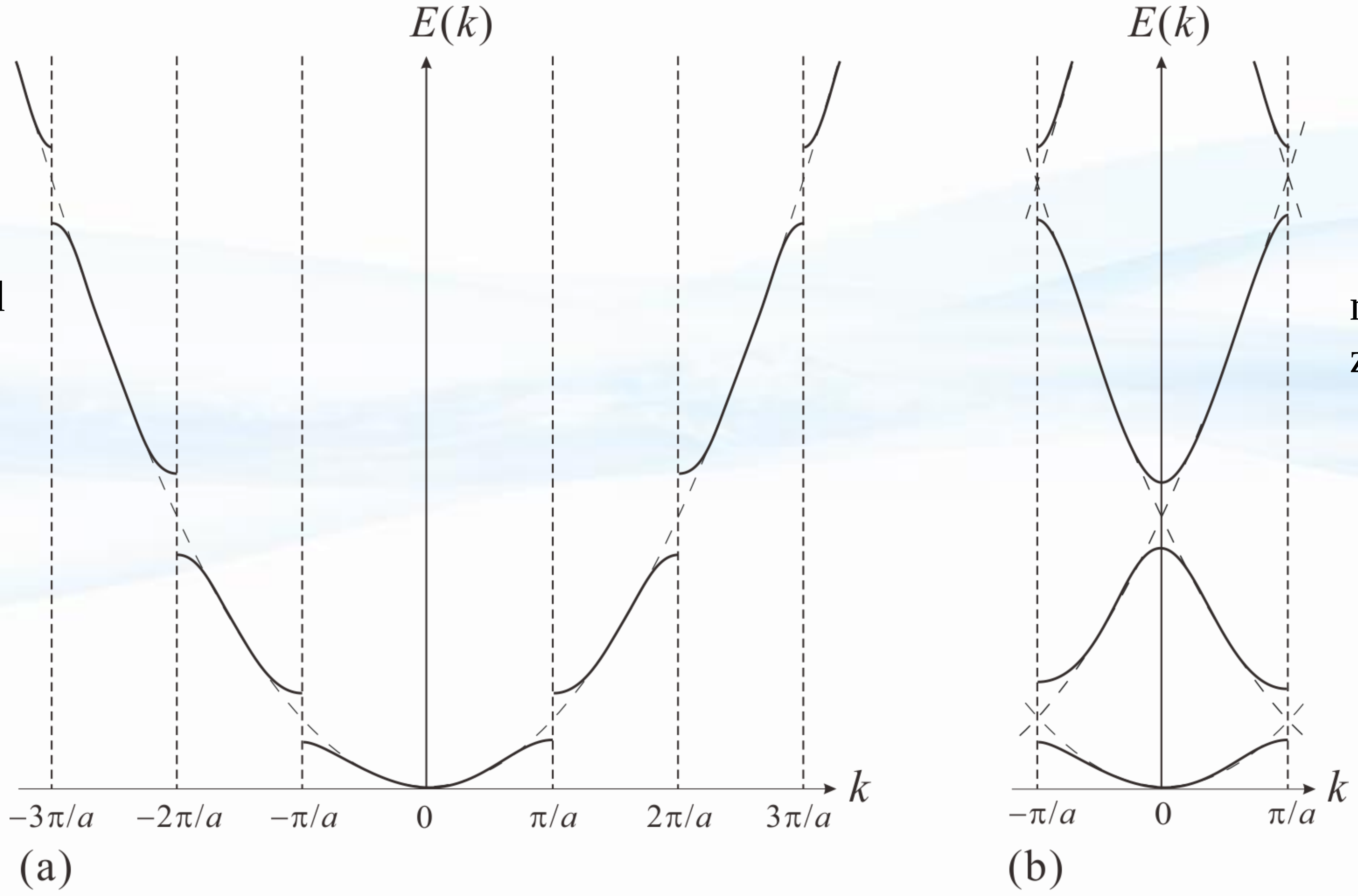
Lattice periodic function

Points $k_w/2$ and $-k_w/2$ are equivalent

Shifts from these points can be renormalized into $u_{nk}(r)$
→
Reduced zone expression

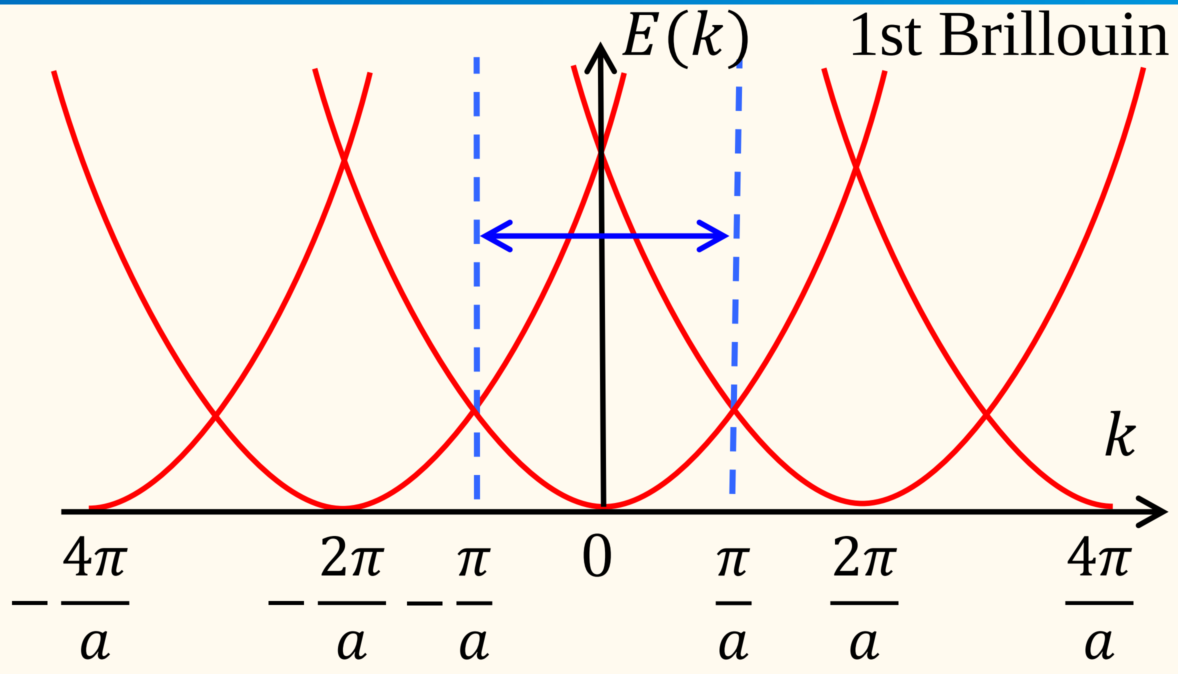
Nearly free electron model (3) Reduced zone expression

extended zone



reduced zone

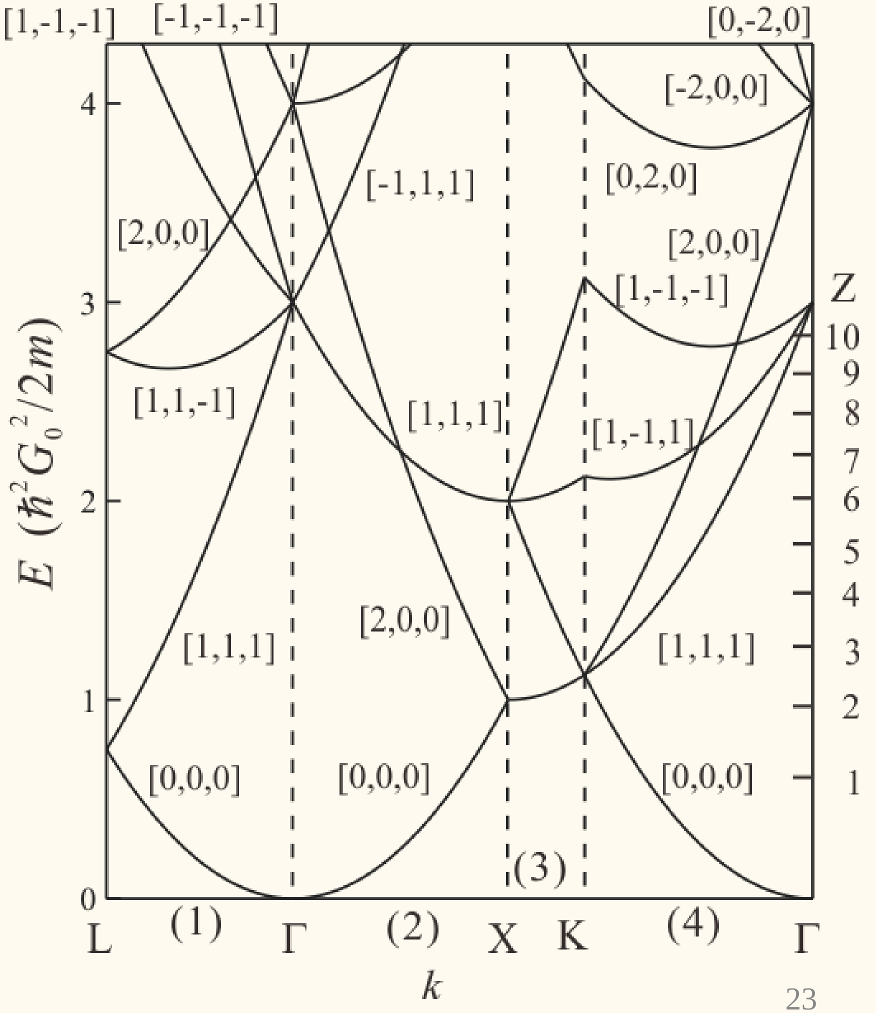
Empty lattice approximation



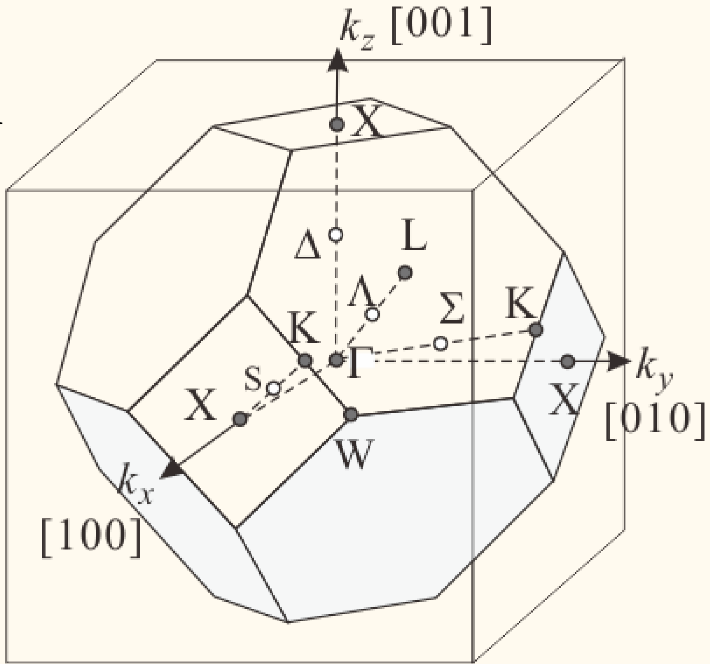
$V_0 \to 0 \qquad e^{ikx} = e^{i(k-k_\mathrm{w})x} e^{ik_\mathrm{w}x}$

The free space has a lattice periodicity.

Empty lattice expression for fcc

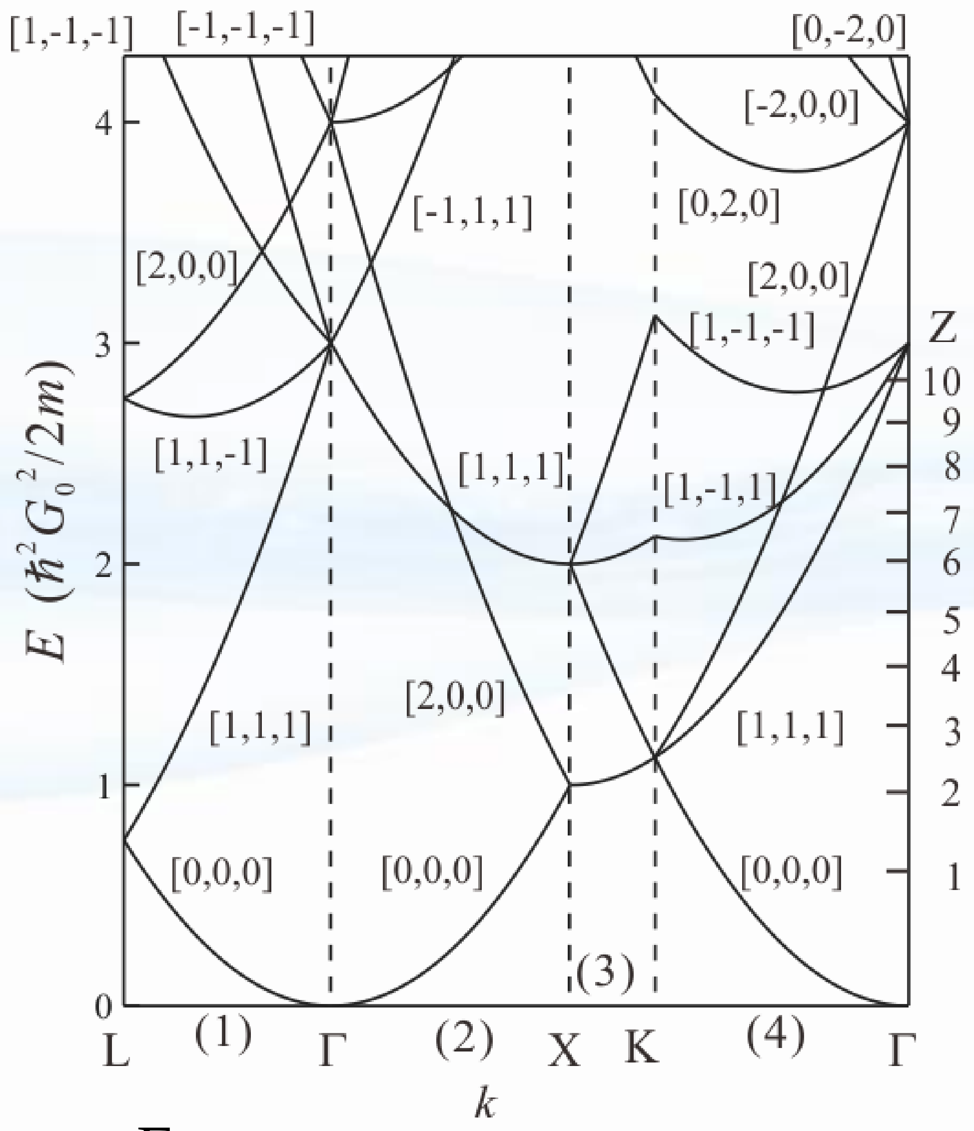


1st Brillouin zone of fcc lattice

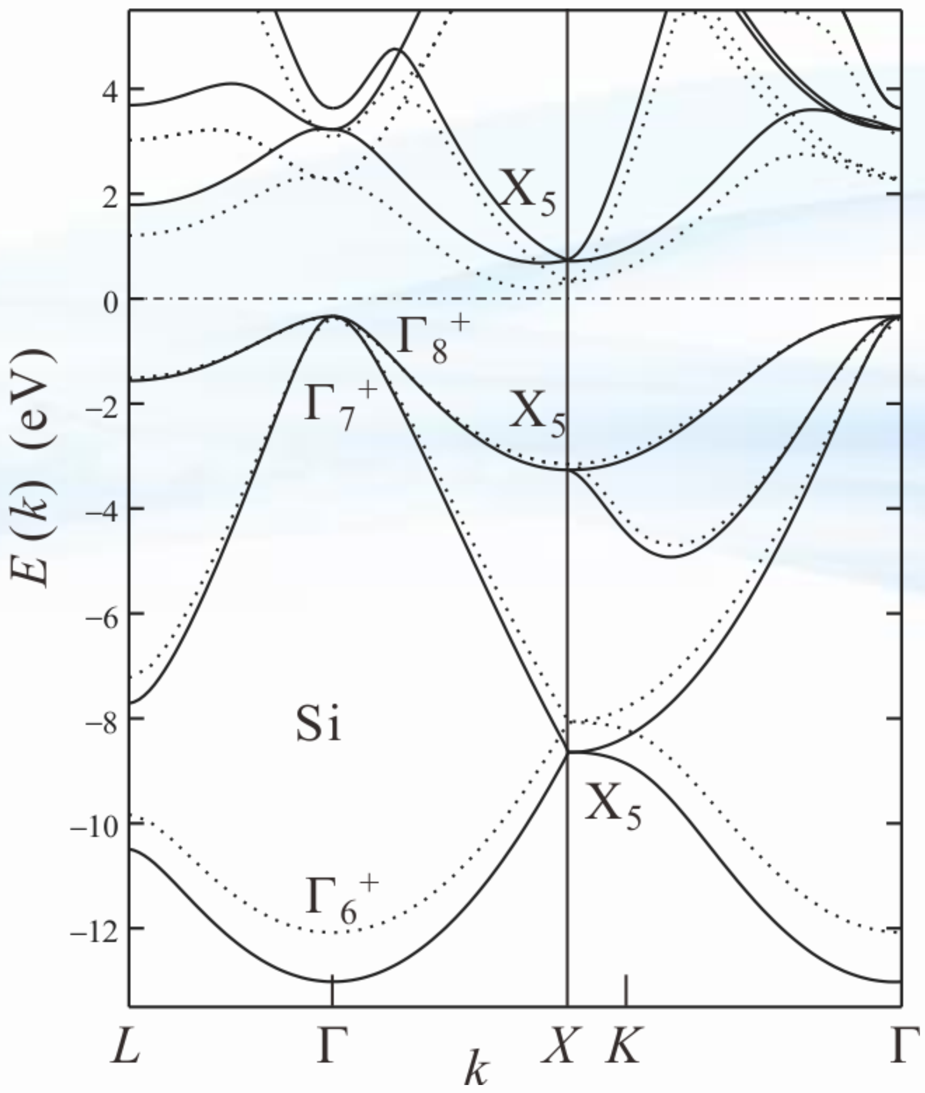


distance	Points	number
0	(0,0,0)	1
$\sqrt{3}$	(1,1,1),…	8
2	(2,0,0),…	6
$\sqrt{8}$	(2,0,2),…	12
$\sqrt{11}$	(3,1,1),…	24

Empty lattice approximation and more realistic band structure



Empty



Si pseudo potential calculation

Tight-binding approximation

Single atom on single unit cell

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

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

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

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

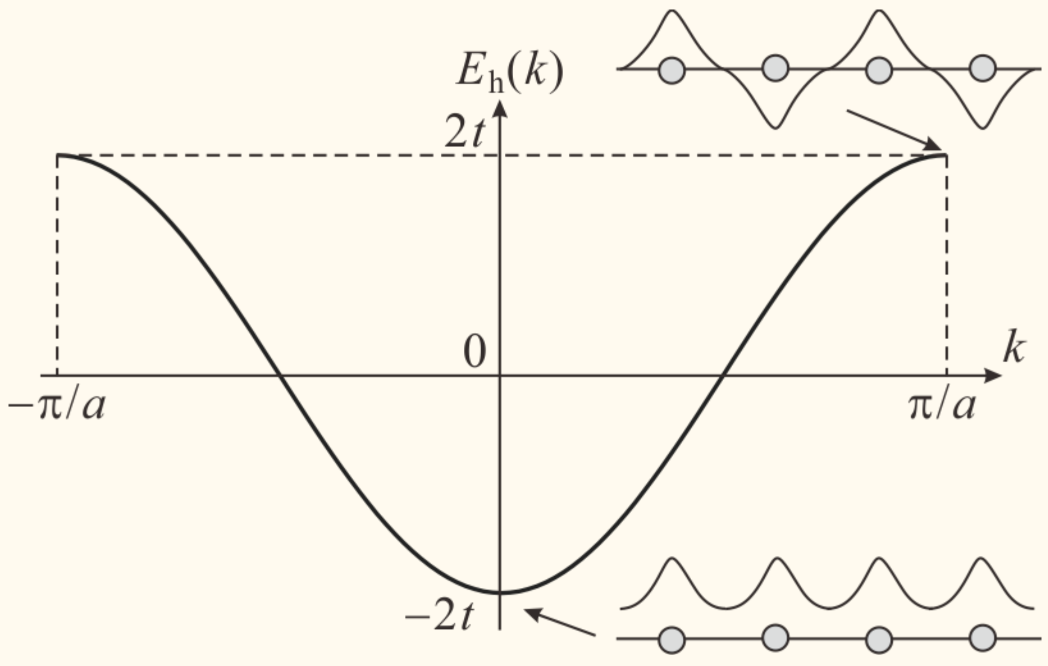
ϕ_n: eigenfunctions for $R_i = 0$

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

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

Lattice periodic function

: Bloch form



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

Tight binding approximation (2)

$$\begin{aligned}\langle\psi_{nk}|\mathscr{H}|\psi_{nk}\rangle &= N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\langle\phi_n(r-R_i)|[\hat{T}_r+V(r)]|\phi_n(r-R_j)\rangle\\ &= N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\\ &\quad\times\langle\phi_n(r-R_i)|[\hat{T}_r+u(r-R_i)+V(r)-u(r-R_i)]|\phi_n(r-R_j)\rangle\\ &= \epsilon_n + N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\langle\phi_n(r-R_i)|[V(r)-u(r-R_i))]|\phi_n(r-R_j)\rangle\\ &= \epsilon_n + \sum_{j} e^{ikR_j}\langle\phi_n(r)|[V(r)-u(r))]|\phi_n(r-R_j)\rangle.\end{aligned}$$

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

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

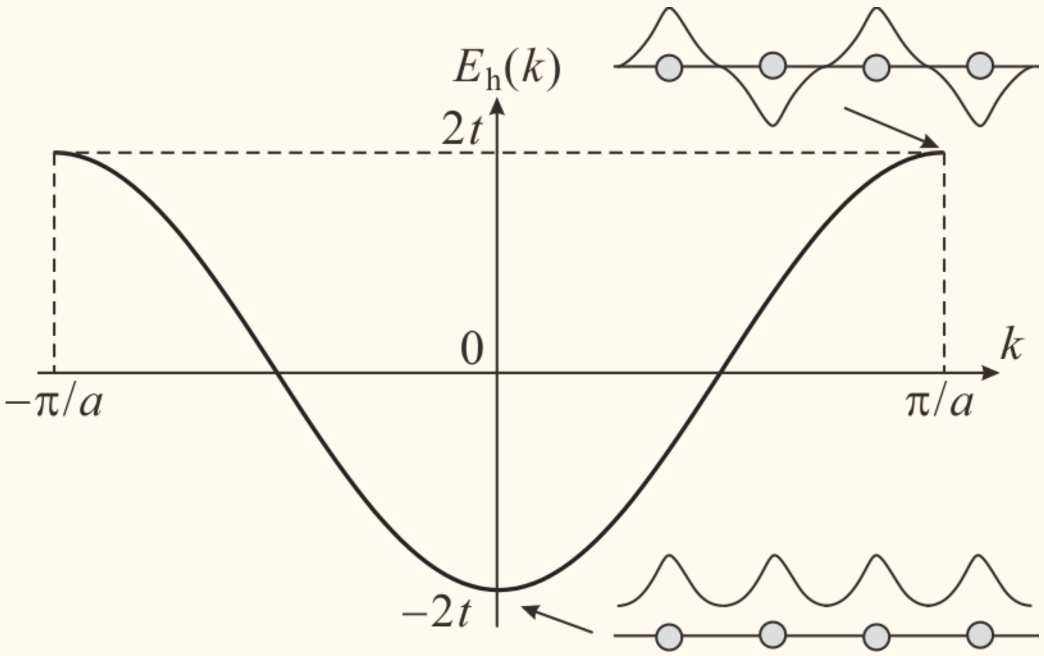
$t_n(R_j) \equiv -\langle\phi_n(r)|v(r)|\phi_n(r-R_j)\rangle$ Hopping integral

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 $4t$.



Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.14 Lecture 02

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

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

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

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

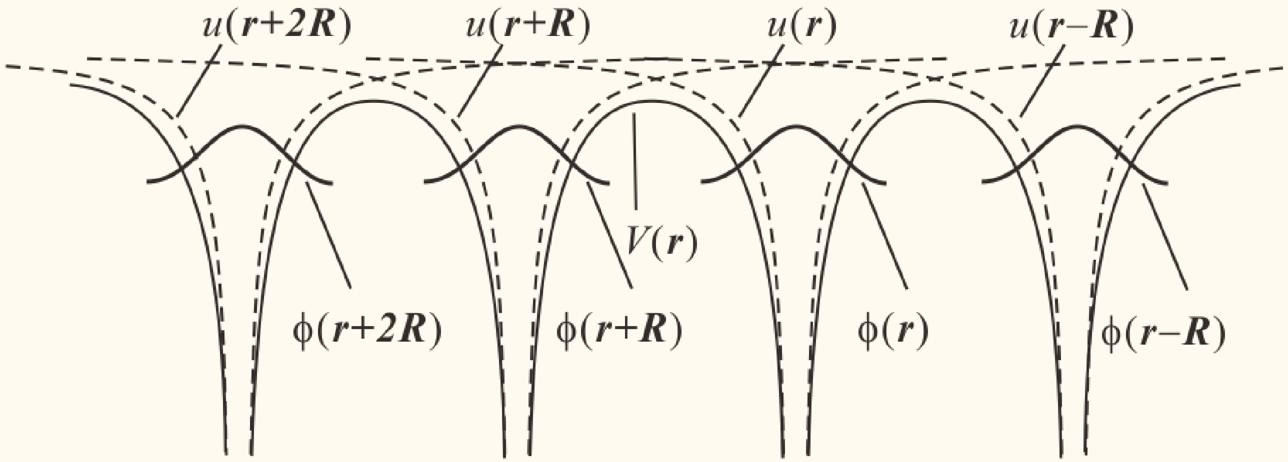
ϕ_n: eigenfunctions for $R_i = 0$

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

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

Lattice periodic function

: Bloch form



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

Tight binding approximation (2)

$$\begin{aligned}
\langle \psi_{nk} | \mathscr{H} | \psi_{nk} \rangle &= N^{-1} \sum_{i,j} e^{ik(R_j - R_i)} \langle \phi_n(r - R_i) | [\hat{T}_r + V(r)] | \phi_n(r - R_j) \rangle \\
&= N^{-1} \sum_{i,j} e^{ik(R_j - R_i)} \\
&\quad \times \langle \phi_n(r - R_i) | [\hat{T}_r + u(r - R_i) + V(r) - u(r - R_i)] | \phi_n(r - R_j) \rangle \\
&= \epsilon_n + N^{-1} \sum_{i,j} e^{ik(R_j - R_i)} \langle \phi_n(r - R_i) | [V(r) - u(r - R_i))] | \phi_n(r - R_j) \rangle \\
&= \epsilon_n + \sum_{j} e^{ikR_j} \langle \phi_n(r) | [V(r) - u(r))] | \phi_n(r - R_j) \rangle .
\end{aligned}$$

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

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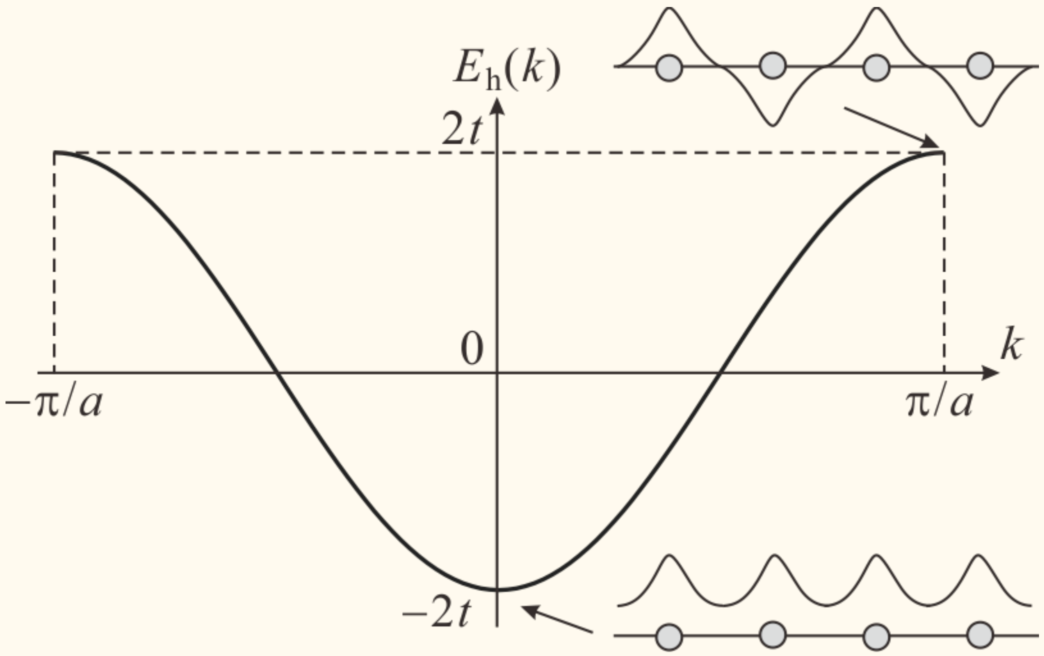
Cosine band with the width of $4t$.



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

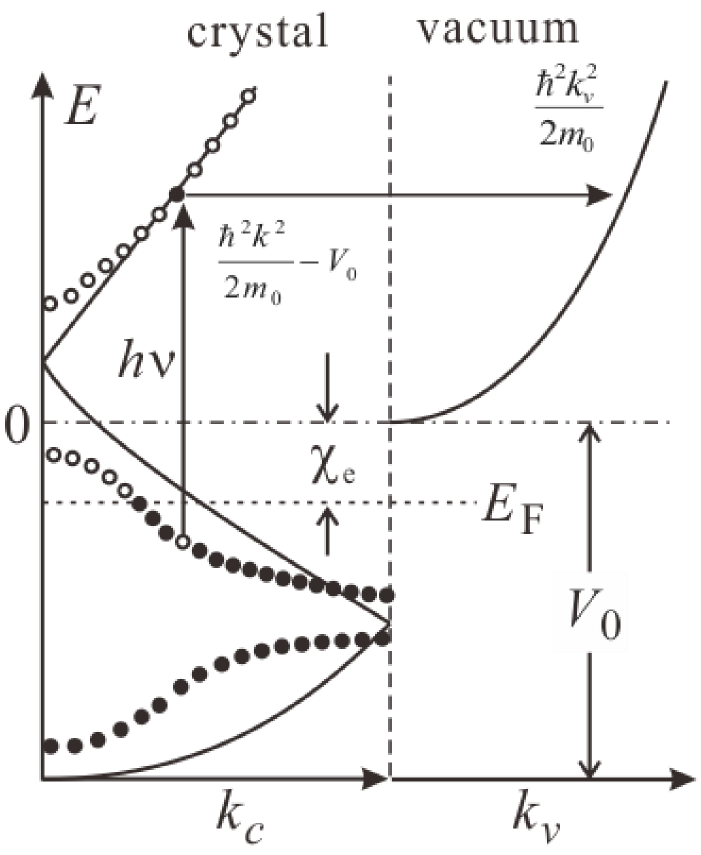
ab-initio calculation

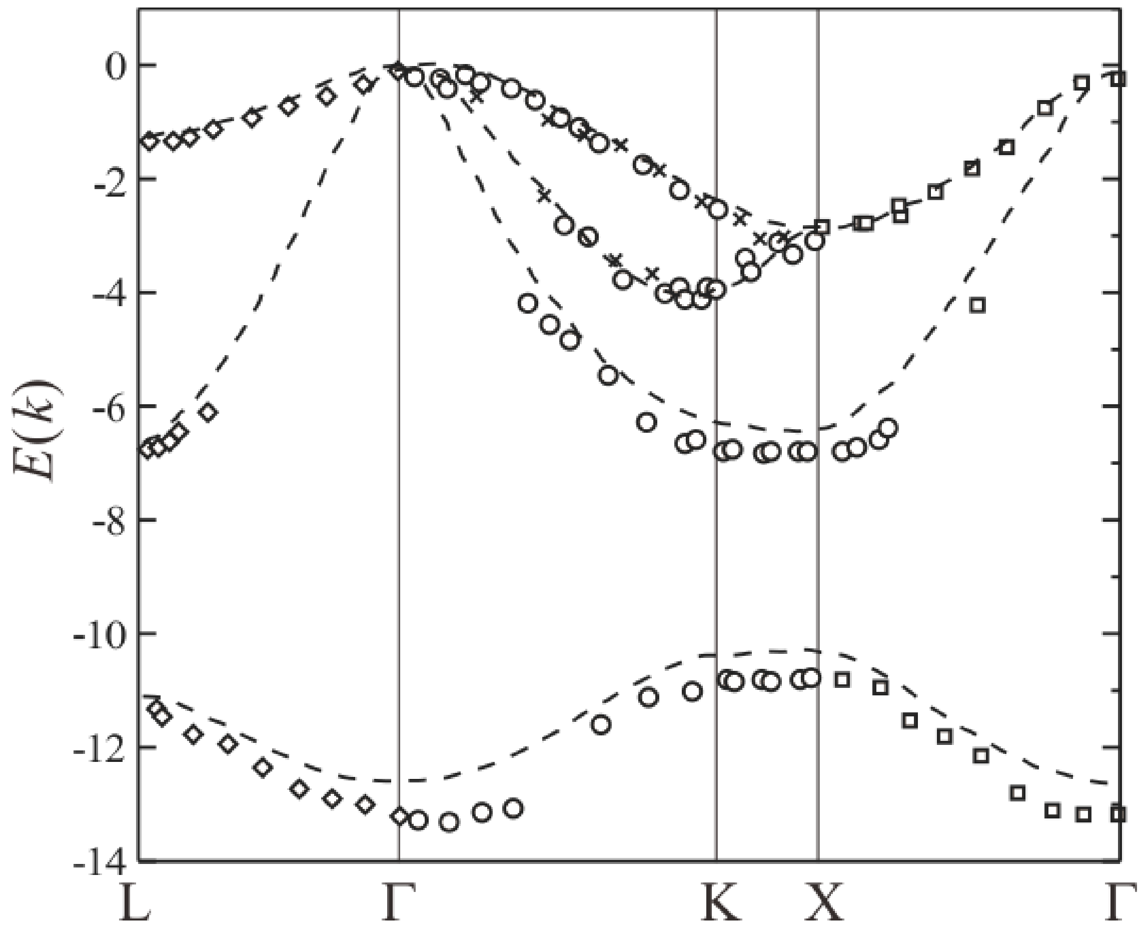
- Local density approximation
- Augmented plane wave
- Generalized gradient approximation

Angle resolved photoemission spectroscopy (ARPES)

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

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



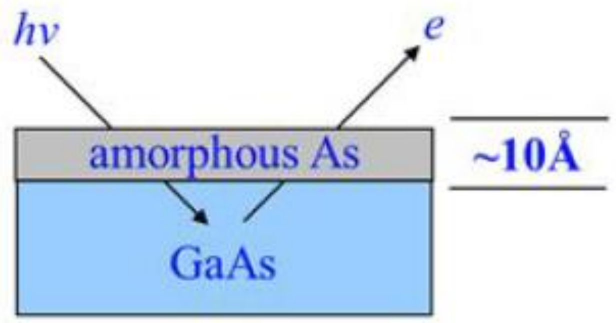


GaAs

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).

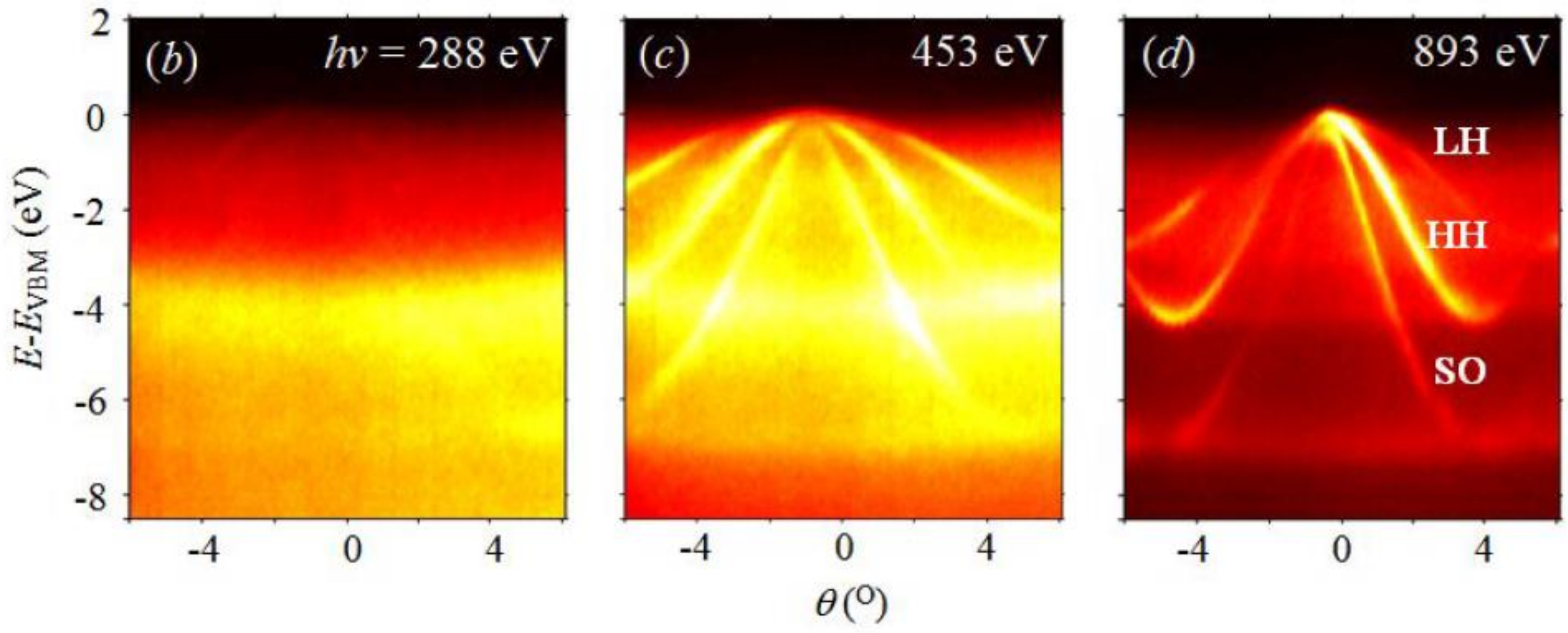
Angle resolved photoemission spectroscopy (ARPES) (2)



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:

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

Bloch function (omit band index)

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

Fourier expansion
(∵ lattice periodicity)

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

(2), (3) → (1)

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

Each term in the sum over ***G*** is zero in (4)

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

For (5) to have non-trivial solution

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

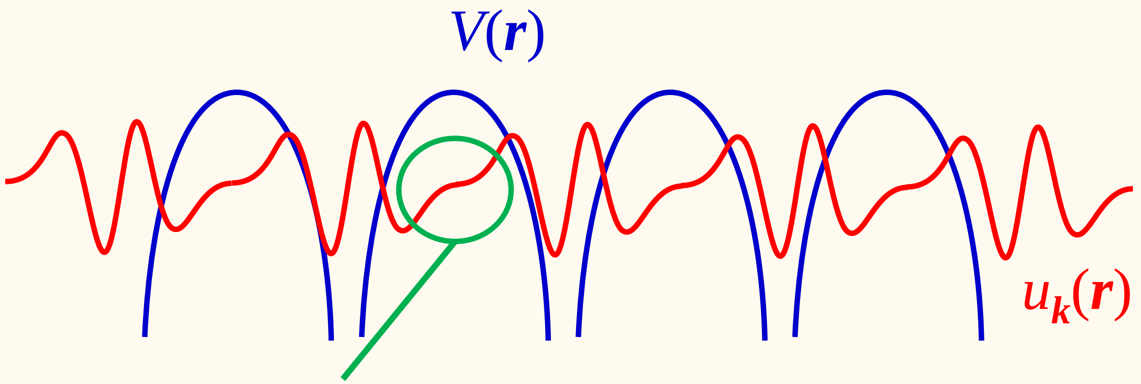
Pseudo-potential calculation method

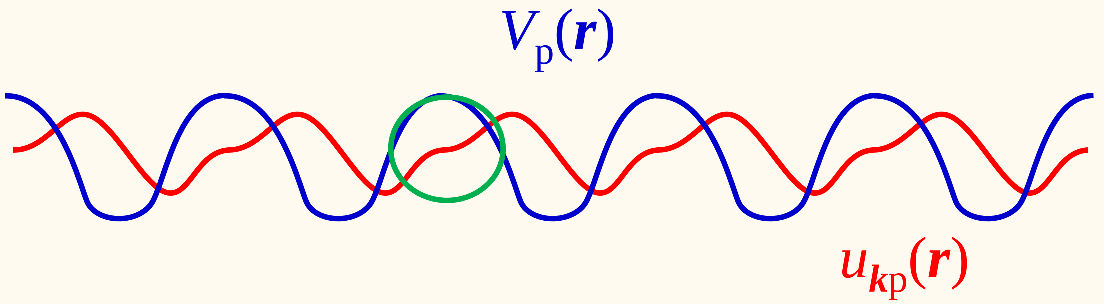
$$\left|\left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E\right\}\delta_{\boldsymbol{G}\boldsymbol{G}'} + V_{\boldsymbol{G}-\boldsymbol{G}'}\right]_{\boldsymbol{G}\boldsymbol{G}'}\right| = 0$$

→ 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.



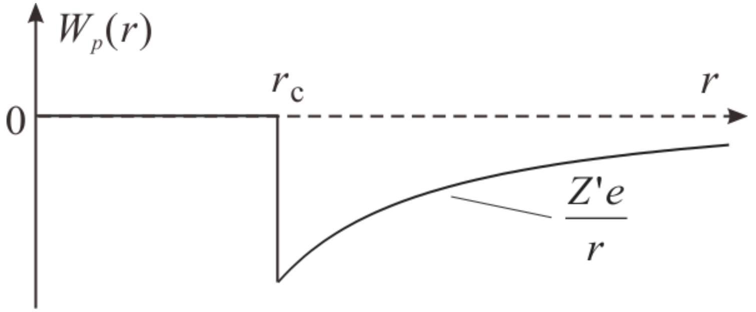


band structure: almost determined in skirt characteristics

Pseudo potential calculation method (2)

Replacement with pseudo potential $V(r) = -\frac{Ze}{r}$ ⇒ $W_p(r) = \begin{cases} 0 & (r < r_c) \\ -\frac{Z'e}{r} & (r \geq r_c) \end{cases}$

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

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

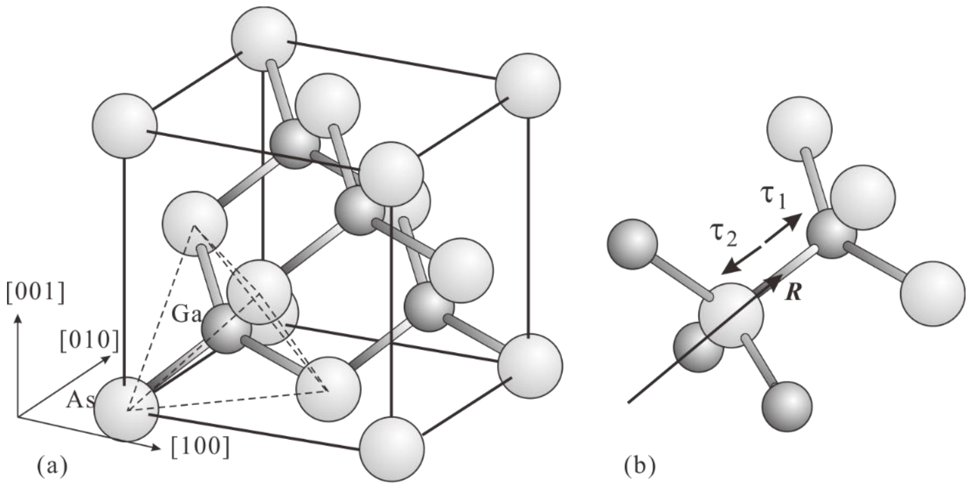
$$= \sum_\alpha e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_\alpha} \frac{1}{\Omega} \int_\Omega W_p^\alpha(\boldsymbol{r}') e^{-i\boldsymbol{K}\cdot\boldsymbol{r}'} d\boldsymbol{r}' \quad \because e^{-i\boldsymbol{K}\cdot\boldsymbol{R}_j} = 1$$

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

$w_p^\alpha(\boldsymbol{K})$: 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 Ga : $\frac{a}{8}(1,1,1)$ As : $-\frac{a}{8}(1,1,1)$

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

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

Distance from the origin and number of points in reciprocal lattice

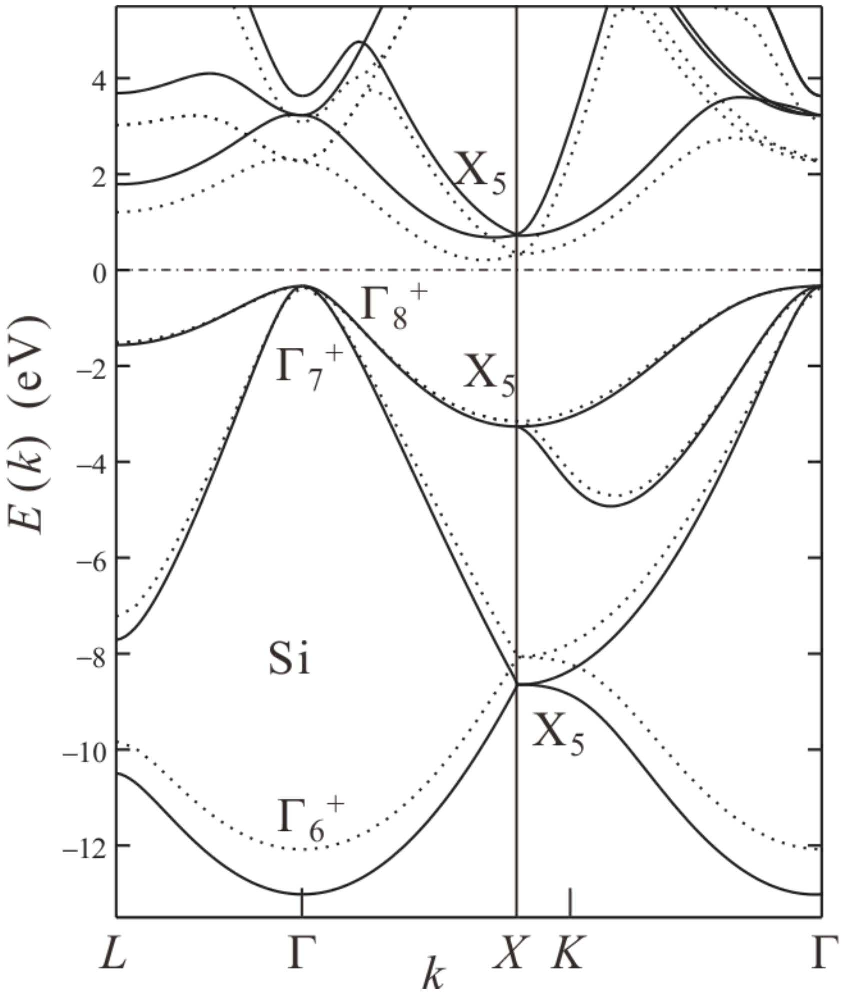
distance	Points	number
0	(0,0,0)	1
$\sqrt{3}$	(1,1,1),…	8
2	(2,0,0),…	6
$\sqrt{8}$	(2,0,2),…	12
$\sqrt{11}$	(3,1,1),…	24

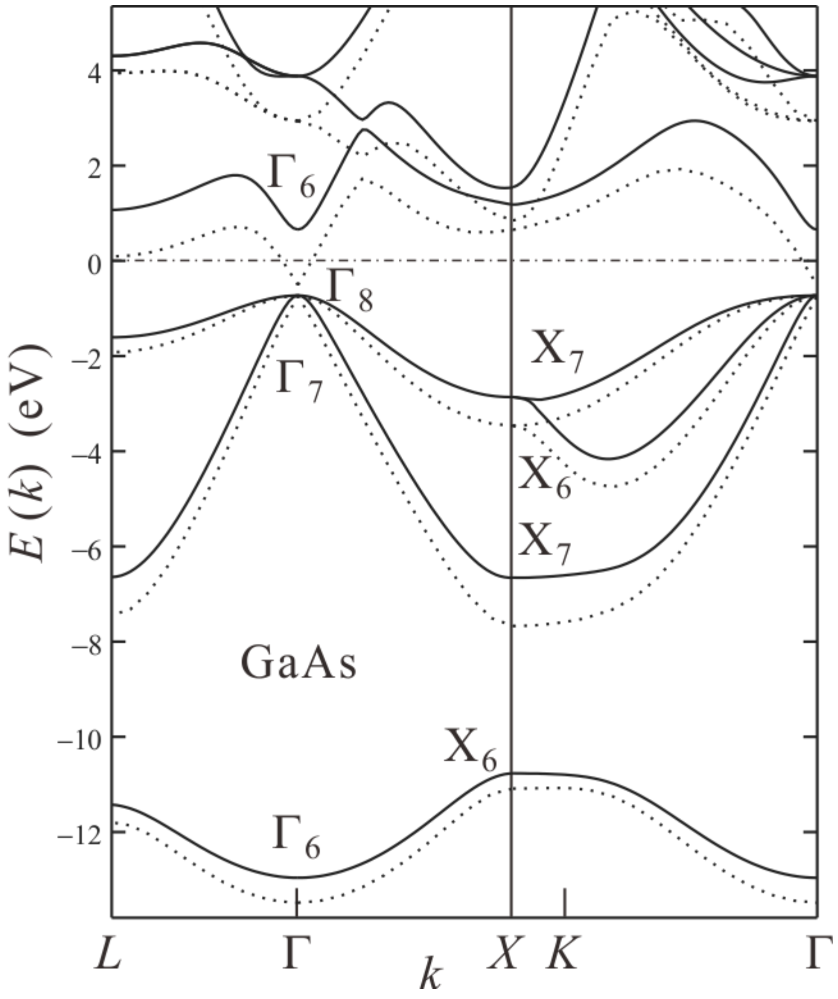
Form factors obtained from fitting to optical experiment

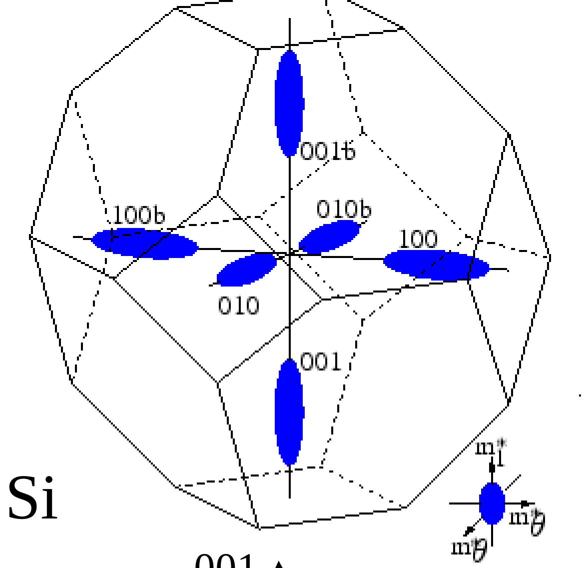
	$v_p^s(111)$	$v_p^s(220)$	$v_p^s(311)$	$v_p^a(111)$	$v_p^a(200)$	$v_p^a(311)$
Si	−2.856	0.544	1.088	0	0	0
Ge	−3.128	0.136	0.816	0	0	0
GaAs	−3.128	0.136	0.816	0.952	0.68	0.136
CdTe	−2.72	0	0.544	2.04	1.224	0.544

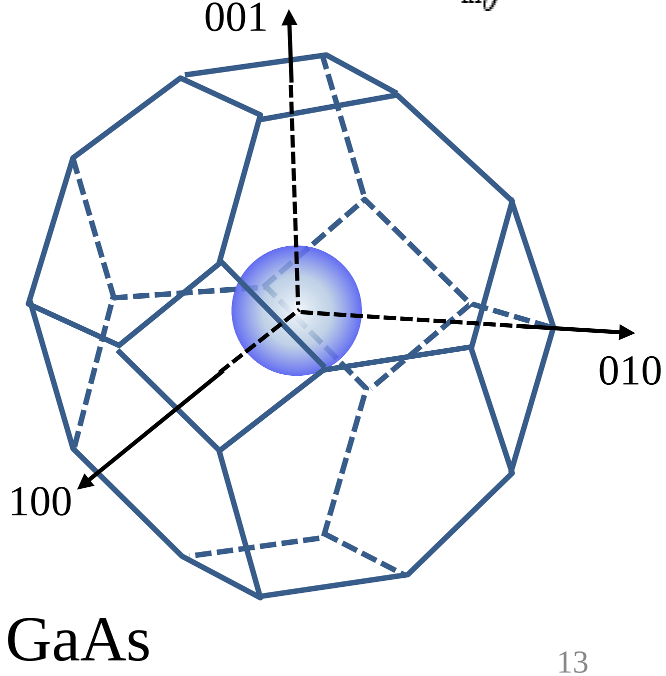
Band structure of Si and GaAs

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

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

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

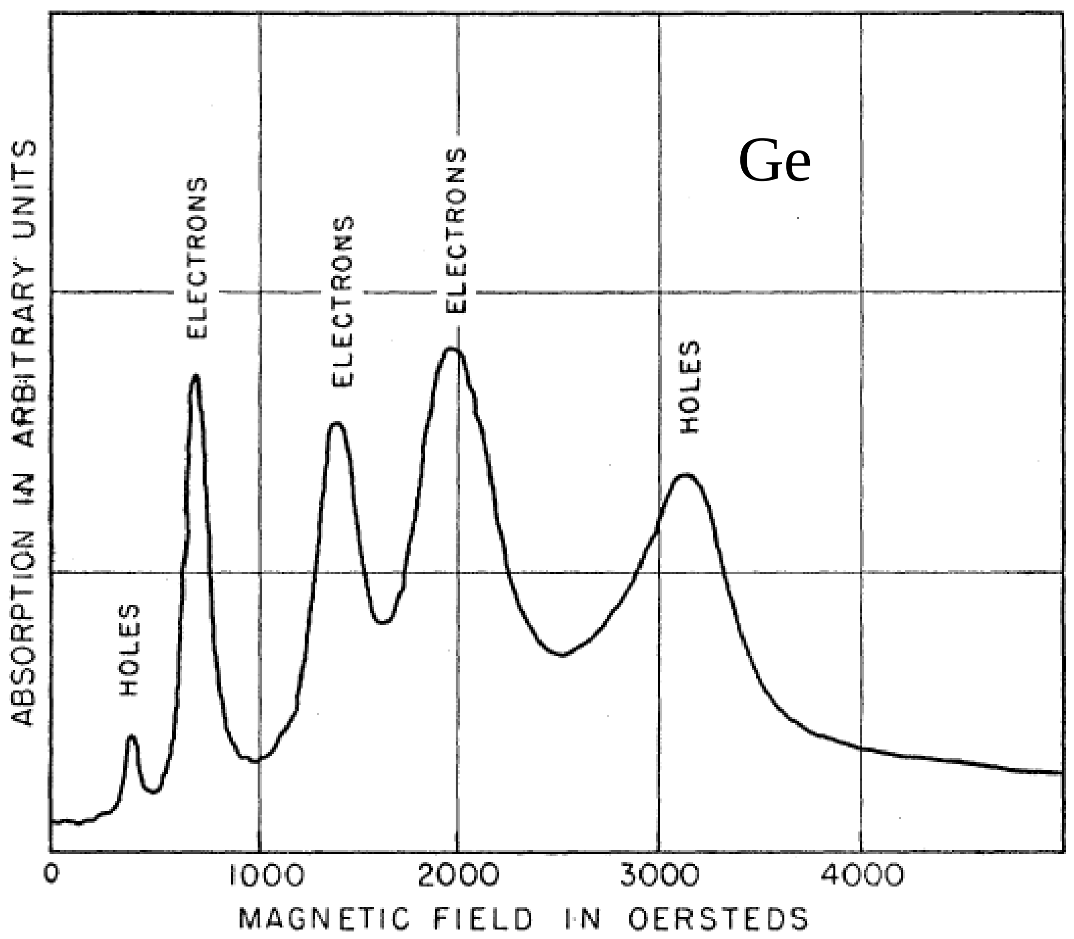
$\frac{1}{m^*}$: inverse effective mass tensor

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

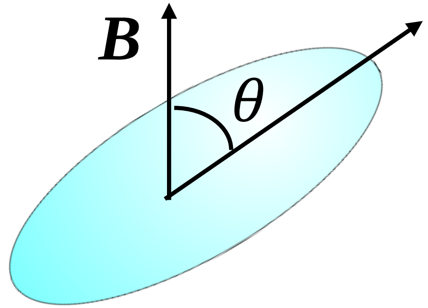


Cyclotron frequency $\omega_c = \frac{qB}{m}$

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

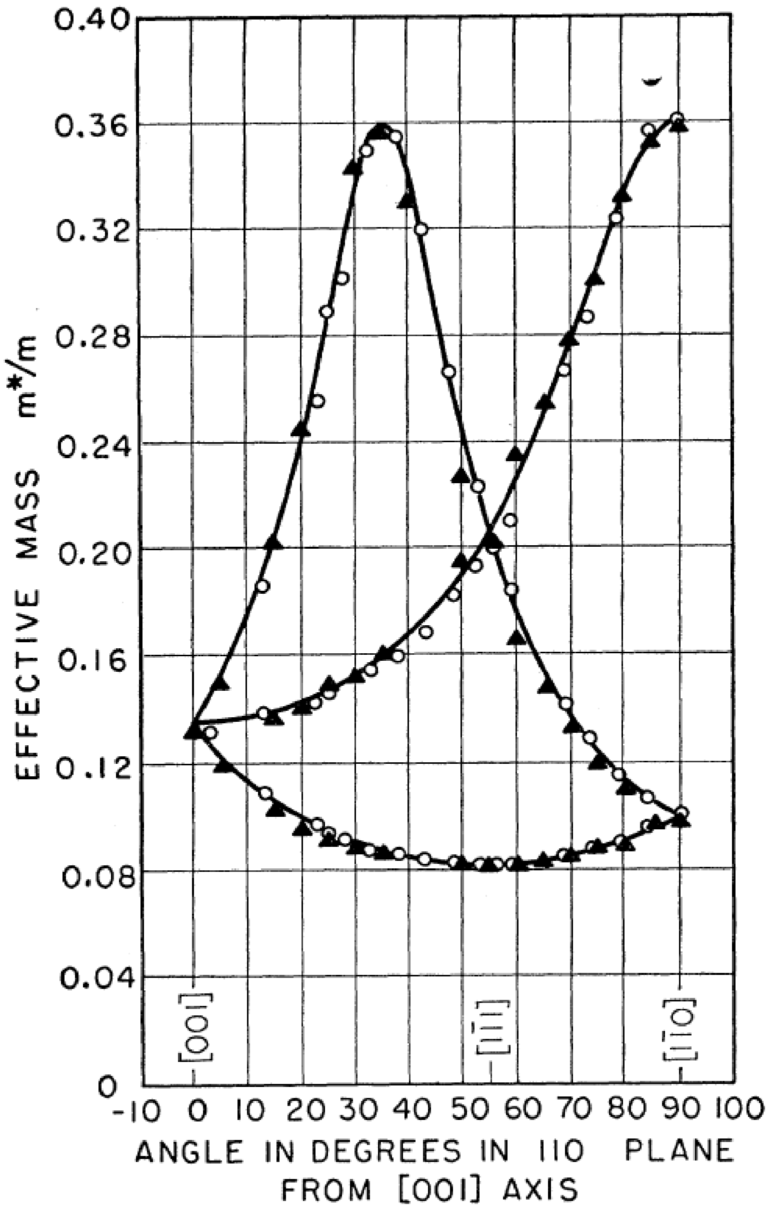
$$\left(\frac{1}{m_c}\right)^2 = \frac{\cos^2\theta}{m_t^2} + \frac{\sin^2\theta}{m_l m_t}$$

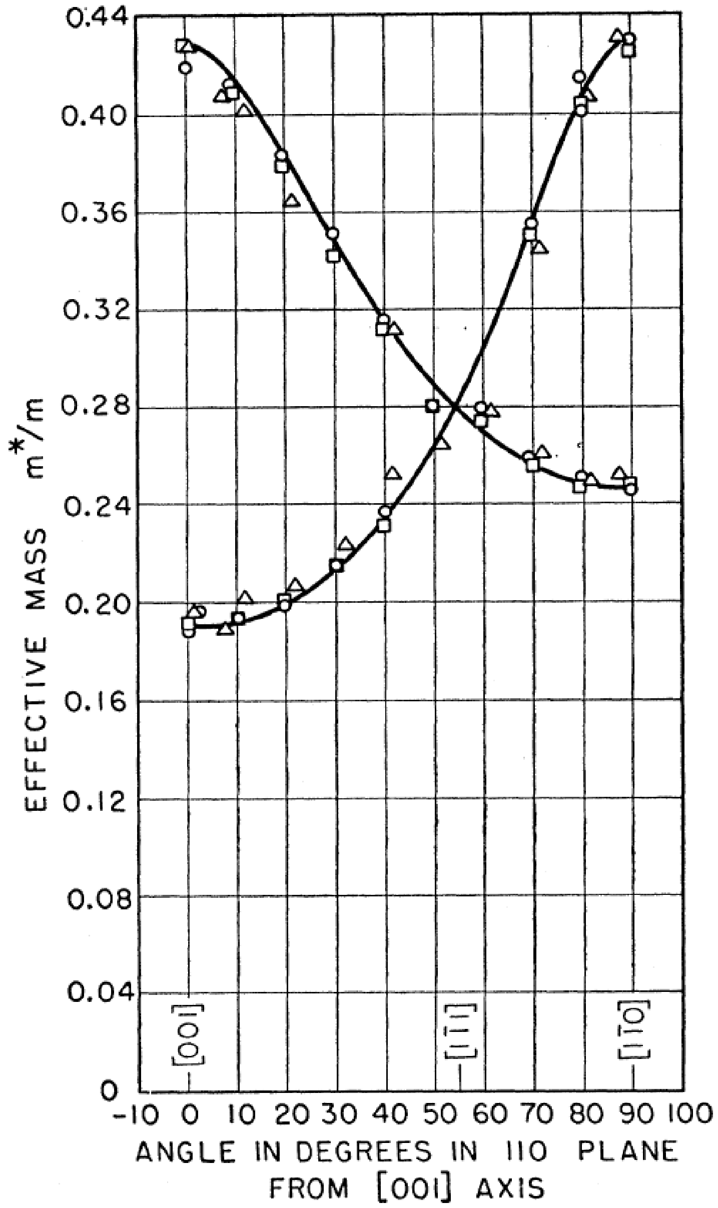
Electron-hole distinction ← circular polarization

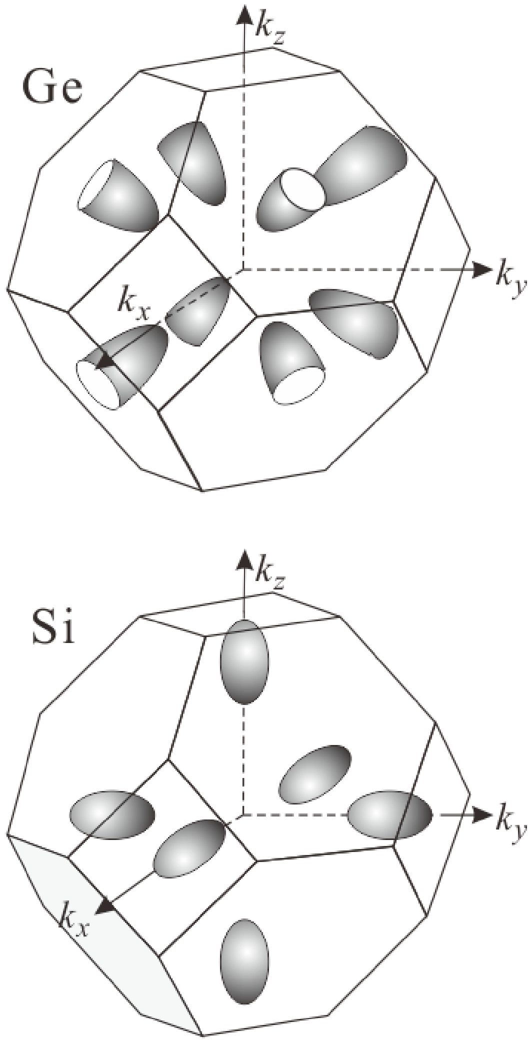
(24 GHz microwave)

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 ***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

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

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

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

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

Approximate the perturbed wavefunction

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

Substitute to the equation for u

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

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 $$\mathscr{H}_{\text{so}} = -\frac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot\boldsymbol{p}\times(\nabla V)$$

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

From identity

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

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

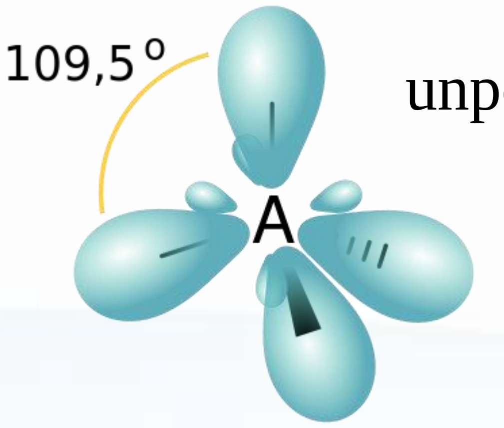
$$\boldsymbol{\pi} \equiv \boldsymbol{p} + \frac{\hbar}{4mc^2}\boldsymbol{\sigma}\times\nabla V$$

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

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

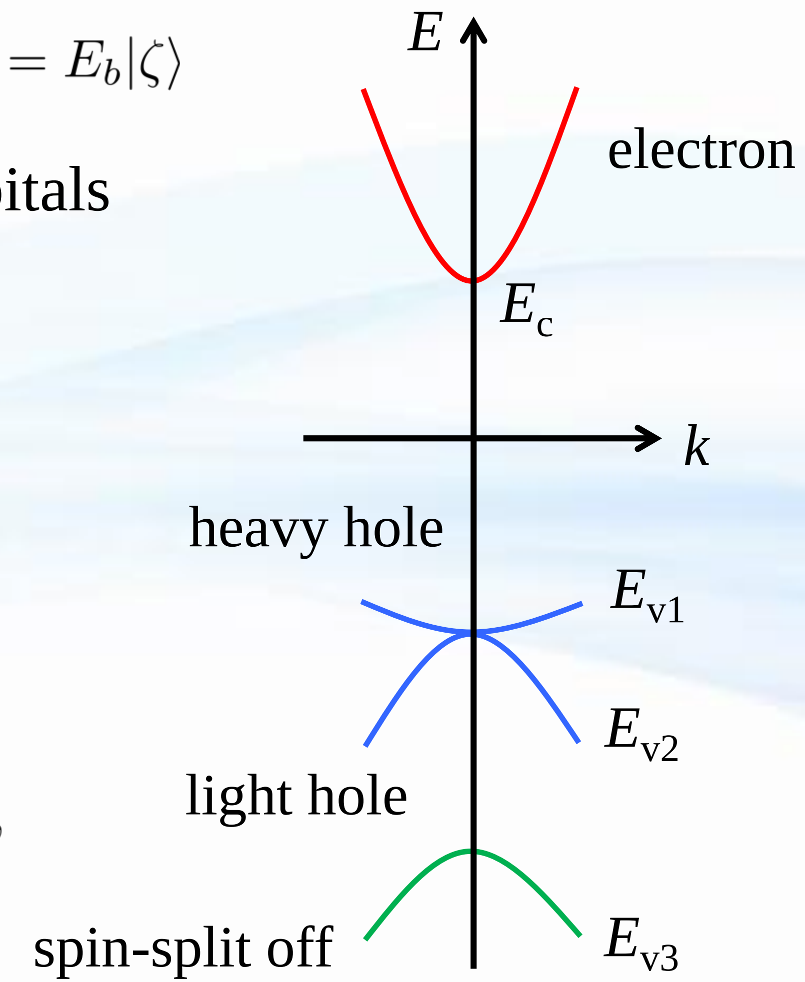
$$\{|S\rangle,|X\rangle,|Y\rangle,|Z\rangle\} \to \{|S\rangle,|\pm\rangle \equiv (|X\rangle \pm i|Y\rangle)/\sqrt{2},|Z\rangle\}$$

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

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

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:

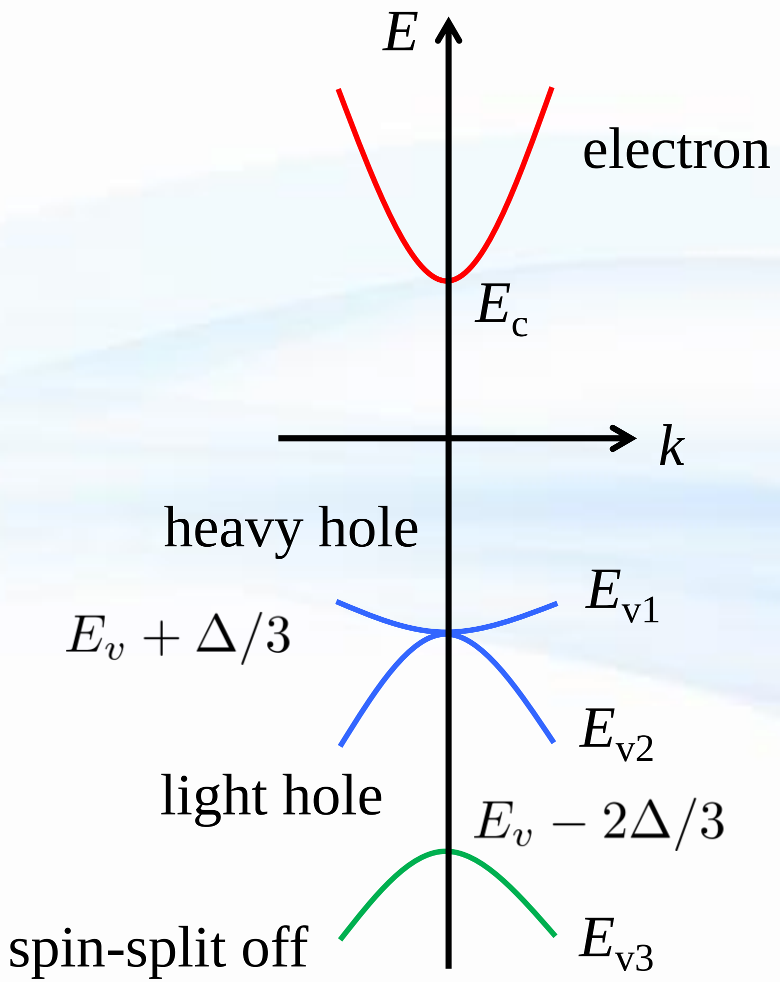
$$E_c(\boldsymbol{k}) = E_c + \frac{\hbar^2 k^2}{2m_0} + \frac{|P|^2 k^2}{3}\left[\frac{2}{E_g} + \frac{1}{E_g + \Delta}\right],$$

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

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

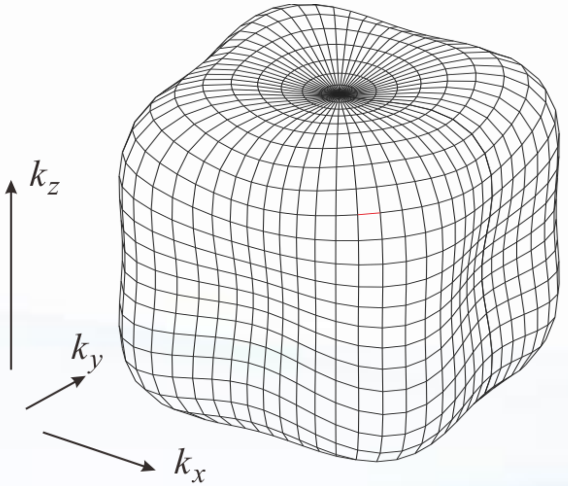
$$E_{v3}(\boldsymbol{k}) = E_v - \frac{2\Delta}{3} + \frac{\hbar^2 k^2}{2m_0} - \frac{|P|^2 k^2}{3(E_g + \Delta)}$$

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

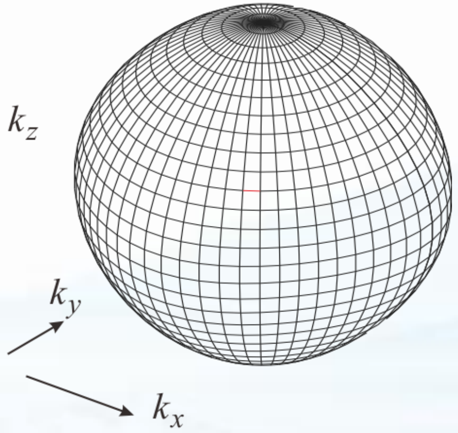


Band warping, a conventional way to get band parameters

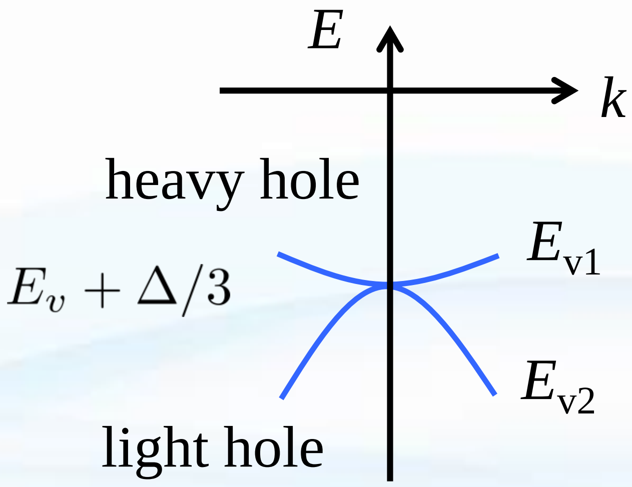
constant-energy surface



heavy hole



light hole



Summary of $k \cdot p$ second order perturbation

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

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

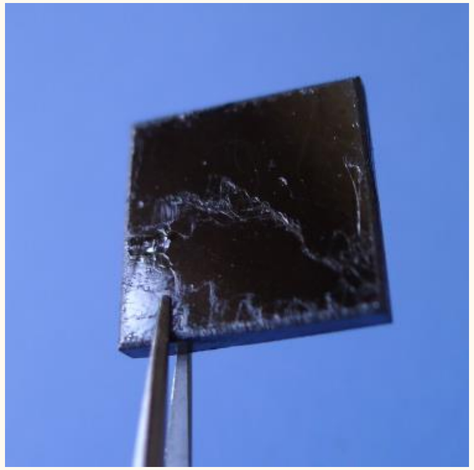
Table of band parameters

	E_r (eV)	E_L (eV)	E_Δ (eV)	E_{so} (eV)	m_t^* (m_0)	m^* (m_0)	m_t^* (m_0)	$\lvert A\rvert$ (eV^{-1})	$\lvert B\rvert$	$\lvert C\rvert$
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

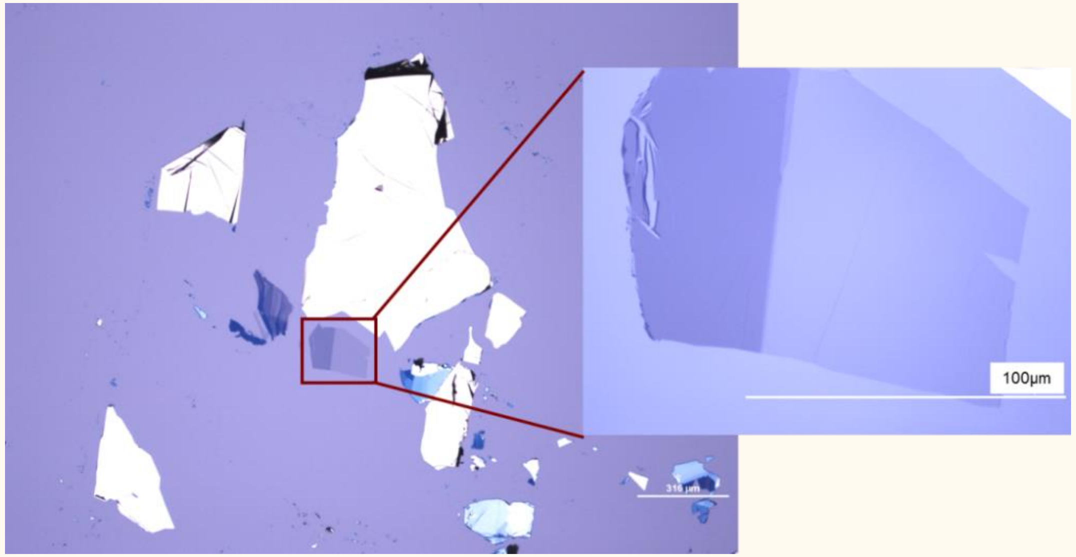
Lundstrom “Fundamentals of Carrier Transport” (Cambridge, 2000).

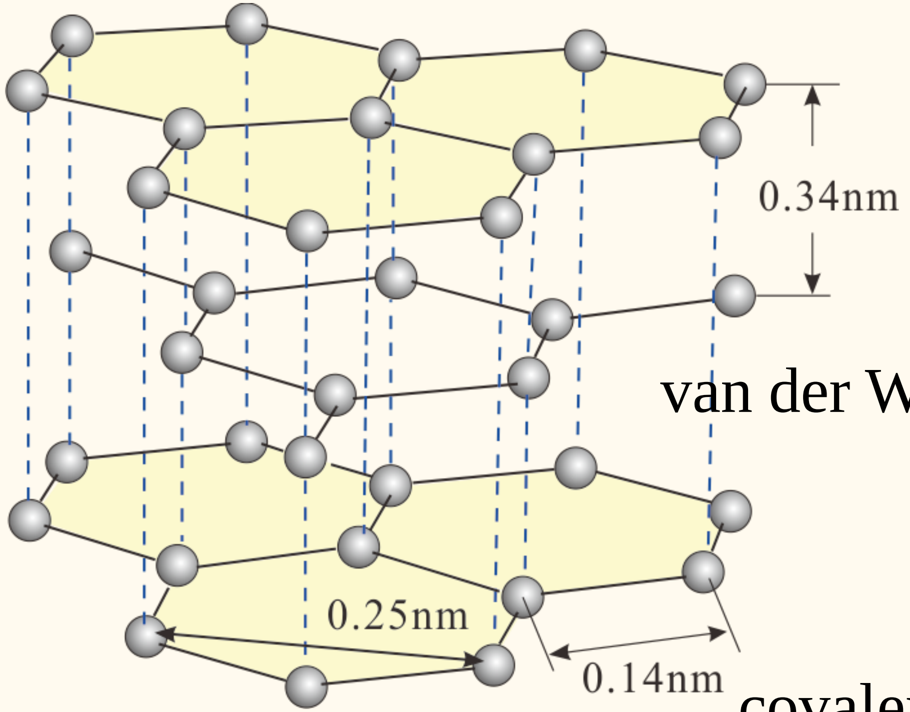
Graphene: A two-dimensional material (another example of TBA)

Graphite



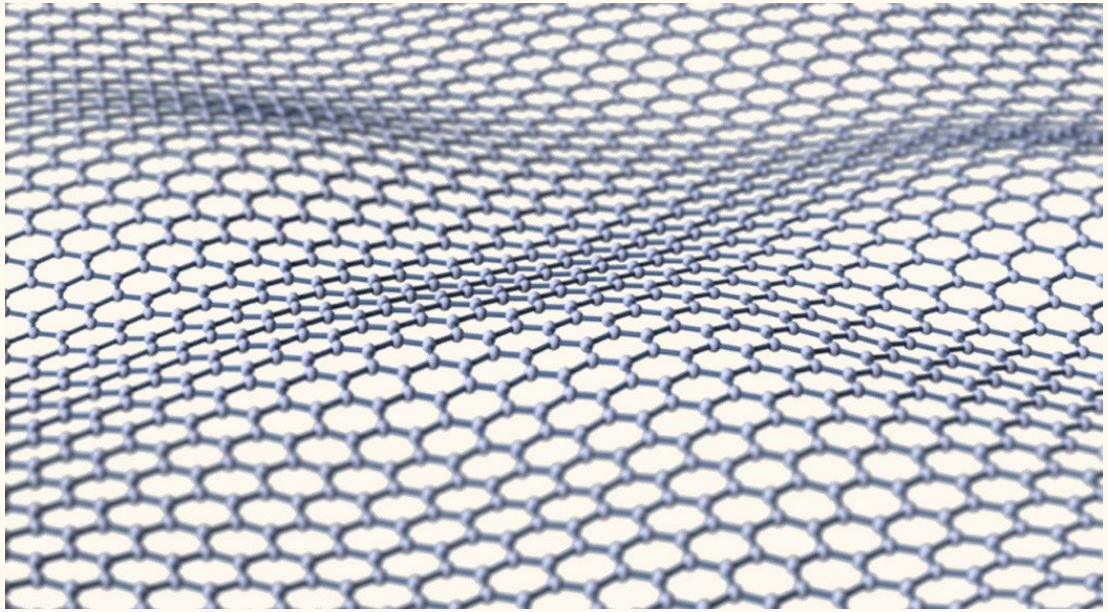
Graphene





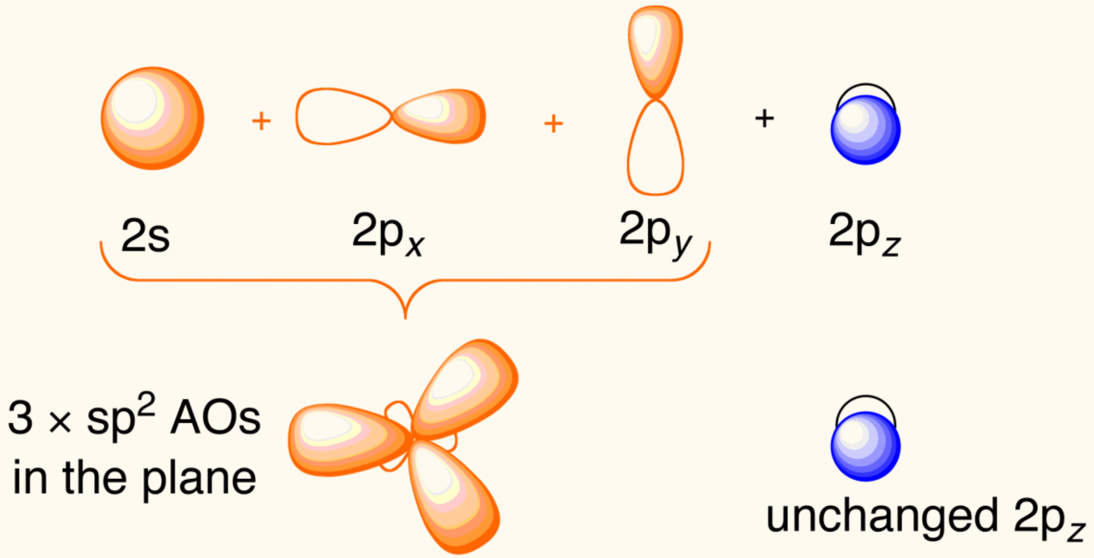
van der Waals

covalent

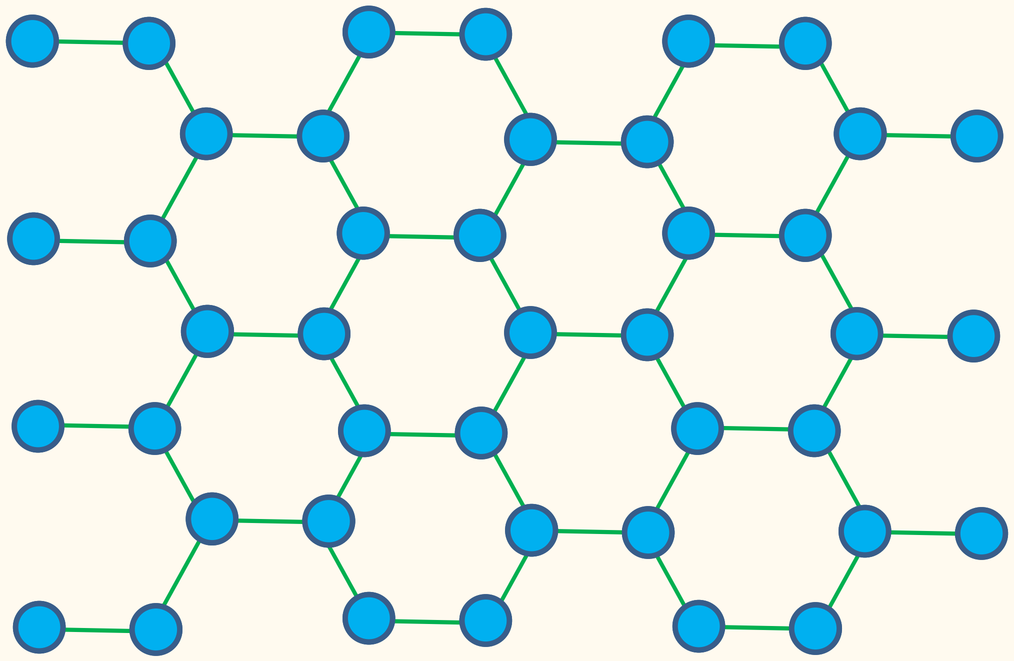


Graphene lattice/reciprocal lattice structure

Atomic orbitals

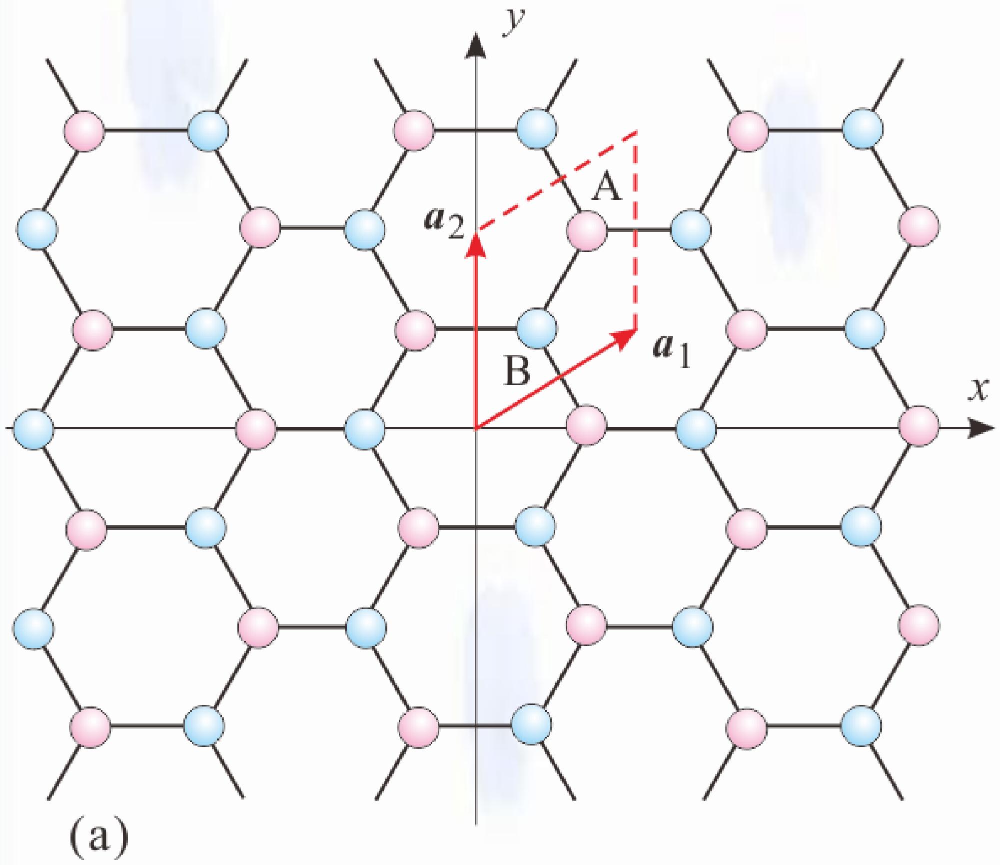


Honeycomb lattice

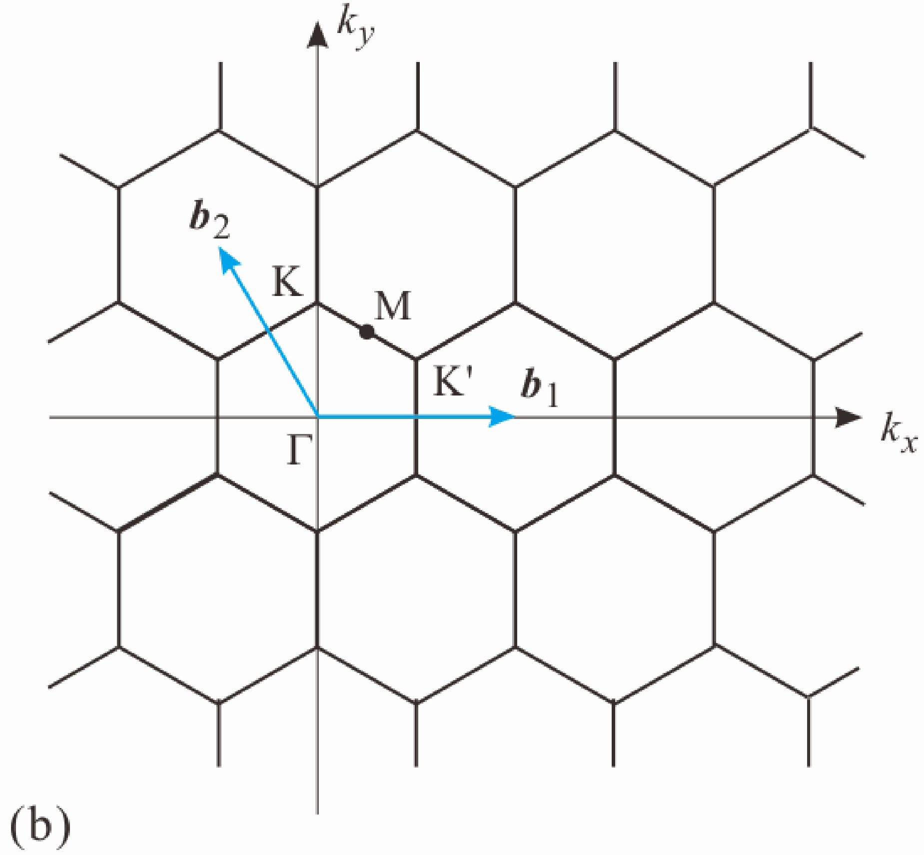


Graphene lattice/reciprocal lattice structure

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

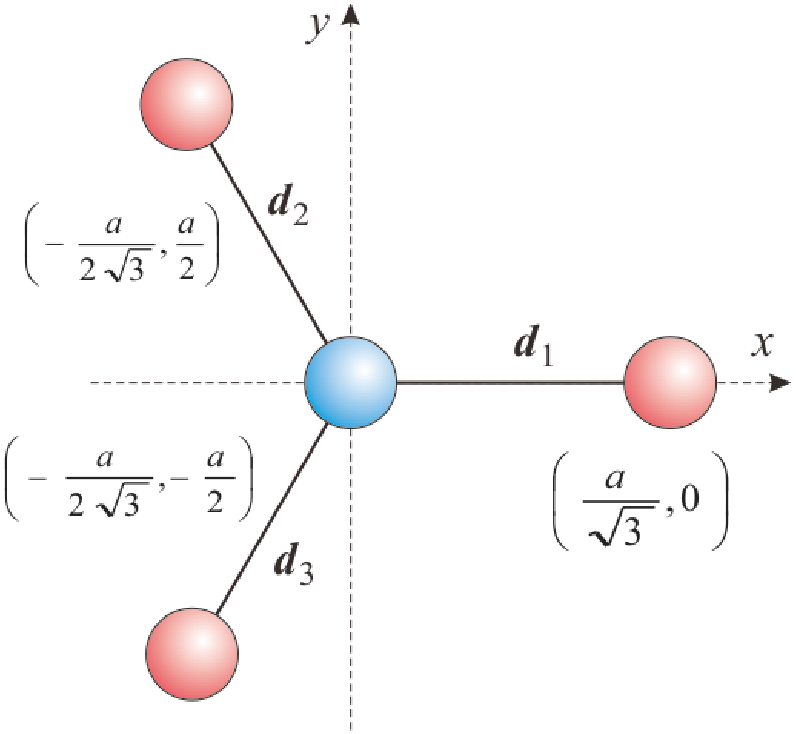
$$H_{\mathrm{AA}} = \langle \psi_{\mathrm{A}} | \mathscr{H} | \psi_{\mathrm{A}} \rangle, \quad H_{\mathrm{BB}} = \langle \psi_{\mathrm{B}} | \mathscr{H} | \psi_{\mathrm{B}} \rangle,$$
$$H_{\mathrm{AB}} = H_{\mathrm{BA}}^* = \langle \psi_{\mathrm{A}} | \mathscr{H} | \psi_{\mathrm{B}} \rangle$$

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

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



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

Take the nearest neighbor approximation:

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

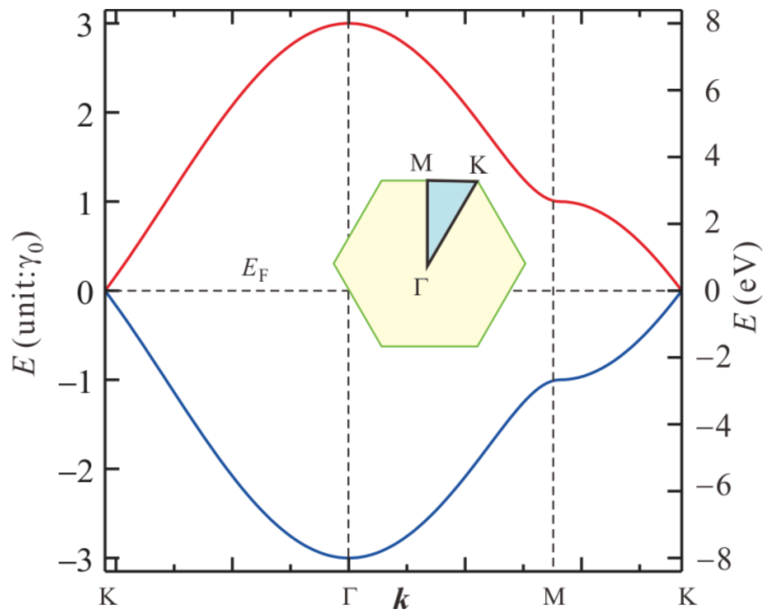
$$\boldsymbol{k}\cdot\boldsymbol{d}_3 = \left(-\frac{k_x}{2\sqrt{3}} - \frac{k_y}{2}\right)a$$

$\langle \phi(\boldsymbol{r}-\boldsymbol{r}_l)|\mathscr{H}|\phi(\boldsymbol{r}-\boldsymbol{r}_j)\rangle_{\boldsymbol{r}} = \xi$: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

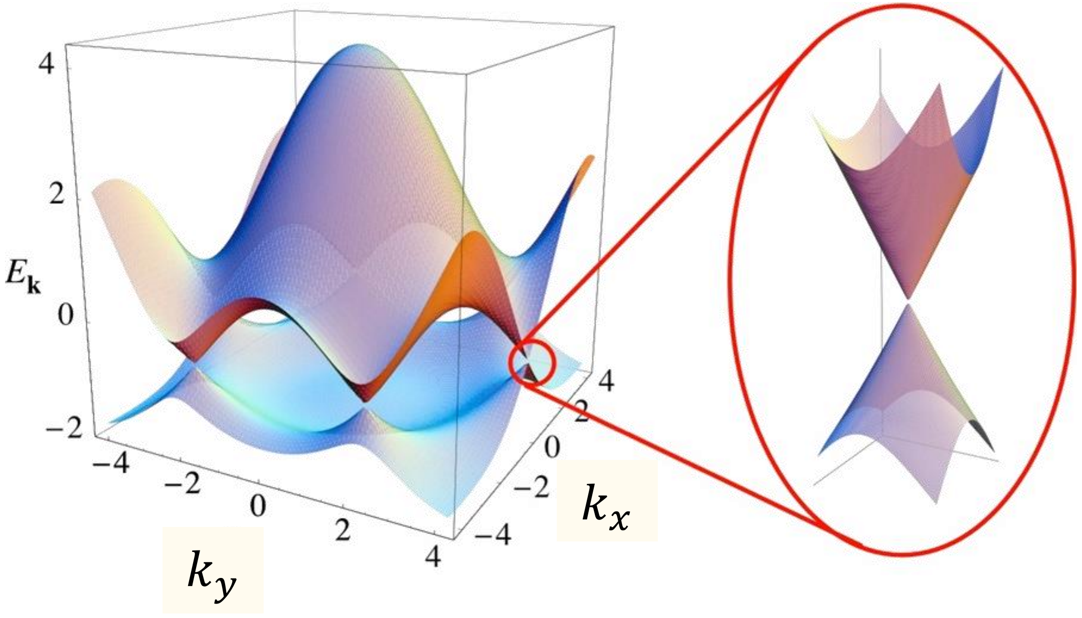


$$E = h_{AA} \pm \xi \sqrt{1 + 4\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2} + 4\cos^2\frac{k_y a}{2}}$$

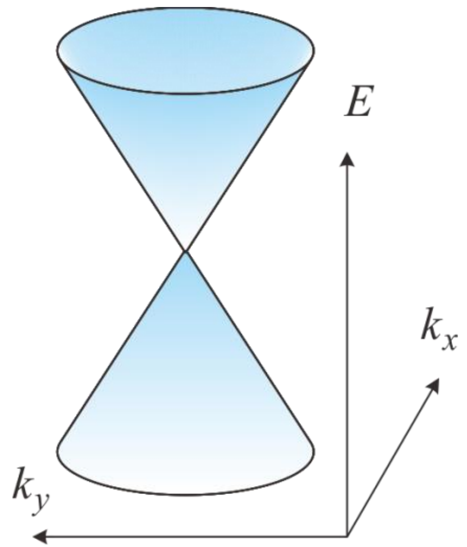
$$k_x = 0$$

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

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



A Dirac point



Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.21 Lecture 03

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Review of lecture in the last week

Chapter 2 Energy bands, effective mass approximation

Energy band calculation

- Nearly free electron approximation
- Tight-binding approximation
- (empirical) Pseudo-potential calculation method
- k·p perturbation method

Energy band measurement

- Angle-resolved photoemission spectroscopy (ARPES)
- Cyclotron resonance

Example of tight-binding approximation: Band structure in graphene

Contents today

Envelope function (effective mass approximation)

Chapter 3 Carrier statistics and chemical doping

Density of states

Definition and properties of valence band hole states

Carrier distribution in intrinsic semiconductors

Shallow hydrogen-like impurity states

Shallow impurity states in Si

Doping and carrier distribution

Envelope function (effective mass approximation)

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

Problem: Non-uniform perturbation potential $U(\boldsymbol{r})$

Schrödinger equation $$\left[-\frac{\hbar^2\nabla^2}{2m} + V(\boldsymbol{r}) + U(\boldsymbol{r})\right]\zeta(\boldsymbol{r}) = [\hat{H}_0 + U(\boldsymbol{r})]\zeta(\boldsymbol{r}) = E\zeta(\boldsymbol{r})$$

Expand $\zeta(\boldsymbol{r})$ with Bloch function $\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = |n, \boldsymbol{k}\rangle$ $$\zeta(\boldsymbol{r}) = \sum_{n,\boldsymbol{k}} f(n,\boldsymbol{k})\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_{n,\boldsymbol{k}} f(n,\boldsymbol{k}) u_{n\boldsymbol{k}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$\langle n', \boldsymbol{k}'| \rightarrow$ $$[E_0(n',\boldsymbol{k}') - E] f(n',\boldsymbol{k}') + \sum_{n,\boldsymbol{k}} \langle n',\boldsymbol{k}'|U|n,\boldsymbol{k}\rangle f(n,\boldsymbol{k}) = 0$$

Fourier transform of $U(\boldsymbol{r})$ $$U(\boldsymbol{r}) = \int d\boldsymbol{q} U_{\boldsymbol{q}} e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}$$

Fourier expansion of $u^*_{n'\boldsymbol{k}'}(\boldsymbol{r}) u_{n\boldsymbol{k}}(\boldsymbol{r})$ $$u^*_{n'\boldsymbol{k}'}(\boldsymbol{r}) u_{n\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} b_{n'\boldsymbol{k}'n\boldsymbol{k}}(\boldsymbol{G}) e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

Envelope function (2)

Ω_0: unit cell space,
v_0: unit cell volume

$$b_{n'\boldsymbol{k}'n\boldsymbol{k}}(\boldsymbol{G}) = \int_{\Omega_0} \frac{d\boldsymbol{r}}{v_0} e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} u^*_{n'\boldsymbol{k}'}(\boldsymbol{r}) u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$\therefore \langle n', \boldsymbol{k}'|U|n, \boldsymbol{k}\rangle = \int d\boldsymbol{q} U_{\boldsymbol{q}} \sum_{\boldsymbol{G}} b_{n'\boldsymbol{k}'n\boldsymbol{k}}(\boldsymbol{G}) \underline{\int d\boldsymbol{r} e^{i(\boldsymbol{k}-\boldsymbol{k}'+\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}}$$

$$= (2\pi)^3 \delta(\boldsymbol{k} - \boldsymbol{k}' + \boldsymbol{q} + \boldsymbol{G})$$

$$= (2\pi)^3 \sum_{\boldsymbol{G}} U_{\boldsymbol{k}'-\boldsymbol{k}-\boldsymbol{G}} b_{n'\boldsymbol{k}'n\boldsymbol{k}}(\boldsymbol{G})$$

Assumption: $U(\boldsymbol{r})$ varies little in the scale of the lattice constant

$$\rightarrow \ U_{\boldsymbol{q}} \text{ is finite only for } |\boldsymbol{q}| \ll \pi/a$$

$$\boldsymbol{k}' - \boldsymbol{k} \sim \boldsymbol{G} < \frac{\pi}{a}$$

$U(\boldsymbol{r})$ is weaker than the lattice potential: Elements between different n are negligible

$$\rightarrow \ \langle n', \boldsymbol{k}'|U|n, \boldsymbol{k}\rangle \approx U_{\boldsymbol{k}'-\boldsymbol{k}} \delta_{n'n}$$

$$[E_0(\boldsymbol{k}') - E] f(n, \boldsymbol{k}') + \sum_{\boldsymbol{k}} U_{\boldsymbol{k}'-\boldsymbol{k}} f(n, \boldsymbol{k}) = 0$$

Envelope function (3)

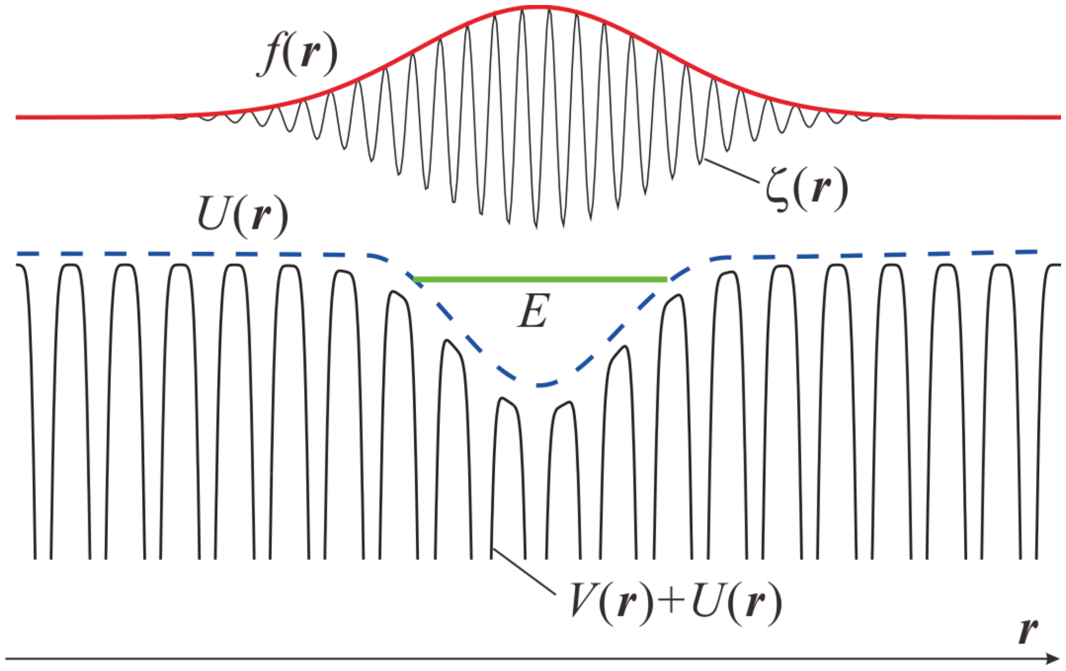
Assumption: $u_{n\boldsymbol{k}} \approx u_{n0}$

$$\zeta_n(\boldsymbol{r}) = u_{n0}\sum_{\boldsymbol{k}} f(n,\boldsymbol{k})e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = u_{n0}f_n(\boldsymbol{r})$$

$$\frac{\hbar^2 k\boldsymbol{k}'^2}{2m^*}f(\boldsymbol{k}) + \sum_{\boldsymbol{k}} U_{\boldsymbol{k}'-\boldsymbol{k}}f(\boldsymbol{k}) = Ef(\boldsymbol{k}')$$

$$\left[\frac{\hbar^2\nabla^2}{2m^*} + U(\boldsymbol{r})\right]f(\boldsymbol{r}) = Ef(\boldsymbol{r})$$

Effective mass equation



Derivation of effective mass equation with Wannier function

Wannier function (WF):

Fourier transform of Bloch function

$$w_n(\boldsymbol{r}-\boldsymbol{R}_j)=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}}\exp(-i\boldsymbol{k}\cdot\boldsymbol{R}_j)\psi_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r})=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}}\exp(i\boldsymbol{k}\cdot\boldsymbol{R}_j)w_n(\boldsymbol{r}-\boldsymbol{R}_j)$$

WF tends to localize around the lattice points.

WF are orthogonal.

$$\langle w^*_{n'}(\boldsymbol{r}-\boldsymbol{R}_{j'})|w_n(\boldsymbol{r}-\boldsymbol{R}_j)\rangle=\delta_{jj'}\delta_{nn'}$$

Effective mass approximation

$$[\mathscr{H}_0+\mathscr{H}_1(\boldsymbol{r})]\phi(\boldsymbol{r})=E\phi(\boldsymbol{r})$$

Expansion by Wannier functions

$$\phi(\boldsymbol{r})=\sum_{n,j}f_n(\boldsymbol{R}_j)w_n(\boldsymbol{r}-\boldsymbol{R}_j)$$

$$\sum_{j'}\langle j|\mathscr{H}_0|j'\rangle f(\boldsymbol{R}_{j'})+\sum_{j'}\langle j|\mathscr{H}_1|j'\rangle f(\boldsymbol{R}_{j'})=Ef(\boldsymbol{R}_j)$$

$$\sum_{j'}\langle j|\mathscr{H}_1|j'\rangle\approx\mathscr{H}_1(\boldsymbol{R}_j)\langle j|j\rangle=\mathscr{H}_1(\boldsymbol{R}_j)$$

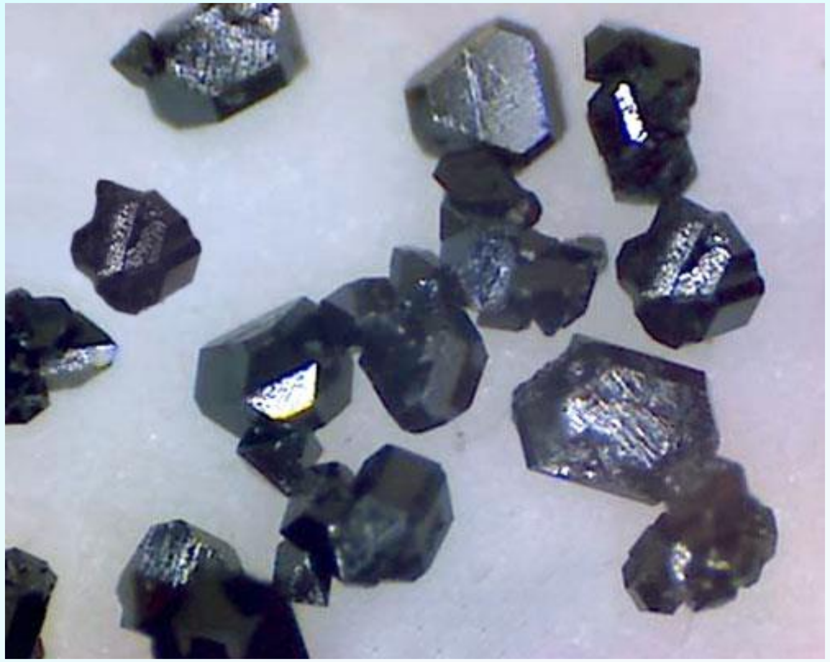
$$\langle j|\mathscr{H}_0|j'\rangle=\langle 0|\mathscr{H}_0|-\boldsymbol{R}_{j'}+\boldsymbol{R}_j\rangle\equiv h_0(\boldsymbol{R}_j-\boldsymbol{R}_{j'})$$

Effective mass equation

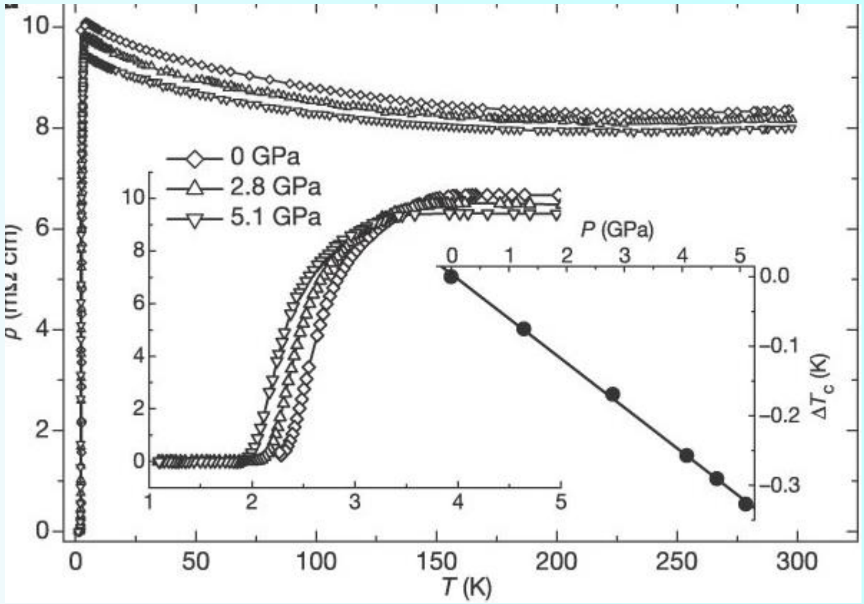
$$\left[-\frac{\hbar^2}{2m^*}\nabla^2+\mathscr{H}_1(\boldsymbol{r})\right]f(\boldsymbol{r})=Ef(\boldsymbol{r})$$

Ekimov et al., Nature **428**, 542 (2004).

Diamond

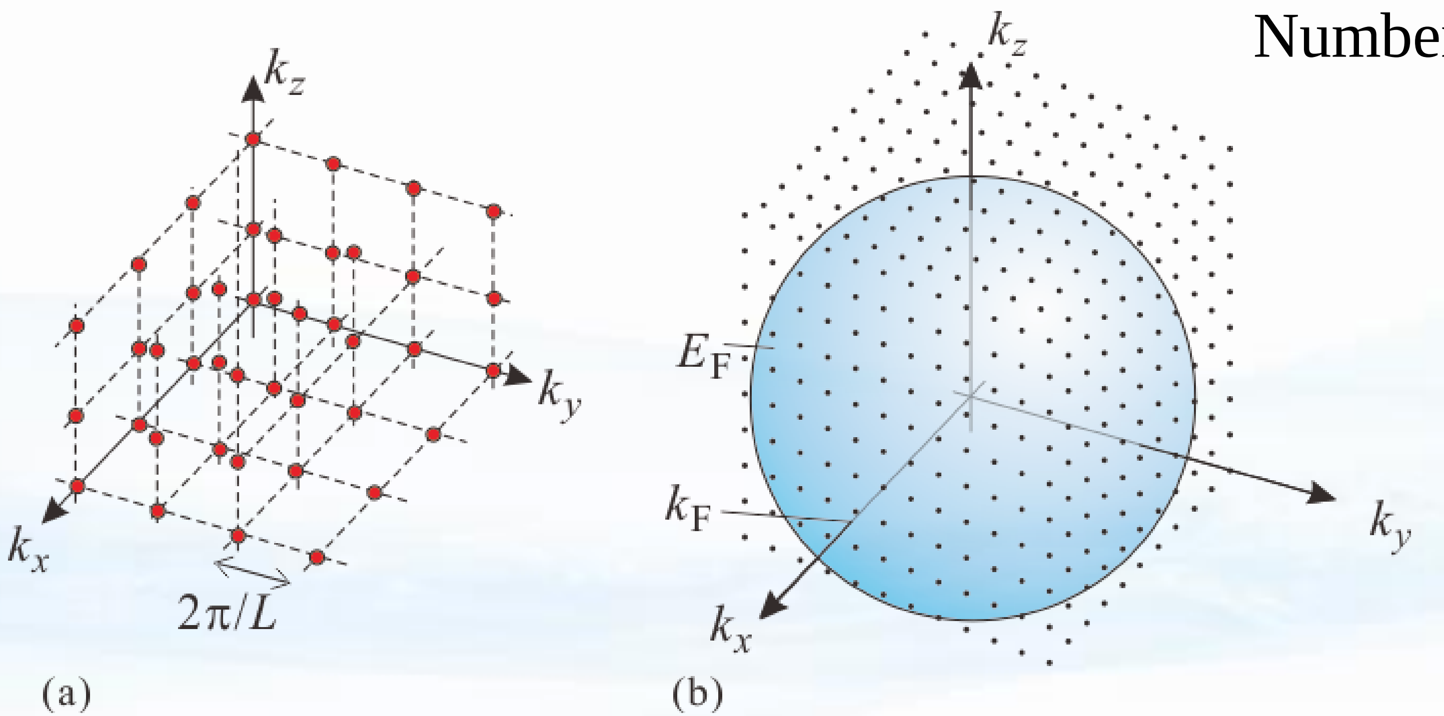


Boron doped diamond



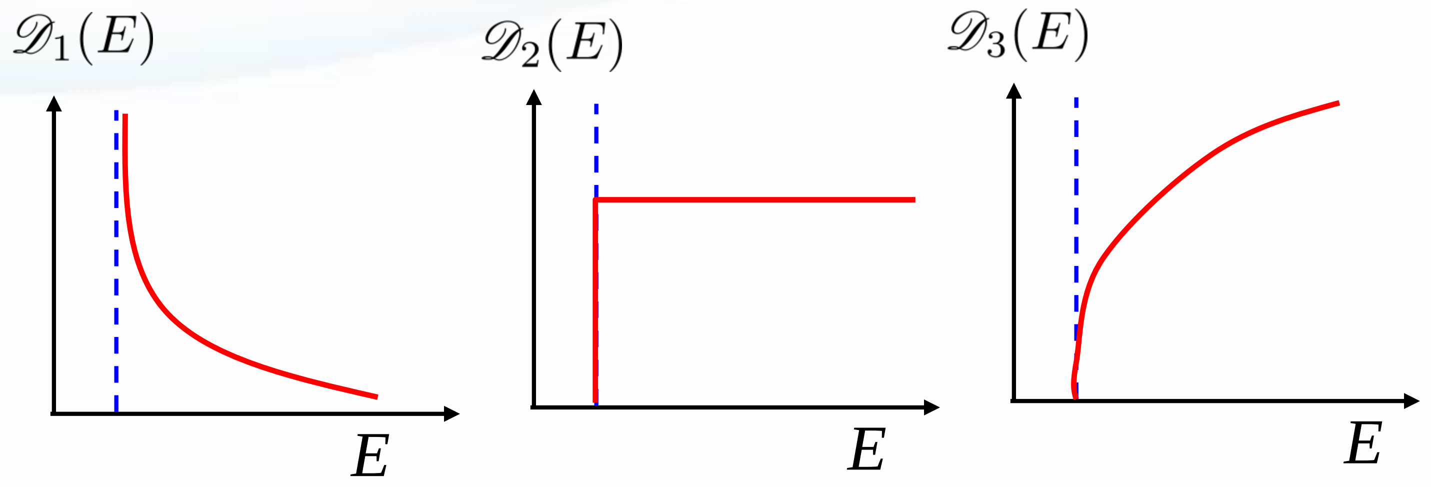
Chapter 3 Carrier statistics and chemical doping

Density of states



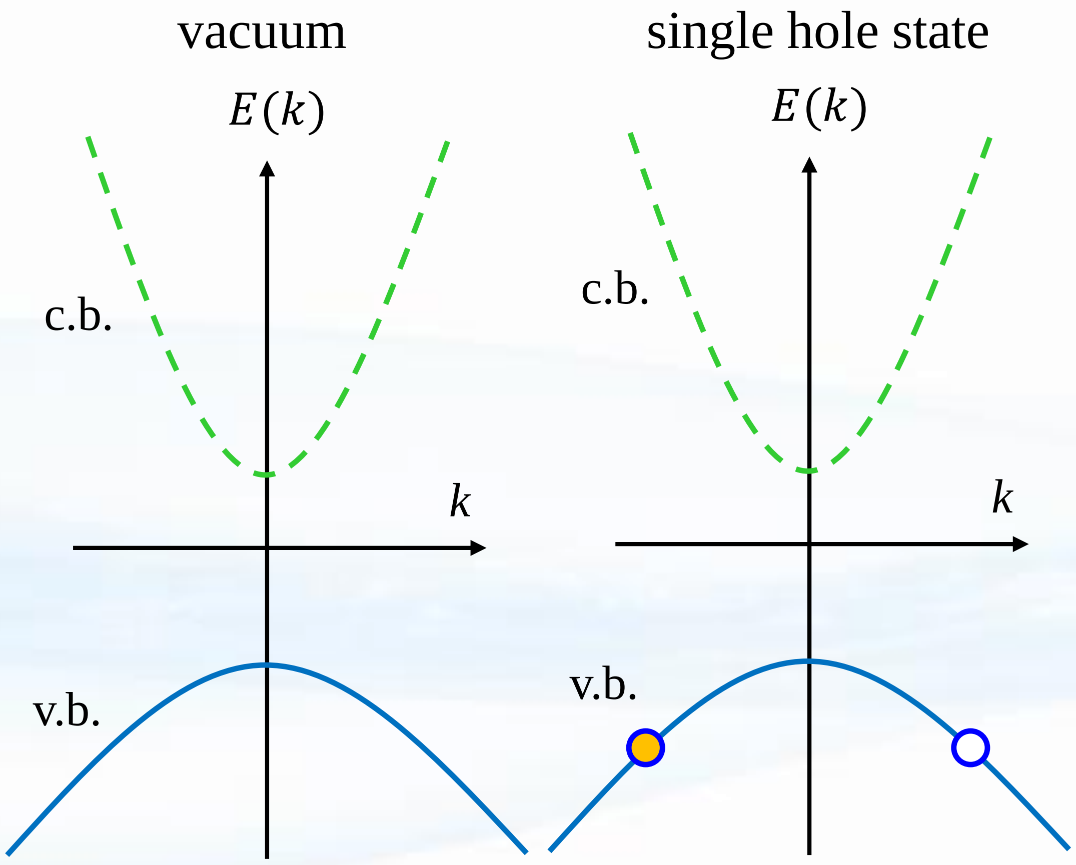
Number of states per energy (per volume)

$$\mathscr{D}(E) = \frac{1}{L^d}\left(\frac{L}{2\pi}\right)^d \frac{dV_d(k)}{dE}$$
$$= \frac{1}{(2\pi)^d}\frac{dV_d(k)}{dk}\frac{dk}{dE}$$
$$= \frac{1}{(2\pi)^d}\frac{m_0}{\hbar^2}\frac{dV_d(k)}{kdk}$$



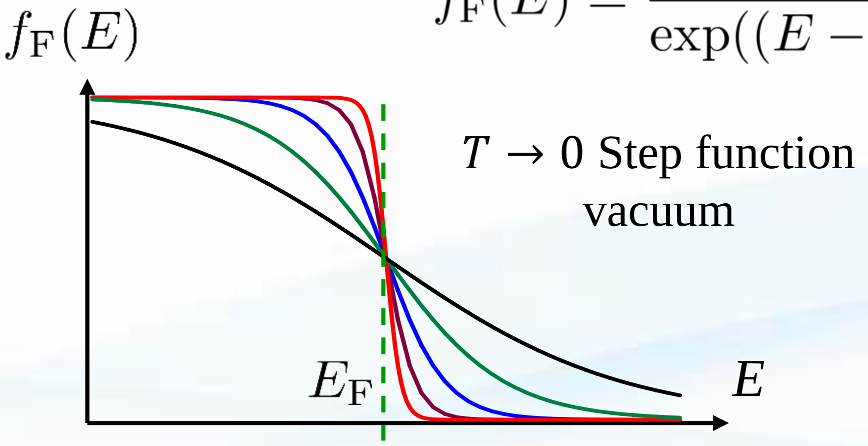
$$\mathscr{D}^{(0)}_{d=1} = \frac{1}{\pi\hbar}\sqrt{\frac{2m_0}{E}},$$
$$\mathscr{D}^{(0)}_{d=2} = \frac{m_0}{\pi\hbar^2},$$
$$\mathscr{D}^{(0)}_{d=3} = \frac{\sqrt{2m_0^3}}{\pi^2\hbar^3}\sqrt{E}$$

Electrons and holes



Fermi (electron) distribution function

$$f_{\mathrm{F}}(E) = \frac{1}{\exp((E - E_{\mathrm{F}})/k_{\mathrm{B}}T) + 1}$$



vacuum total current $\boldsymbol{J} = \sum_{\boldsymbol{k}} (-e)\boldsymbol{v}_{\boldsymbol{k}} = 0$

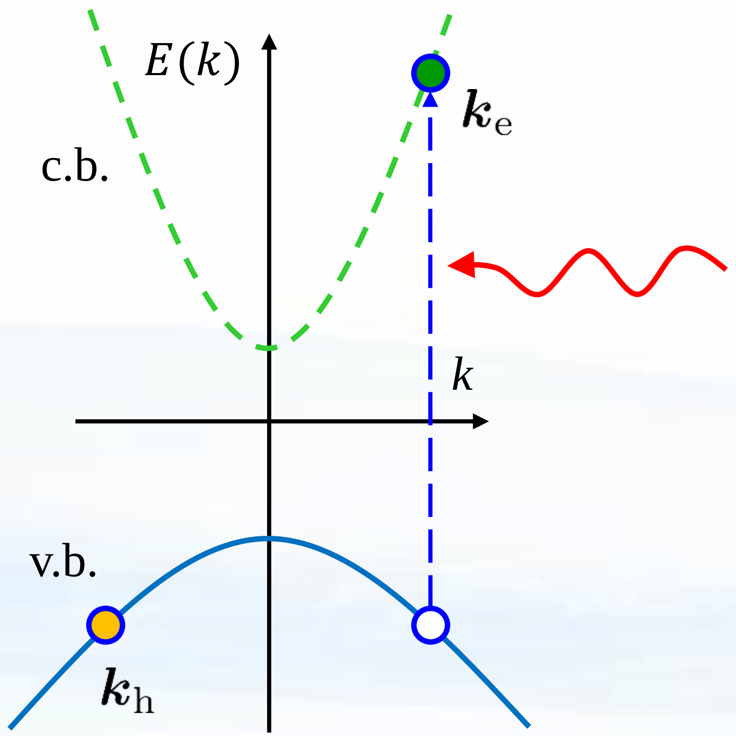
single empty state at $\boldsymbol{k}$ in valence band $\boldsymbol{J}(\boldsymbol{k}) = \sum_{\boldsymbol{k}'} (-e)\boldsymbol{v}_{\boldsymbol{k}'} - (-e)\boldsymbol{v}_{\boldsymbol{k}} = e\boldsymbol{v}_{\boldsymbol{k}}$

Electric field $\boldsymbol{E}$ $\quad \frac{d\boldsymbol{k}}{dt} = (-e)\frac{\boldsymbol{E}}{\hbar}$

All the electrons in the v.b. move in k-space in this way. So does the empty state.

Equation of motion of the empty state $\quad m^* \frac{d\boldsymbol{v}}{dt} = (-e)\boldsymbol{E} \rightarrow (-m^*)\frac{d\boldsymbol{v}}{dt} = e\boldsymbol{E}$

Definition and properties of valence band hole states



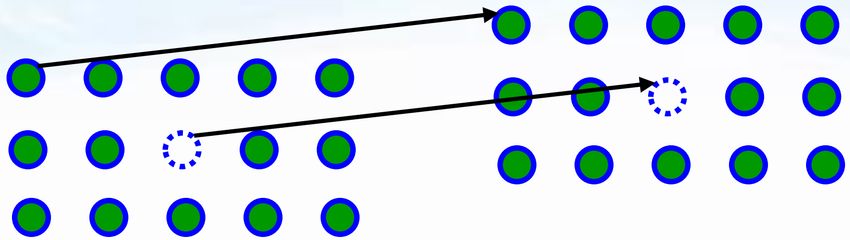
Definition: single hole

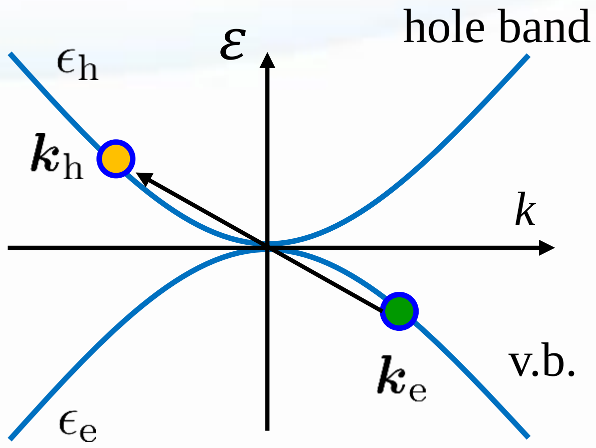
valence band electrons with a single empty Bloch state

(i) $\boldsymbol{k}_\mathrm{h} = -\boldsymbol{k}_\mathrm{e}$ Because $\sum \boldsymbol{k}_\mathrm{e} = 0$ in the vacuum state.

(ii) $\epsilon_\mathrm{h}(\boldsymbol{k}_\mathrm{h}) = -\epsilon_\mathrm{e}(\boldsymbol{k}_\mathrm{e})$ Energy measured from the valence top

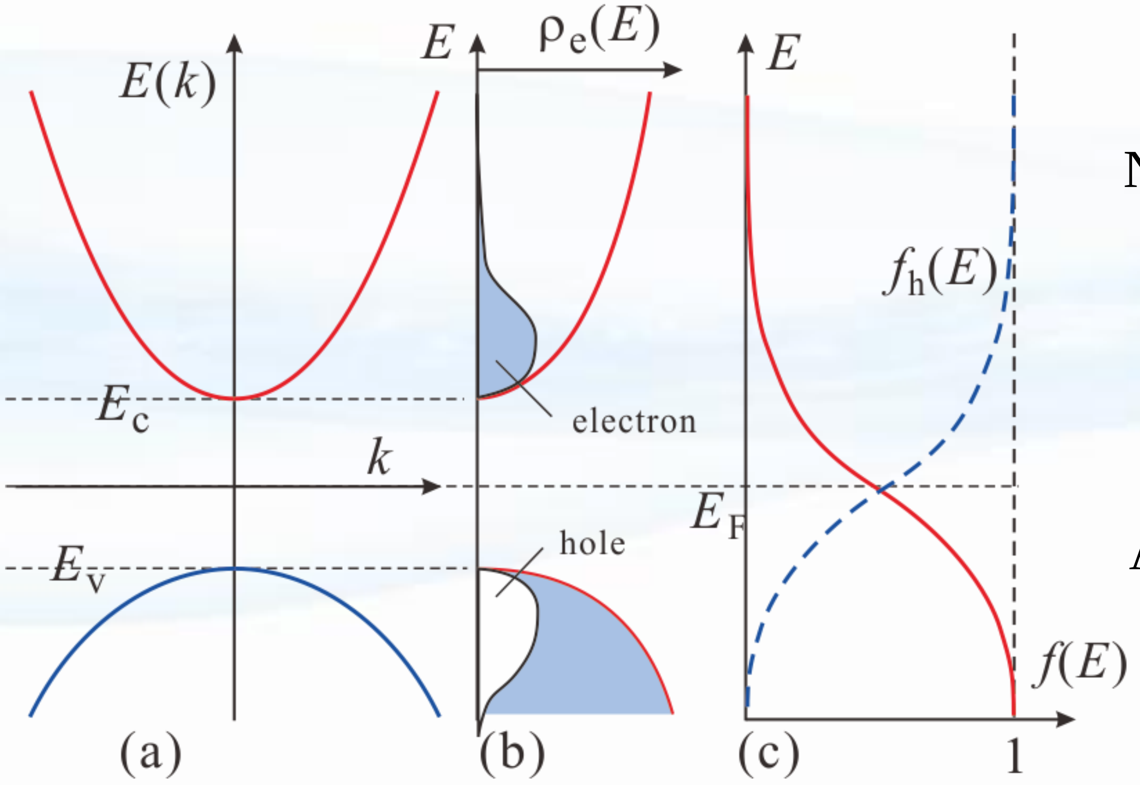
(iii) $\boldsymbol{v}_\mathrm{h} = \boldsymbol{v}_\mathrm{e}$





(iv) $m_\mathrm{h} = -m_\mathrm{e}$

Carrier distribution in intrinsic semiconductors



Hole distribution function

$$f_h(E) = 1 - f(E) = \frac{1}{1 + \exp(E_\mathrm{F} - E)/k_\mathbf{B}T)}$$

Numbers of electrons and holes exist between E and $E + dE$

$$g_e(E)dE = \mathscr{D}_e(E)f(E)dE,$$

$$g_h(E)dE = \mathscr{D}_h(E)[1 - f(E)]dE \equiv \mathscr{D}_h(E)f_h(E)dE$$

Approximate density of states with those of free particles

$$\mathscr{D}_e(E) = \frac{\sqrt{2m_e^{*3}}}{\pi^2\hbar^3}\sqrt{E - E_c} \quad \text{(conduction band)},$$

$$\mathscr{D}_h(E) = \frac{\sqrt{2m_h^{*3}}}{\pi^2\hbar^3}\sqrt{E_v - E} \quad \text{(valence band)}$$

Carrier distribution in intrinsic semiconductors (2)

$$n = \int_{E_c}^{\infty} g_e(E)dE = \frac{\sqrt{2m_e^{*3}}}{\pi^2\hbar^3}\int_{E_c}^{\infty}\frac{\sqrt{E-E_c}dE}{1+\exp(E-E_\mathrm{F})/k_\mathrm{B}T},$$

$$p = \int_{-\infty}^{E_v} g_h(E)dE = \frac{\sqrt{2m_h^{*3}}}{\pi^2\hbar^3}\int_{-\infty}^{E_v}\frac{\sqrt{E_v-E}dE}{1+\exp(E_\mathrm{F}-E)/k_\mathrm{B}T}$$

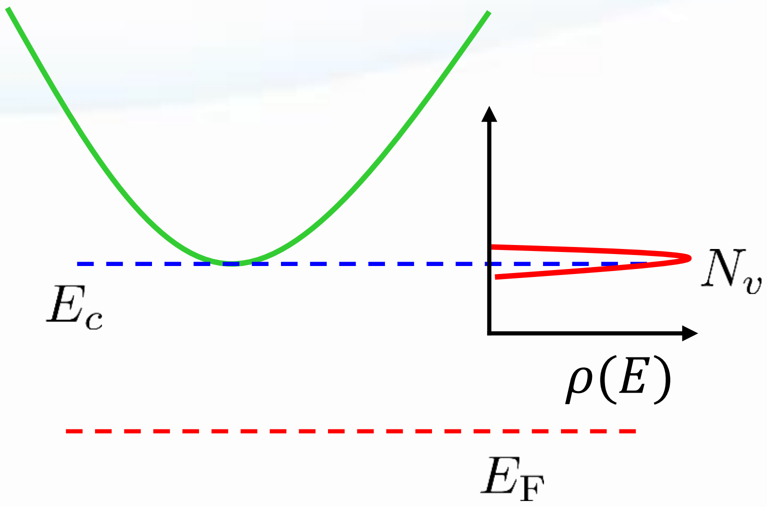
Maxwellian approximation

$$f_\mathrm{F}(E) \ll 1 (E \geq E_c)$$

$$f_h(E) \ll 1 (E \leq E_v)$$

$$f_\mathrm{F}(E) \sim \exp(E_\mathrm{F}-E)/k_\mathrm{B}T$$

$$f_h(E) \sim \exp(E-E_\mathrm{F})/k_\mathrm{B}T$$



$$n = 2\left(\frac{m_e^* k_\mathrm{B}T}{2\pi\hbar}\right)^{3/2}\exp\left(\frac{E_\mathrm{F}-E_c}{k_\mathrm{B}T}\right) \equiv N_c\exp\left(\frac{E_\mathrm{F}-E_c}{k_\mathrm{B}T}\right)$$

$$p = 2\left(\frac{m_h^* k_\mathrm{B}T}{2\pi\hbar}\right)^{3/2}\exp\left(\frac{E_v-E_\mathrm{F}}{k_\mathrm{B}T}\right) \equiv N_v\exp\left(\frac{E_v-E_\mathrm{F}}{k_\mathrm{B}T}\right)$$

$N_c,\ N_v$: effective density of states

Carrier distribution in intrinsic semiconductors (3)

Mass-action law

$$np = N_c N_v \exp\left(\frac{E_v - E_c}{k_\mathrm{B}T}\right) = N_c N_v \exp\left(-\frac{E_g}{k_\mathrm{B}T}\right) = n_i^2$$

n_i: intrinsic carrier density

The charge neutrality condition $n = p$

$$E_\mathrm{F} = \frac{E_c + E_v}{2} + \frac{k_\mathrm{B}T}{2}\ln\frac{N_v}{N_c} = \frac{E_c + E_v}{2} + \frac{3k_\mathrm{B}T}{4}\ln\frac{m_h}{m_e} \equiv E_i$$

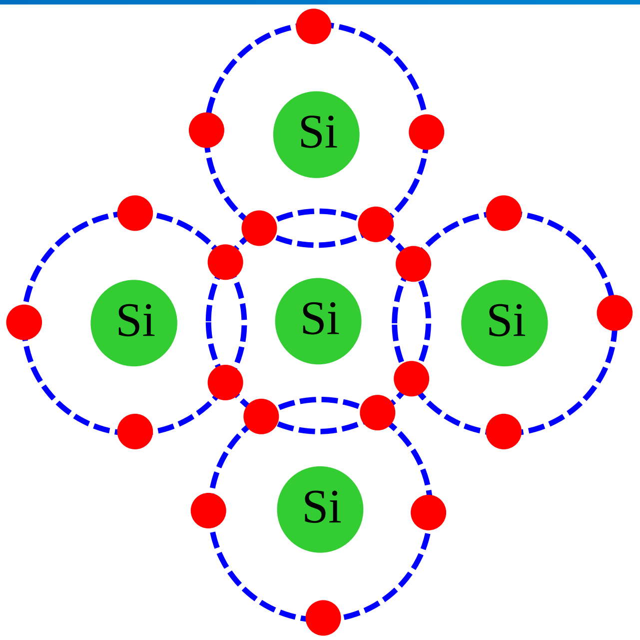
$$T \to 0:\ E_\mathrm{F} \to \frac{E_c + E_v}{2}$$

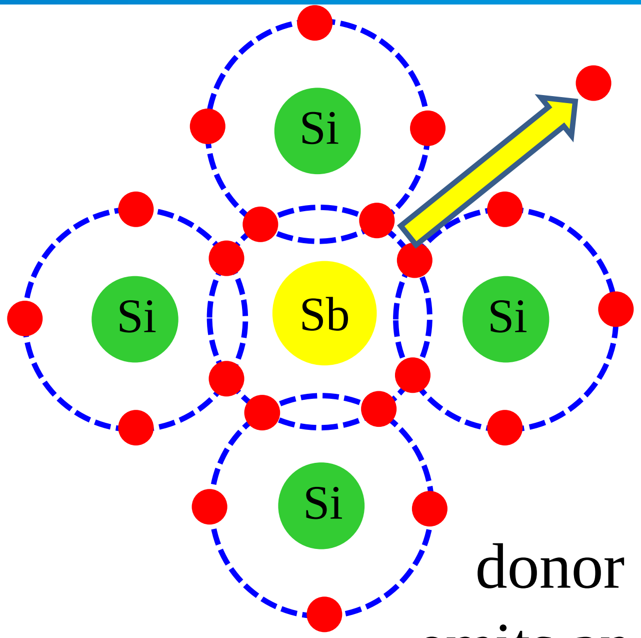
General expressions

$$n = n_i \exp\left(\frac{E_\mathrm{F} - E_i}{k_\mathrm{B}T}\right) \qquad E_\mathrm{F} - E_i = k_\mathrm{B}T\ln\frac{n}{n_i}$$

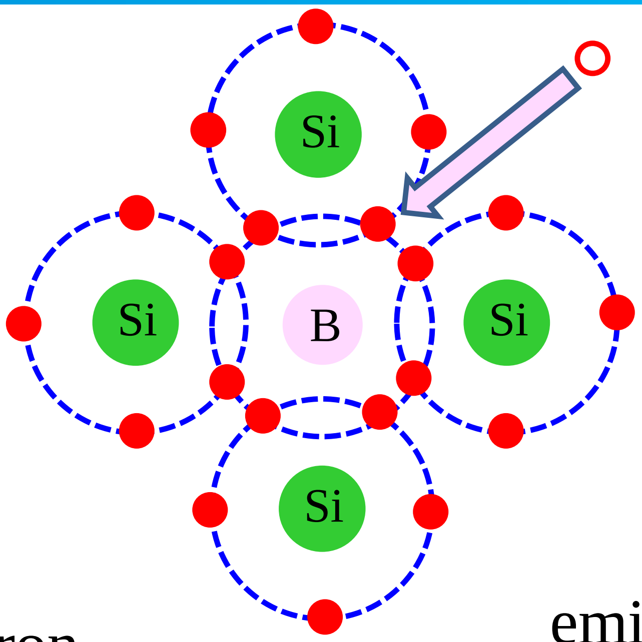
$$p = n_i \exp\left(\frac{E_i - E_\mathrm{F}}{k_\mathrm{B}T}\right) \qquad E_i - E_\mathrm{F} = k_\mathrm{B}T\ln\frac{p}{n_i}$$

Doping and carrier distribution





donor
emits an electron



acceptor
emits a hole

II	III	IV	V	VI
4 Be ベリリウム 9.012182	5 B ホウ素 10.811	6 C 炭素 12.0107	7 N 窒素 14.0067	8 O 酸素 15.9994
12 Mg マグネシウム 24.305	13 Al アルミニウム 26.98153...	14 Si ケイ素 28.0855	15 P リン 30.973762	16 S 硫黄 32.065
30 Zn 亜鉛 65.38	31 Ga ガリウム 69.723	32 Ge ゲルマニウム 72.63	33 As ヒ素 74.9216	34 Se セレン 78.96
48 Cd カドミウム 112.411	49 In インジウム 114.818	50 Sn スズ 118.71	51 Sb アンチモン 121.76	52 Te テルル 127.6

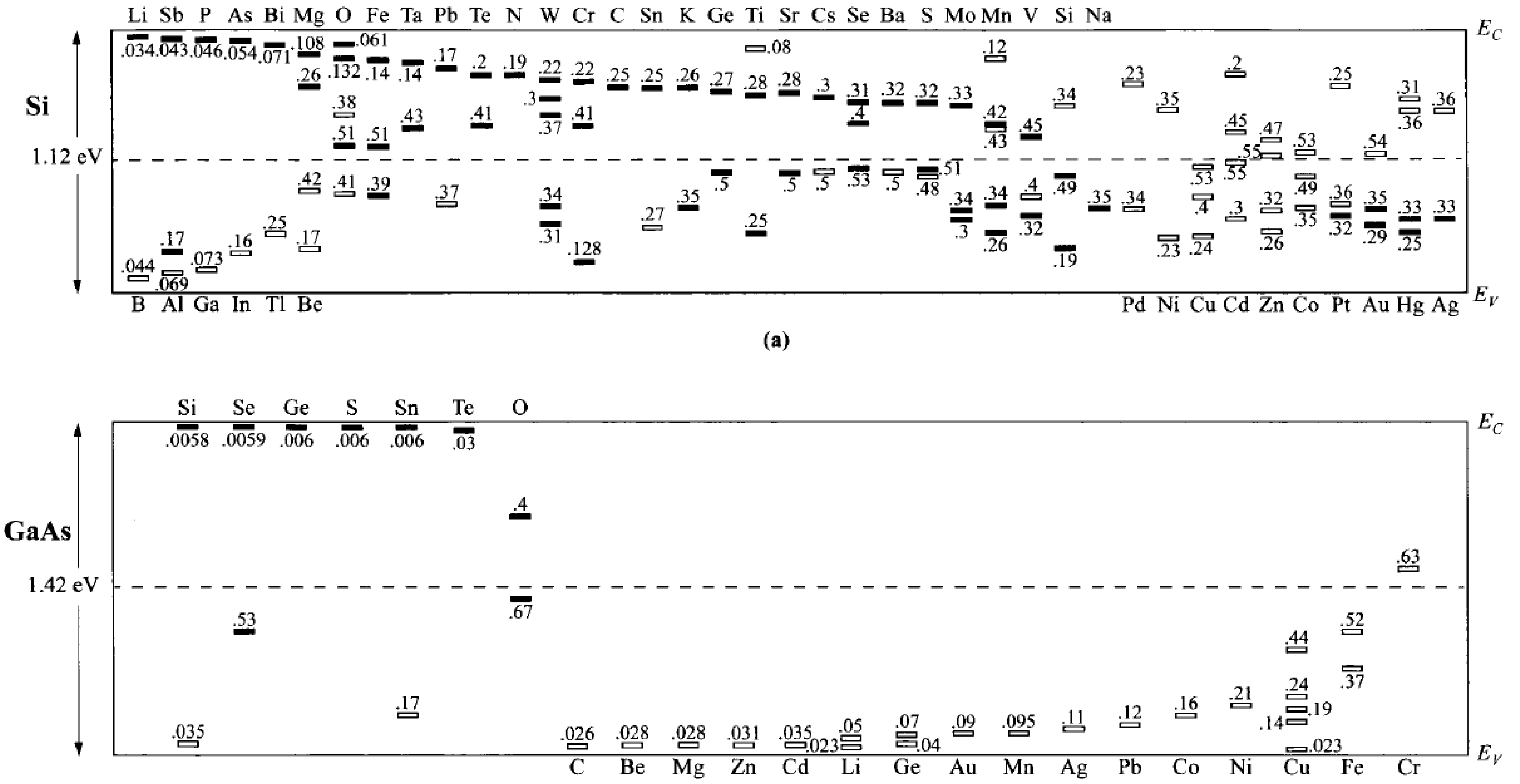
Donor concentration is higher: *n*-type
Acceptor concentration is higher: *p*-type

Donors and acceptors compensate each other.

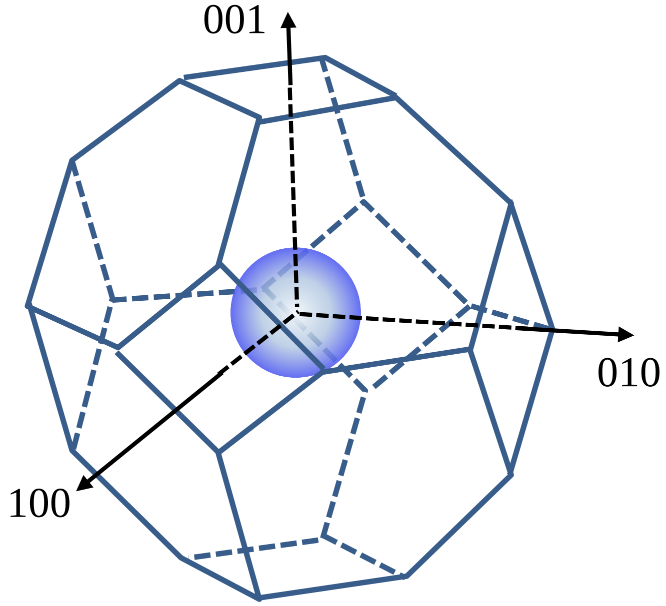
For silicon Donors: P, As, Sb
Acceptors: B, Al, Ga

Impurity levels in Si and GaAs

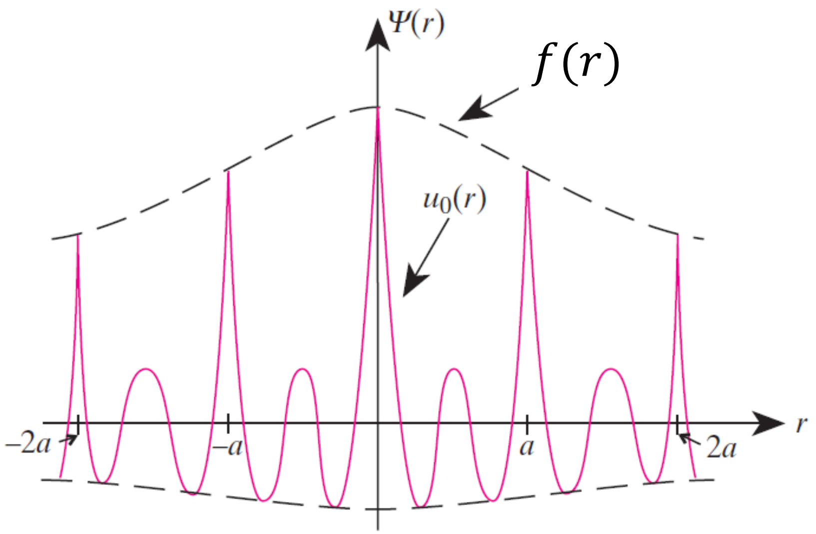
S. M. Sze, Physics of semiconductor devices



Shallow hydrogen-like impurity states



GaAs



Conduction mass is isotropic and unique.

Effective mass equation
$$\left[-\frac{\hbar^2\nabla^2}{2m^*}-\frac{e^2}{4\pi\epsilon_0\epsilon r}\right]f(\boldsymbol{r})=Ef(\boldsymbol{r})$$

We can readily use the results of the hydrogen atom with replacing the mass and the dielectric constant.

$$E_n=E_c-\frac{Ry^*}{n^2}\quad(n=1,2,\cdots)$$

1*s* wavefunction
$$\psi_{1s}(\boldsymbol{r})=\sqrt{\frac{1}{\pi a_{\mathrm{B}}^{*3}}}\exp\left(-\frac{\boldsymbol{r}}{a_{\mathrm{B}}^*}\right)$$

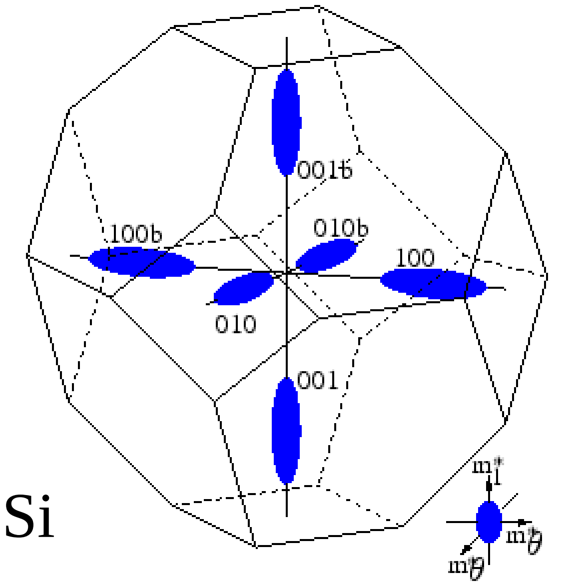
Effective Rydberg constant:
$$Ry^*=\frac{e^2m^*}{2(4\pi\epsilon\epsilon_0)^2\hbar^2}=\frac{m^*}{m}\frac{1}{\epsilon^2}Ry,$$

Effective Bohr radius:
$$a_{\mathrm{B}}^*=\frac{4\pi\epsilon\epsilon_0\hbar^2}{m^*e^2}=\frac{m}{m^*}\epsilon a_{\mathrm{B}}$$

How good is the approximation

Semiconductor	Binding energy from (4.24) [meV]	Experimental binding energy of common donors [meV]
GaAs	5.72	Si_{Ga}(5.84); Ge_{Ga}(5.88) S_{As}(5.87); Se_{As}(5.79)
InP	7.14	7.14
InSb	0.6	Te_{Sb}(0.6)
CdTe	11.6	In_{Cd}(14); Al_{Cd}(14)
ZnSe	25.7	Al_{Zn}(26.3); Ga_{Zn}(27.9) F_{Se}(29.3); Cl_{Se}(26.9)

Shallow impurity states in Si



Donor biding energy in Si (meV)

Measurement

Dopant	Li	P	As	Sb	Bi
Thermal		44	55	39	69
Optical	32.8	45	53.7	43	70.6

For [001] spheroid $$E_1(\boldsymbol{k}) = \frac{\hbar^2}{2}\left[\frac{k_x^2 + k_y^2}{m_t} + \frac{(k_z - k_0)^2}{m_l}\right]$$

Effective mass equation $$\left[-\frac{\hbar^2}{2m_t}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\hbar^2}{2m_l}\frac{\partial^2}{\partial z^2} - \frac{e^2}{4\pi\epsilon_0\epsilon r}\right] f(\boldsymbol{r}) = Ef(\boldsymbol{r})$$

Variational method $$f_{1s}(\boldsymbol{r}) = \sqrt{\frac{1}{\pi a^2 b}}\exp\left(-\sqrt{\frac{x^2+y^2}{a^2} + \frac{z^2}{b^2}}\right)$$

	a (10^{-8} cm)	*b* (10^{-8} cm)	E (1s) (meV)
Si	25	14.2	29
Ge	64.5	22.7	9.2

Not sufficient agreements.
Need more accurate calculations.

Doping and carrier distribution

Uniform donor concentration N_D

n: excited electrons,
n_D: captured electrons

$$n + n_D = N_D$$

Entropy

$$S = k_B \ln W$$

Helmholtz free energy

$$F = U - TS = E_D n_D - k_B T \ln \left[2^{n_D} \frac{N_D!}{n_D!(N_D - n_D)!} \right]$$

Starling approximation

$\ln N! \sim N \ln N - N$

$$\mu = E_F = \frac{\partial F}{\partial n_D} = E_D - k_B T \ln \left[\frac{2(N_D - n_D)}{n_D} \right]$$

Donor level

$$n_D = N_D \left[1 + \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_B T} \right) \right]^{-1}$$

For acceptors

$$n_A = N_A \left[1 + 2 \exp\left(\frac{E_A - E_F}{k_B T} \right) \right]^{-1}$$

note: the formula is symmetric if we introduce captured hole concentration $p_A = N_A - n_A$

Doping and carrier distribution

E_F is given from n or p as

$$E_\mathrm{F} \approx E_C + k_\mathrm{B}T\left[\ln\left(\frac{n}{N_C}\right) + 2^{-3/2}\left(\frac{n}{N_C}\right)\right],$$

$$E_\mathrm{F} \approx E_V - k_\mathrm{B}T\left[\ln\left(\frac{p}{N_V}\right) + 2^{-3/2}\left(\frac{p}{N_V}\right)\right]$$

In the case of n-type semiconductor with compensation $n + N_A = N_\mathrm{D} - n_\mathrm{D}$

$$\frac{n + N_\mathrm{A}}{N_\mathrm{D} - N_\mathrm{A} - n} = \frac{1}{2}\exp\left(\frac{E_\mathrm{D} - E_\mathrm{F}}{k_\mathrm{F}T}\right)$$

$$\frac{n(n + N_\mathrm{A})}{N_\mathrm{D} - N_\mathrm{A} - n} = \frac{1}{2}N_c\exp\left(-\frac{\Delta E_\mathrm{D}}{k_\mathrm{B}T}\right), \quad \Delta E_\mathrm{D} \equiv E_c - E_\mathrm{D}$$

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.28 Lecture 04

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Review of lecture in the last week

Envelope function (effective mass approximation)

Chapter 3 Carrier statistics and chemical doping

Density of states

Definition and properties of valence band hole states

Carrier distribution in intrinsic semiconductors

Shallow hydrogen-like impurity states

Shallow impurity states in Si

Contents today

Doping and carrier distribution

Temperature dependence of carrier concentration

Exciton

Chapter 4 Optical properties (bulk)

Quantization of electromagnetic field

Number state, coherent state

Optical response of two-level system

Optical absorption with inter-band transition

Doping and carrier distribution

Uniform donor concentration N_D

n: excited electrons,
n_D: captured electrons

$$n + n_D = N_D$$

Entropy $S = k_B \ln W$

Helmholtz free energy

$$F = U - TS = E_D n_D - k_B T \ln \left[2^{n_D} \frac{N_D!}{n_D!(N_D - n_D)!} \right]$$

Starling approximation

$\ln N! \sim N \ln N - N$

$$\mu = E_F = \frac{\partial F}{\partial n_D} = E_D - k_B T \ln \left[\frac{2(N_D - n_D)}{n_D} \right]$$

Donor level

$$n_D = N_D \left[1 + \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_B T} \right) \right]^{-1}$$

For acceptors

$$n_A = N_A \left[1 + 2 \exp\left(\frac{E_A - E_F}{k_B T} \right) \right]^{-1}$$

note: the formula is symmetric if we introduce captured hole concentration $p_A = N_A - n_A$

Doping and carrier distribution

E_F is given from n or p as $\begin{cases} E_F \approx E_C + k_B T \left[\ln\left(\frac{n}{N_C}\right) + 2^{-3/2}\left(\frac{n}{N_C}\right) \right], \\ E_F \approx E_V - k_B T \left[\ln\left(\frac{p}{N_V}\right) + 2^{-3/2}\left(\frac{p}{N_V}\right) \right] \end{cases}$

In the case of n-type semiconductor with compensation $n + N_A = N_D - n_D$

$$\frac{n + N_A}{N_D - N_A - n} = \frac{1}{2}\exp\left(\frac{E_D - E_F}{k_F T}\right)$$

$$\frac{n(n + N_A)}{N_D - N_A - n} = \frac{1}{2} N_c \exp\left(-\frac{\Delta E_D}{k_B T}\right), \quad \Delta E_D \equiv E_c - E_D$$

Temperature dependence of carrier concentration

(I) Impurity regime I: Temperature is very low.

$$n \ll N_A \ll N_D$$

$$n \approx \frac{N_D N_c}{2N_A} \exp\left(-\frac{\Delta E_D}{k_B T}\right)$$

(II) Impurity regime II:

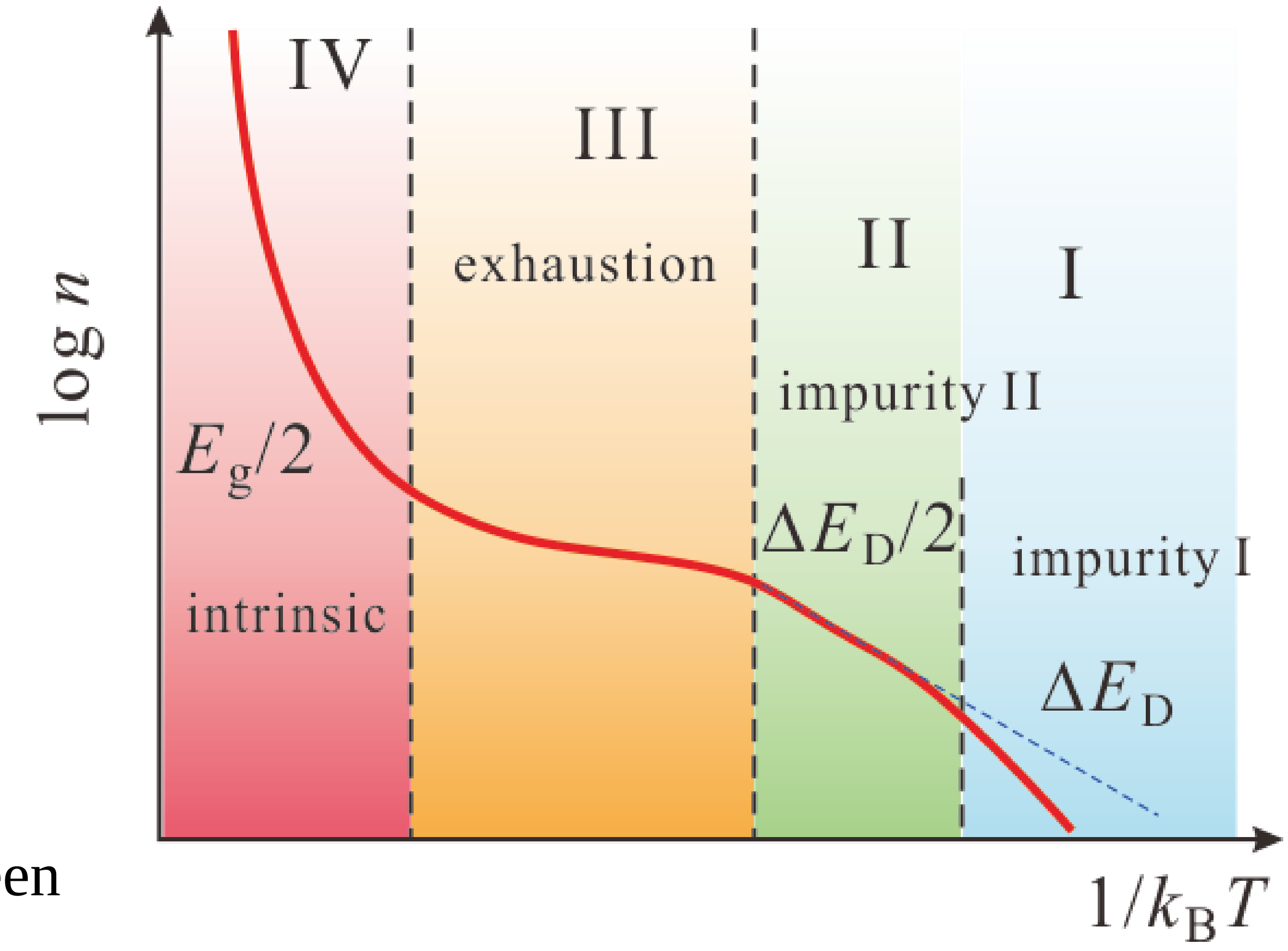
T is a bit higher. $N_A \ll n \ll N_D$

$$n \approx \left(\frac{N_c N_D}{2}\right)^{1/2} \exp\left(-\frac{\Delta E_D}{2k_B T}\right)$$

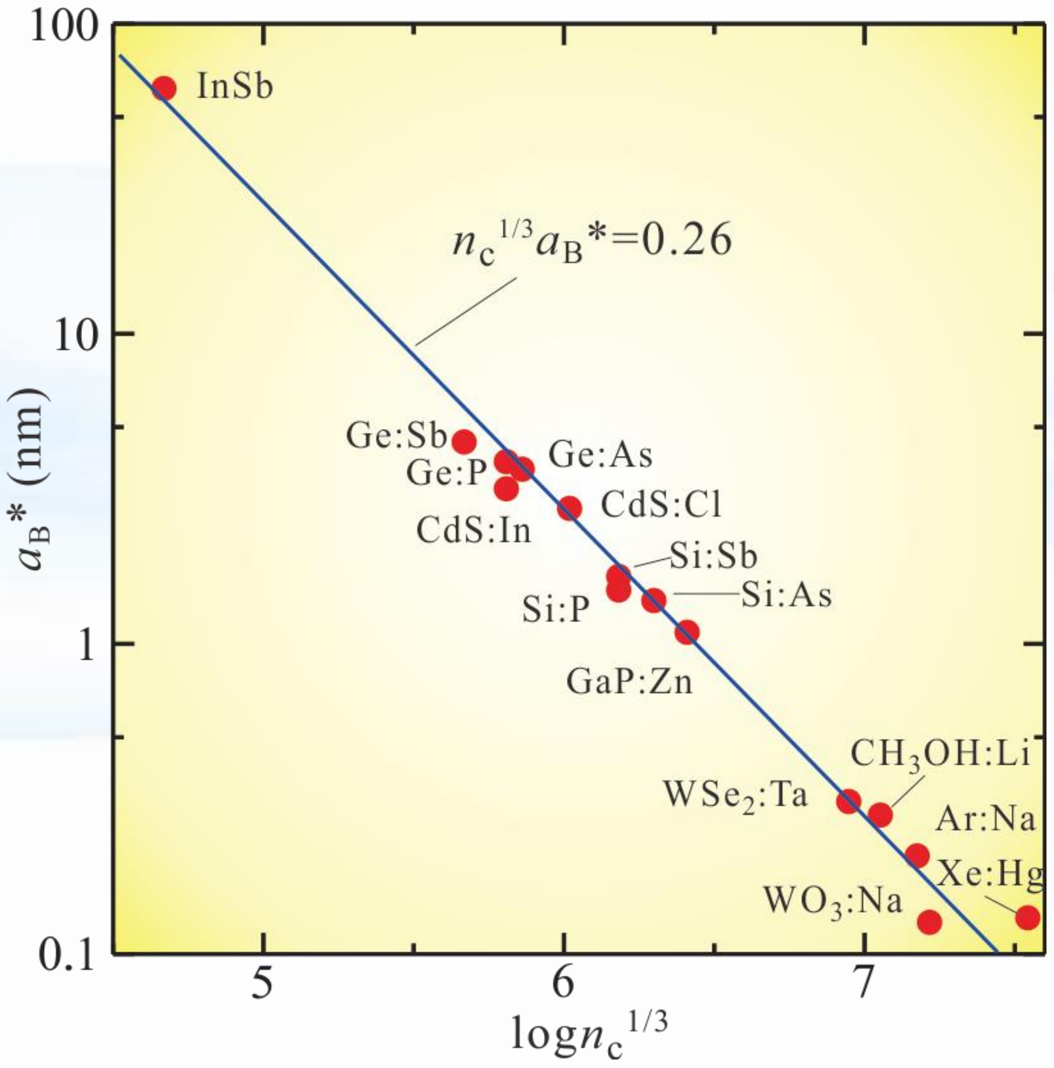
(III) Exhaustion regime:

$k_B T > \Delta E_D$ $\quad n \approx N_D - N_A$

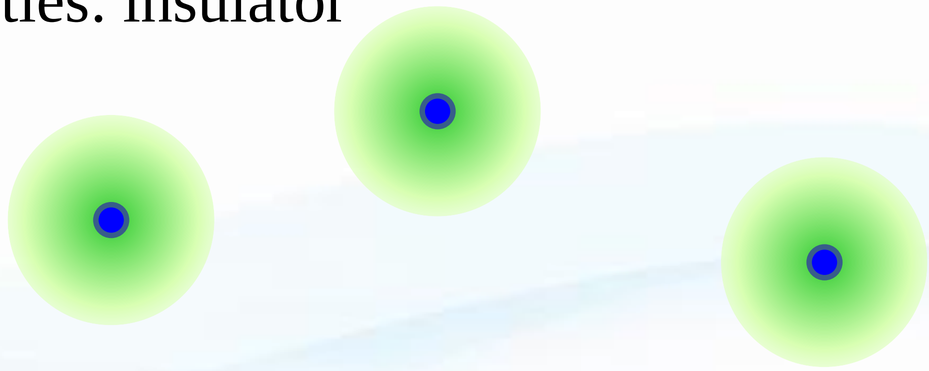
(IV) Intrinsic regime: direct excitation between the v.b. and the c.b. is not negligible.



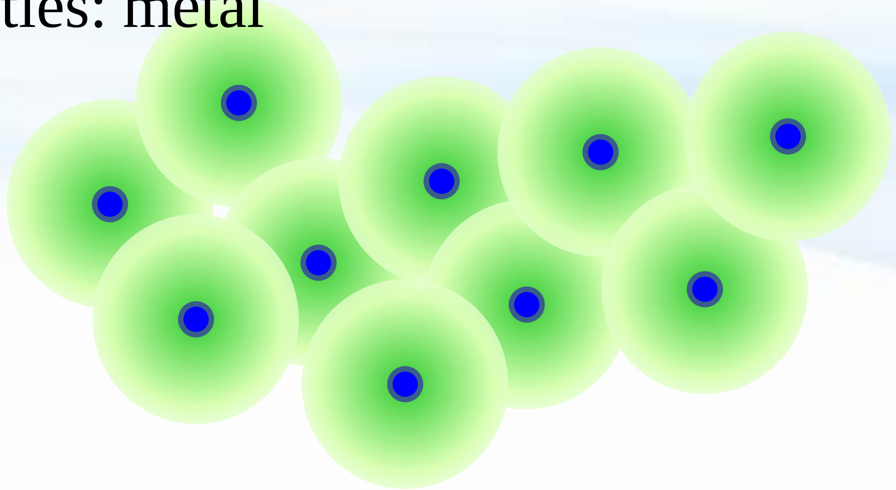
Degenerate semiconductors



sparse impurities: insulator



dense impurities: metal

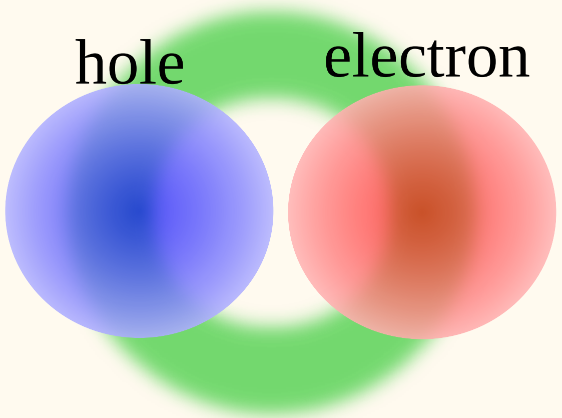


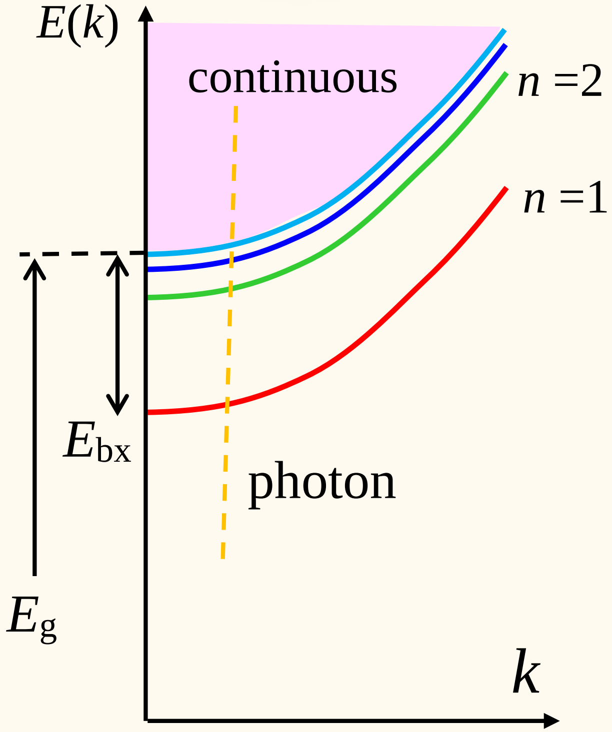
Empirical metal-insulator criterion

$$n_c^{1/3} a_{\mathrm{B}}^* = 0.26$$

Excitons (Wannier type)

Free excitons





Binding energy $$E_{bx} = -\frac{m_r^* e^4}{8h^2(\epsilon_0\epsilon)^2}\frac{1}{n^2}$$

Reduced mass $$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Exciton kinetic energy $$E_{kx} = \frac{\hbar^2 k^2}{2(m_e + m_h)}$$

Energy for exciton creation $$E_{ex} = E_g + \frac{\hbar^2 k^2}{2(m_e + m_h)} - \frac{m_r^* e^4}{8h^2(\epsilon_0\epsilon)^2}\frac{1}{n^2}$$

Excitonic complexes

(+) : donor + : hole – : electron

(+)	+	–		H_2^+	Excitonic ions
(+)	–	–		H^-	
+	+	–		H_2^+	
+	+	–	–	H_2	Excitonic molecule (bi-exciton, trion)
(+)	+	–	–	H_2	

Chapter 4 Optical properties (bulk)

Luminescence from CdTe quantum dots (Sigma-Aldrich)

Quantization of electromagnetic field

1-d harmonic oscillator $\frac{\hbar\omega}{2}\left(-\frac{d^2}{dq^2}+q^2\right)\phi = E\phi \;\rightarrow\; \hbar\omega\left(a^\dagger a+\frac{1}{2}\right)\phi = E\phi$

up/down operators $a = \frac{1}{\sqrt{2}}\left(\frac{d}{dq}+q\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{dq}+q\right), \quad [a, a^\dagger] = 1$

Eigenenergy $E_n = \hbar\omega\left(n+\frac{1}{2}\right) \quad (n = 0, 1, 2, \cdots)$ $\quad \frac{\hbar\omega}{2}$: Zero-point energy

Starting point: Electro-magnetic field is a set of harmonic oscillators (Jeans theorem)

$$E = \int\left(\epsilon_0 \boldsymbol{E}^2 + \frac{\boldsymbol{H}^2}{\mu_0}\right)\frac{d\boldsymbol{r}}{4} \;\rightarrow\; \boldsymbol{A}_{\boldsymbol{k}\lambda} = \frac{\boldsymbol{e}_{\boldsymbol{k}\lambda}}{\sqrt{4\epsilon_0 V\omega_{\boldsymbol{k}}^2}}(iP_{\boldsymbol{k}\lambda}+\omega_{\boldsymbol{k}}Q_{\boldsymbol{k}\lambda}), \quad E = \frac{1}{2}\sum_{\boldsymbol{k}\lambda}(P_{\boldsymbol{k}\lambda}^2+\omega_{\boldsymbol{k}}^2Q_{\boldsymbol{k}\lambda}^2)$$

Quantization: $\rightarrow \hat{H} = \frac{1}{2}\sum_{\boldsymbol{k}\lambda}(\hat{P}_{\boldsymbol{k}\lambda}^2+\omega_{\boldsymbol{k}}^2\hat{Q}_{\boldsymbol{k}\lambda}^2), \quad [\hat{Q}_{\boldsymbol{k}'\lambda'}, \hat{P}_{\boldsymbol{k}\lambda}] = i\hbar\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\delta\delta'}$

Creation/annihilation operators

$$a_{\boldsymbol{k}\lambda}^\dagger = \frac{1}{\sqrt{2\hbar\omega_{\boldsymbol{k}}}}(\omega_{\boldsymbol{k}}\hat{Q}_{\boldsymbol{k}\lambda}-i\hat{P}_{\boldsymbol{k}\lambda}), \quad a_{\boldsymbol{k}\lambda} = \frac{1}{\sqrt{2\hbar\omega_{\boldsymbol{k}}}}(\omega_{\boldsymbol{k}}\hat{Q}_{\boldsymbol{k}\lambda}+i\hat{P}_{\boldsymbol{k}\lambda})$$

$$[a_{\boldsymbol{k}\lambda}, a_{\boldsymbol{k}'\lambda'}^\dagger] = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'}, \quad \text{(others)} = 0$$

Quantization of electromagnetic field (2)

$$\hat{H} = \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}} \left(a^\dagger_{\boldsymbol{k}\lambda} a_{\boldsymbol{k}\lambda} + \frac{1}{2} \right)$$

$$\hat{\boldsymbol{A}}(\boldsymbol{r}, t) = \sum_{\boldsymbol{k}\lambda} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_{\boldsymbol{k}} V}} \boldsymbol{e}_{\boldsymbol{k}\lambda} \left[a_{\boldsymbol{k}\lambda} e^{i(\boldsymbol{k}\boldsymbol{r} - \omega_{\boldsymbol{k}} t)} + a^\dagger_{\boldsymbol{k}\lambda} e^{-i(\boldsymbol{k}\boldsymbol{r} - \omega_{\boldsymbol{k}} t)} \right]$$

$$|\{n_{\boldsymbol{k}\lambda}\}\rangle = \left[\prod_{\boldsymbol{k}\lambda} \frac{(a^\dagger_{\boldsymbol{k}\lambda})^{n_{\boldsymbol{k}\lambda}}}{\sqrt{n_{\boldsymbol{k}\lambda}!}} \right] |0\rangle$$

$$\langle \{n_{\boldsymbol{k}\lambda}\} | \hat{H} | \{n_{\boldsymbol{k}\lambda}\} \rangle = \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}} \left(n_{\boldsymbol{k}\lambda} + \frac{1}{2} \right)$$

$$|v\rangle = \exp(-|v|^2/2) \exp(v a^\dagger) |0\rangle = \exp(-|v|^2/2) \sum_{n=0}^{\infty} \frac{v^n}{\sqrt{n!}} |n\rangle$$

Properties of number state, coherent state

Number state

Expectation value of electromagnetic field is zero

$$\langle\{n_{\boldsymbol{k}\lambda}\}|\hat{\boldsymbol{E}}|\{n_{\boldsymbol{k}\lambda}\}\rangle = -\langle\{n_{\boldsymbol{k}\lambda}\}|(\partial\hat{\mathbf{A}}/\partial t)|\{n_{\boldsymbol{k}\lambda}\}\rangle = 0$$

Quantum fluctuation is non-zero even for |0⟩

$$\langle\{n_{\boldsymbol{k}\lambda}\}|\hat{\boldsymbol{E}}^2|\{n_{\boldsymbol{k}\lambda}\}\rangle = \sum_{\boldsymbol{k}\lambda}\frac{\hbar\omega_{\boldsymbol{k}}}{\epsilon_0 V}\left(n_{\boldsymbol{k}\lambda}+\frac{1}{2}\right) = \frac{1}{\epsilon_0 V}\langle\{n_{\boldsymbol{k}\lambda}\}|H|\{n_{\boldsymbol{k}\lambda}\}\rangle$$

Coherent state

$$|\alpha\rangle = \exp\left(-\frac{|\alpha|^2}{2}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

Probability of *n*-photons $P(n) = \dfrac{e^{-|\alpha|^2}|\alpha|^{2n}}{n!}$ Poisson distribution

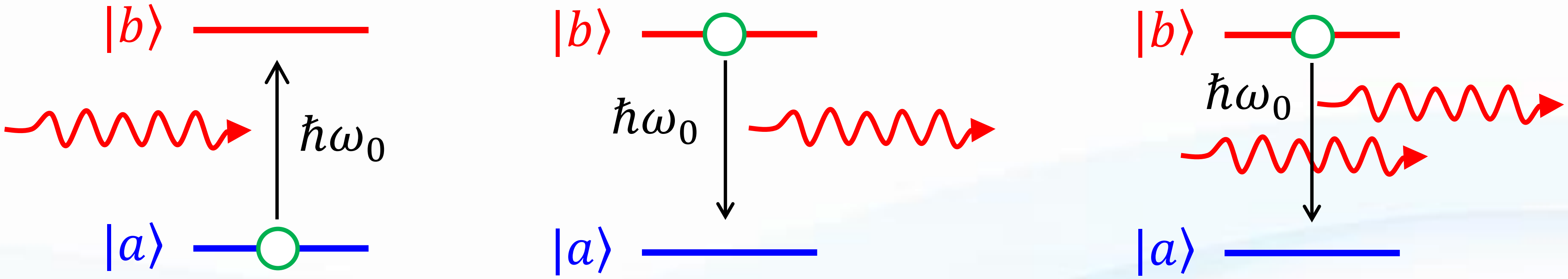
If we write $\alpha = |\alpha|e^{i\phi}$

$$\begin{cases}\langle\alpha|\hat{\boldsymbol{E}}(\boldsymbol{r},t)|\alpha\rangle = -\sqrt{\dfrac{2\hbar\omega_{\boldsymbol{k}}}{\epsilon_0 V}}|\alpha|\boldsymbol{e}_{\boldsymbol{k}\lambda}\sin(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t+\phi) \\ \langle\alpha|\hat{\boldsymbol{B}}(\boldsymbol{r},t)|\alpha\rangle = -\sqrt{\dfrac{2\hbar}{\epsilon_0\omega_{\boldsymbol{k}}V}}|\alpha|\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k}\lambda}\sin(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t+\phi)\end{cases}$$

Expectation value: classical electromagnetic field

Optical response of two-level system

Three fundamental processes



(a) absorption (b) spontaneous emission (c) stimulated emission

$$\mathscr{H}_0|a\rangle = E_a|a\rangle, \quad \mathscr{H}_0|b\rangle = E_b|b\rangle$$

$$\psi(t) = c_a(t)e^{-E_a t/\hbar}|a\rangle + c_b(t)e^{-E_b t/\hbar}|b\rangle$$

Hamiltonian with electromagnetic field $\mathscr{H}_{\mathrm{op}} = \frac{(\boldsymbol{p} + e\boldsymbol{A})^2}{2m} + V(\boldsymbol{r}) \approx \mathscr{H}_0 + \frac{e}{m}\boldsymbol{A}\cdot\boldsymbol{p}$

Light absorption process $\boldsymbol{A} = A_0\vec{e}\cos(\boldsymbol{k}_{\mathrm{p}}\cdot\boldsymbol{r} - \omega t)$

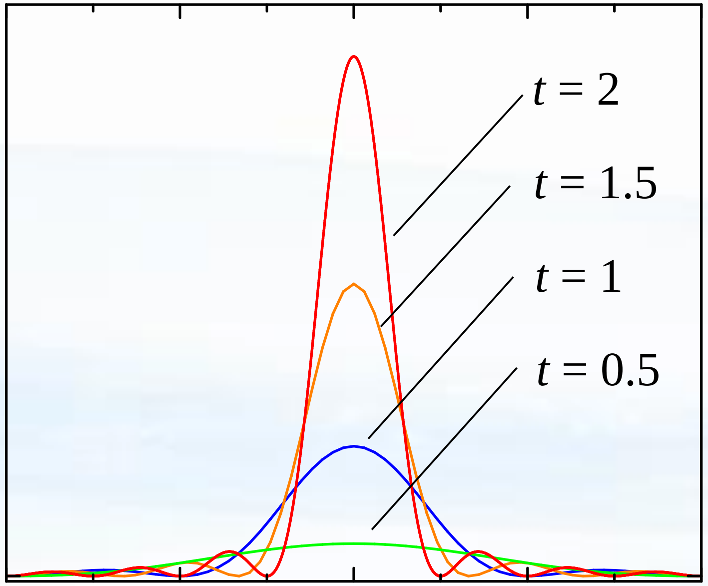
Perturbation part in $\mathscr{H}_{\mathrm{op}}$ $\mathscr{H}' = \frac{eA_0}{m}\vec{e}\cdot\hat{\boldsymbol{p}}\cos(\boldsymbol{k}_{\mathrm{p}}\cdot\boldsymbol{r} - \omega t)$

assumption

$$\langle a|\mathscr{H}'|a\rangle = \langle b|\mathscr{H}'|b\rangle = 0$$

Optical response of two-level system (2)

Schrödinger equation: $i\hbar\left[\frac{dc_a}{dt}|a\rangle e^{-iE_at/\hbar}+\frac{dc_b}{dt}|b\rangle e^{-iE_bt/\hbar}\right]=c_a\mathscr{H}'|a\rangle e^{-iE_at/\hbar}+c_b\mathscr{H}'|b\rangle e^{-iE_bt/\hbar}$



$$\begin{cases}\dfrac{dc_a}{dt}=-\dfrac{i}{\hbar}c_b\langle a|\mathscr{H}'|b\rangle e^{-i\omega_0 t},\\[2mm] \dfrac{dc_b}{dt}=-\dfrac{i}{\hbar}c_a\langle b|\mathscr{H}'|a\rangle e^{i\omega_0 t}.\end{cases}\qquad \omega_0\equiv\frac{E_b-E_a}{\hbar}$$

$$c_a^{(1)}(t)=1,\quad c_b^{(1)}(t)=-\frac{i}{\hbar}\int_0^t\langle b|\mathscr{H}'|a\rangle(t')e^{i\omega_0t'}dt'(=c_b^{(2)}(t))$$

$$c_a^{(2)}(t)=1-\frac{1}{\hbar^2}\int_0^t dt'\langle a|\mathscr{H}'|b\rangle(t')e^{-i\omega_0t'}\left[\int_0^{t'}dt''\langle b|\mathscr{H}'|a\rangle(t'')e^{i\omega_0t''}\right]$$

$$\mathscr{H}'=\frac{eA_0}{m}\vec{e}\cdot\hat{\mathbf{p}}\cos(\boldsymbol{k}_\mathrm{p}\cdot\boldsymbol{r}-\omega t)$$

Ignore $\boldsymbol{k}_\mathrm{p}$

$$V_{ba}\equiv\langle b|\frac{eA_0}{m}\vec{e}\cdot\hat{\mathbf{p}}|a\rangle$$

$$c_b(t)\simeq-\frac{i}{\hbar}V_{ba}\int_0^t dt'\cos\omega t'e^{i\omega_0t'}=-\frac{V_{ba}}{2\hbar}\left[\frac{e^{i(\omega_0+\omega)t}-1}{\omega_0+\omega}+\frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}\right]$$

$$\simeq-i\frac{V_{ba}}{\hbar}\frac{\sin[(\omega_0-\omega)t/2]}{\omega_0-\omega}e^{i(\omega_0-\omega)t/2}$$

$$P_b(t)=|c_b(t)|^2\simeq\frac{|V_{ba}|^2}{\hbar^2}\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$$

Energy conservation

Rabi oscillation

Rotating wave approximation (drop $e^{-i\omega t}$)

$$\langle a|\mathscr{H}'|b\rangle = \frac{V_{ab}}{2}e^{i\omega t}$$

$$\begin{cases} \dfrac{dc_a}{dt} = -\dfrac{i}{2\hbar}c_b V_{ab} e^{-i(\omega_0-\omega)t}, \\ \dfrac{dc_b}{dt} = -\dfrac{i}{2\hbar}c_a V_{ba} e^{i(\omega_0-\omega)t}. \end{cases}$$

$$\frac{d^2c_b}{dt^2} + i(\omega-\omega_0)\frac{dc_a}{dt} + \frac{|V_{ab}|^2}{(2\hbar)^2} = 0$$

solution $c_b(t) = c_+e^{i\lambda_+t} + c_-e^{\lambda_-t}$ $\quad \lambda_\pm \equiv \frac{1}{2}(\delta \pm \sqrt{\delta^2 + |V_{ab}|^2/\hbar^2}), \quad \delta \equiv \omega_0 - \omega$

initial condition $|c_a(0)| = 1,\ c_b(0) = 0$

Rabi oscillation

$$\begin{cases} c_b(t) = \dfrac{i|V_{ab}|}{\omega_R \hbar}e^{i\delta t/2}\sin(\omega_R t/2), \\ c_a(t) = e^{i\delta t/2}\left[\cos\left(\dfrac{\omega_R t}{2}\right) - i\dfrac{\delta}{\omega_R}\sin\left(\dfrac{\omega_R t}{2}\right)\right] \end{cases}$$

Rabi frequency $\omega_R \equiv \sqrt{\delta^2 + |V_{ab}|^2/\hbar^2}$

Oscillator strength and selection rule

Oscillation strength for $|0\rangle \to |\Phi_{\rm ex}\rangle$

$$\frac{|V_{ba}|^2}{\hbar^2} = \left(\frac{eA_0}{m\hbar}\right)^2 |\langle\Phi_{\rm ex}|\vec{e}\cdot\hat{p}\,|0\rangle|^2 \equiv \left(\frac{eA_0}{m\hbar}\right)^2 P_{\rm p}$$

Application to an electron-hole localized system (with main, angular momentum quantum number)

(wavefunction)=(lattice periodic)×(envelope) $\Phi_{\rm e}(\boldsymbol{r}_{\rm e}) = u_{\rm c} f_{\rm e}(\boldsymbol{r}_{\rm e}), \quad \Phi_{\rm h}(\boldsymbol{r}_{\rm h}) = u_{\rm v} f_{\rm h}(\boldsymbol{r}_{\rm h})$

Envelope functions varies slowly
→ the momentum can be ignored

$$P_{\rm p} = |\langle\Phi_{\rm e}|\vec{e}\cdot\hat{p}\,|\Phi_{\rm h}\rangle|^2 = |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 |\langle f_{\rm e}|f_{\rm h}\rangle|^2$$
$$= |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 \delta_{n_{\rm e},n_{\rm h}}\delta_{L_{\rm e},L_{\rm h}}$$

Selection rule

$n_{\rm e} = n_{\rm h},\ L_{\rm e} = L_{\rm h}$

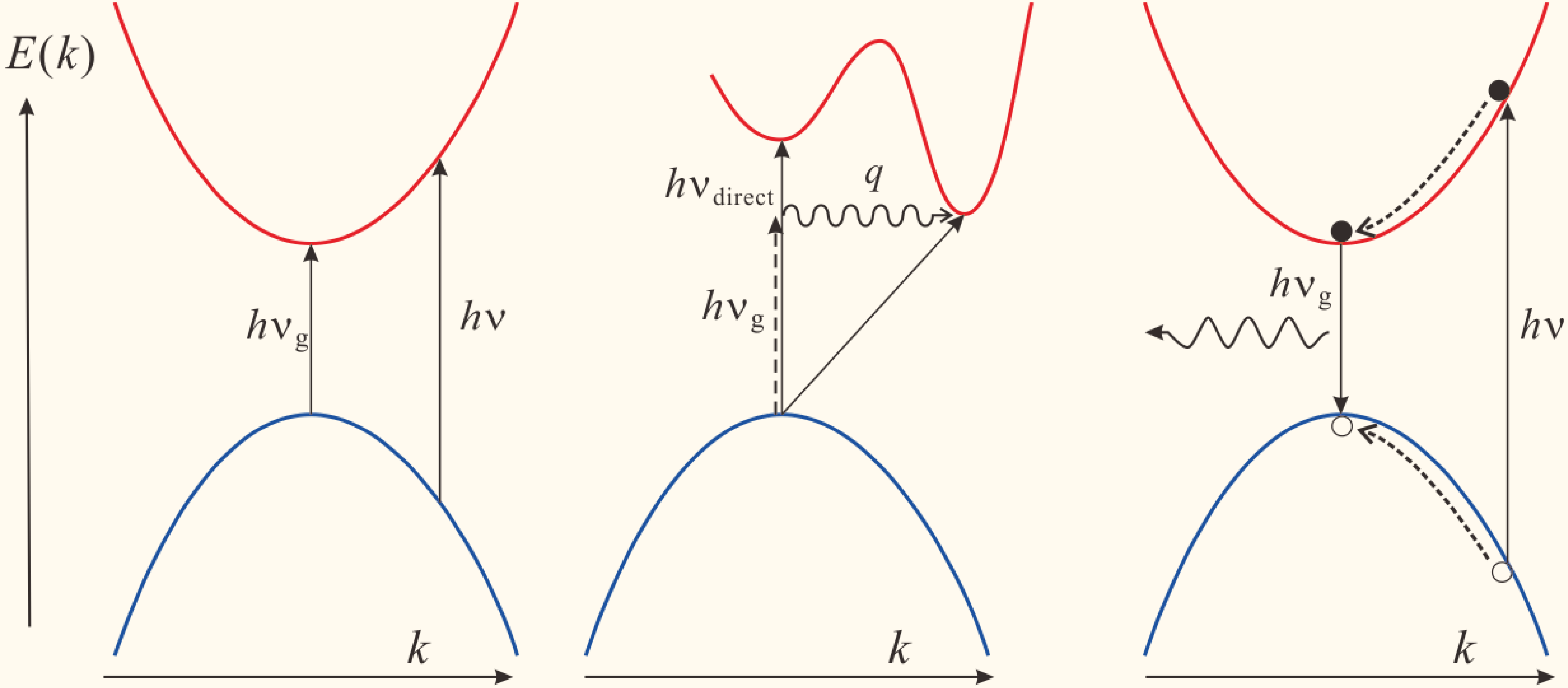
Oscillation strength
(absorption, stimulated emission)

$$\left(\frac{eA_0}{m\hbar}\right)^2 |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 \delta_{n_{\rm e},n_{\rm h}}\delta_{L_{\rm e},L_{\rm h}} \frac{\sin^2[(\omega_{\rm g}-\omega)t/2]}{(\omega_{\rm g}-\omega)^2}$$

For spontaneous emission
(photon number part → 1/2)

$$\frac{e^2}{2m^2\epsilon_0\hbar\omega} |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 \delta_{n_{\rm e},n_{\rm h}}\delta_{L_{\rm e},L_{\rm h}} \frac{\sin^2[(\omega_{\rm g}-\omega)t/2]}{(\omega_{\rm g}-\omega)^2}$$

Application to extended states



(a) direct absorption (b) indirect absorption (c) photoluminescence

Optical absorption with transition from valence to conduction

Plane wave vector potential $\boldsymbol{A} = A_0 \boldsymbol{e} \cos(\boldsymbol{k}_p \cdot \boldsymbol{r} - \omega t)$ $\quad \boldsymbol{k}_{\rm p} = (0, 0, k_{\rm p}), \ \boldsymbol{e} = (1, 0, 0)$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t}, \quad \boldsymbol{H} = \frac{\mathrm{rot}\boldsymbol{A}}{\mu}$$

Poyinting vector $\boldsymbol{I} = \langle \boldsymbol{E} \times \boldsymbol{H} \rangle = \dfrac{\epsilon_0 c \bar{n} \omega^2 A_0^2}{2} \boldsymbol{e}_z$ $\quad \bar{n} = c/c' = \sqrt{\epsilon_1 \mu_1}$

$I(z) = I_0 \exp(-\alpha z)$ Definition of absorption coefficient α

W: number of photons absorbed per unit time $\alpha = \dfrac{\hbar \omega W}{I} = \dfrac{2\hbar\omega W}{\epsilon_0 c \bar{n} \omega^2 A_0^2}$

perturbation $\mathscr{H}' = \dfrac{e A_0}{m_0} \boldsymbol{e} \cdot \boldsymbol{p}$

Conduction electron $|c\boldsymbol{k}\rangle$, valence hole $|v\boldsymbol{k}'\rangle$
Transition probability is

$$W_{\rm vc} = \frac{2\pi e A_0^2}{\hbar m_0} |\langle c\boldsymbol{k}|\boldsymbol{e}\cdot\boldsymbol{p}|v\boldsymbol{k}'\rangle|^2 \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

$$= \frac{\pi e^2 A_0^2}{2\hbar m_0^2} |M|^2 \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

Optical absorption with transition from valence to conduction (2)

Bloch electrons

$$|c\boldsymbol{k}\rangle = u_{c\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}}, \quad |v\boldsymbol{k}\rangle = u_{v\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}}$$

$$\begin{aligned} M &= \int_V \frac{d^3 r}{V} e^{i(\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k})\cdot\boldsymbol{r}} u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot(\boldsymbol{p} + \hbar\boldsymbol{k}') u_{v\boldsymbol{k}'}(\boldsymbol{r}) \\ &= \frac{\sum_l e^{i(\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k})\cdot\boldsymbol{R}_l}}{V} \int_\Omega d^3 r u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot(\boldsymbol{p} + \hbar\boldsymbol{k}') u_{v\boldsymbol{k}'}(\boldsymbol{r}) \\ &= \frac{N}{V} \delta_{\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k}, \boldsymbol{K}} \int_\Omega d^3 r u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot(\boldsymbol{p} + \hbar\boldsymbol{k}') u_{v\boldsymbol{k}'}(\boldsymbol{r}) \end{aligned}$$

$$M = \int_\Omega \frac{d^3 r}{\Omega} u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot\boldsymbol{p} u_{v\boldsymbol{k}}(\boldsymbol{r})$$

Absorption coefficient for direct absorption

$$\alpha_{\rm da} = \frac{\pi e^2}{\bar{n}\epsilon_0 \omega c m_0^2} |M|^2 \underline{\sum_{\boldsymbol{k}} \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}) - \hbar\omega)}$$

joint density of states $\equiv J_{cv}(\hbar\omega)$

$$E_{cv}(\boldsymbol{k}) \equiv E_c(\boldsymbol{k}) - E_v(\boldsymbol{k})$$

Γ point $\quad E_{cv}(\vec{0}) = E_{\rm g}(\Gamma)$

$$J_{cv}(\hbar\omega) = \sum_{\boldsymbol{k}} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega) = 2\int \frac{d^3 k}{(2\pi)^3} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega)$$

Optical absorption with transition from valence to conduction (3)

$$d^3k = dS dk_\perp = dS \frac{dk_\perp}{dE_{cv}} dE_{cv} = dS|\boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv}|^{-1} dE_{cv}$$

$$\therefore\ J_{cv}(\hbar\omega) = \frac{2}{(2\pi)^3} \int \frac{dS}{|\boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv}(\boldsymbol{k})|_{E_{cv}=\hbar\omega}}$$

Minimum at $\boldsymbol{k}_0$

$$E_{cv}(\boldsymbol{k}_0) = E_\mathrm{g}, \quad \boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv} = \boldsymbol{0}$$

$$E_{cv}(\boldsymbol{k}) = E_\mathrm{g} + \sum_i \frac{\hbar^2}{2\xi_i}(k_i - k_{i0})^2, \quad \xi_i > 0 (i = 1, 2, 3) \text{ for simplicity.}$$

Change of variables

$$(\hbar/(2\xi_i)^{1/2})(k_i - k_{i0}) = s_i$$

$$E_{cv} = E_\mathrm{g} + \sum_i s_i^2 \equiv E_\mathrm{g} + s^2, \quad d^3k = \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} ds_1 ds_2 ds_3$$

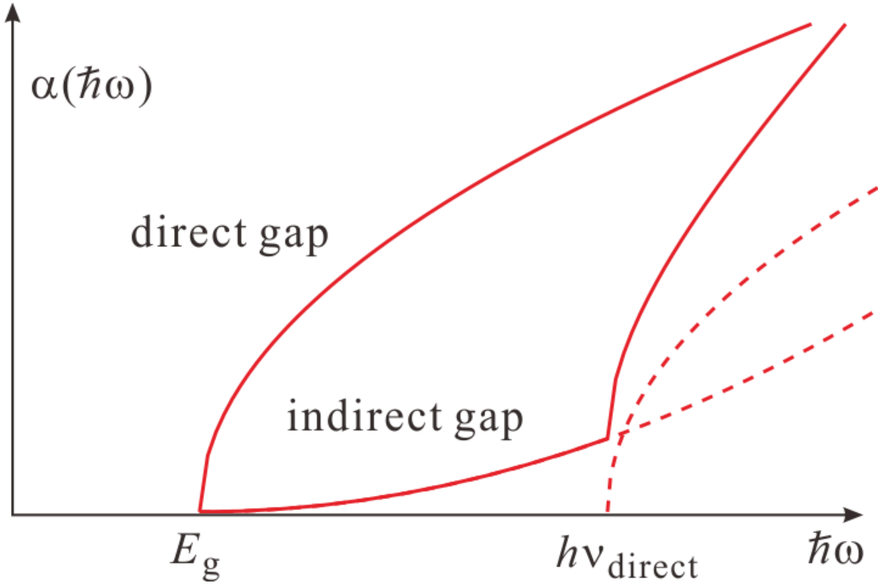
$$|\boldsymbol{\nabla}_{\boldsymbol{s}} E_{cv}| = 2s$$

$$J_{cv} = \frac{2}{(2\pi)^3} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \int \frac{dS}{2s} = \frac{1}{2\pi^2} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \sqrt{\hbar\omega - E_\mathrm{g}}$$

$$= \frac{\sqrt{2}}{\pi^2} \frac{m_r^{3/2}}{\hbar^3} \sqrt{\hbar\omega - E_\mathrm{g}}$$

$$\frac{1}{m_r} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Optical absorption with transition from valence to conduction (4)

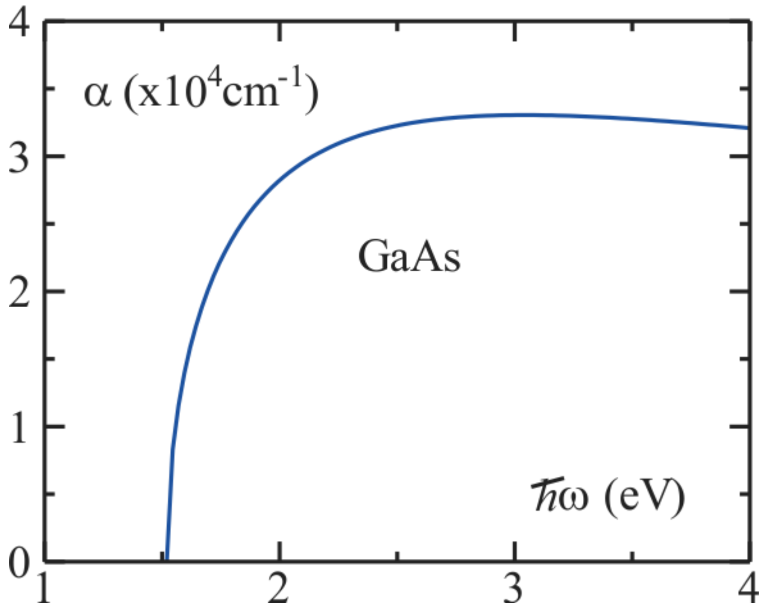


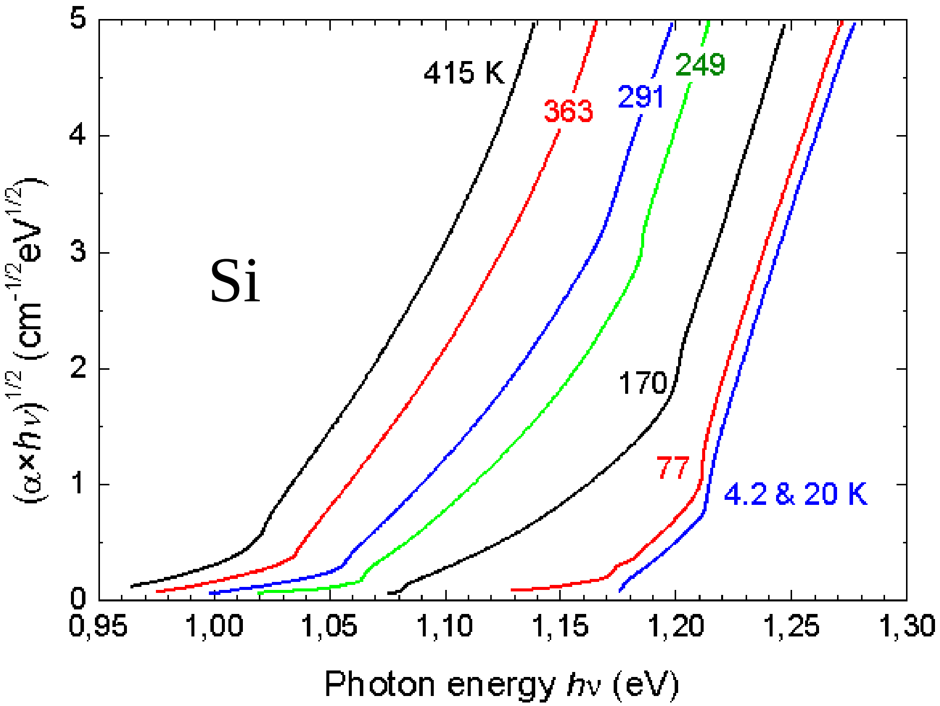
Absorption coefficient $\alpha(\hbar\omega) = \frac{e^2(2m_r)^{3/2}|M|^2}{2\pi\epsilon_0 m_0^2 \bar{n}\omega c\hbar^3}\sqrt{\hbar\omega - E_g}$

Oscillator strength $f_{vc} = \frac{2|M|^2}{m_0\hbar\omega}$

Indirect gap semiconductors $\alpha_{id}(\hbar\omega) \propto (\hbar\omega - E_g)^2$

Example GaAs





Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.5.12 Lecture 05

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Review of lecture in the last week

Doping and carrier distribution

Temperature dependence of carrier concentration

Exciton

Chapter 4 Optical properties (bulk)

Quantization of electromagnetic field

Number state, coherent state

Optical response of two-level system

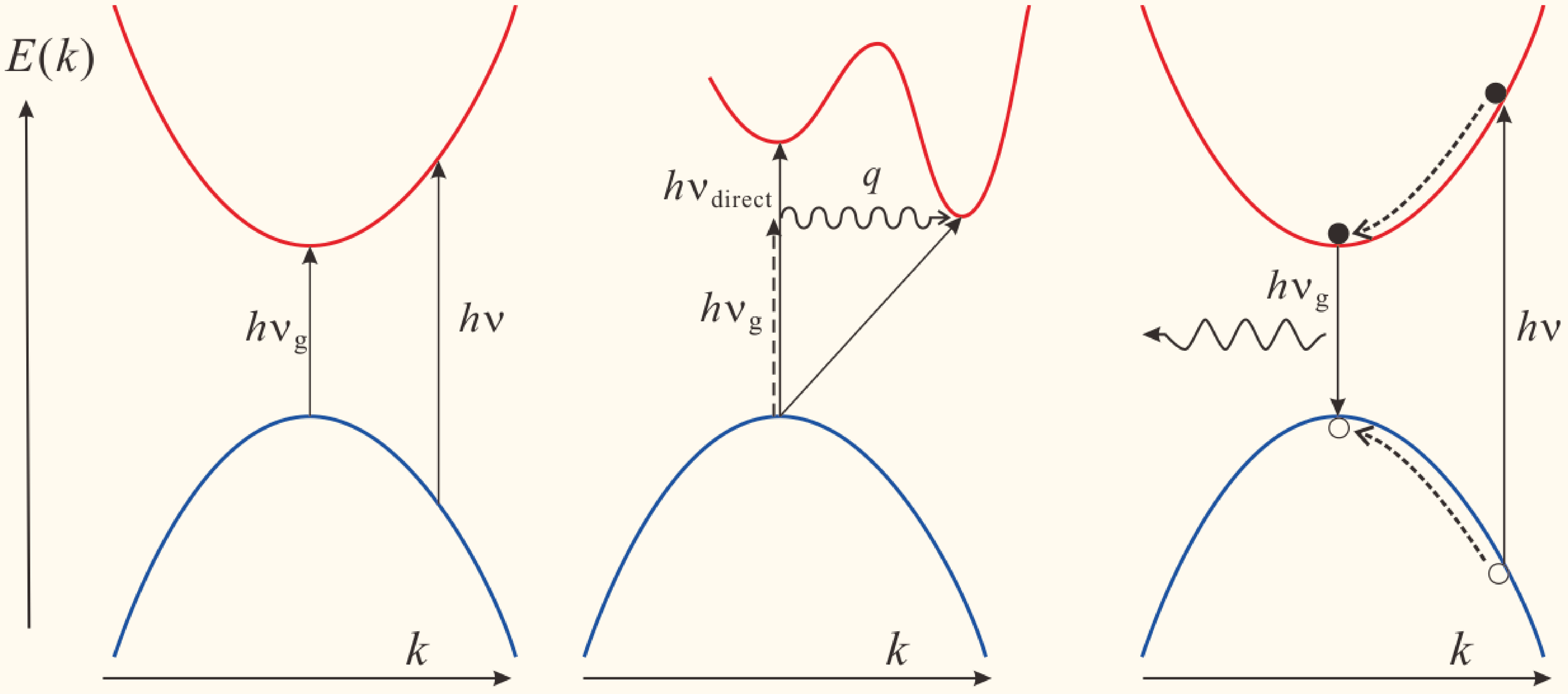
Optical absorption with inter-band transition

Contents today

- Optical absorption with inter-band transition
- Photon emission from inter-band transition
- Optical absorption with exciton formation
- Photon emission from exciton recombination
- Concept of exciton-polariton

Light absorption and luminescence in semiconductors

Application to extended states



(a) direct absorption (b) indirect absorption (c) photoluminescence

Photon momentum $\hbar k_p$ can be ignored in most cases.

Optical absorption with transition from valence to conduction

Plane wave vector potential $\boldsymbol{A} = A_0 \boldsymbol{e} \cos(\boldsymbol{k}_p \cdot \boldsymbol{r} - \omega t)$ $\quad \boldsymbol{k}_\mathrm{p} = (0, 0, k_\mathrm{p}), \ \boldsymbol{e} = (1, 0, 0)$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t}, \quad \boldsymbol{H} = \frac{\mathrm{rot}\boldsymbol{A}}{\mu}$$

Poyinting vector $\boldsymbol{I} = \langle \boldsymbol{E} \times \boldsymbol{H} \rangle = \frac{\epsilon_0 c \bar{n} \omega^2 A_0^2}{2} \boldsymbol{e}_z$ $\quad \bar{n} = c/c' = \sqrt{\epsilon_1 \mu_1}$

$I(z) = I_0 \exp(-\alpha z)$ Definition of absorption coefficient α

W: number of photons absorbed per unit time

$$\alpha = \frac{\hbar \omega W}{I} = \frac{2\hbar\omega W}{\epsilon_0 c \bar{n} \omega^2 A_0^2}$$

perturbation

$$\mathscr{H}' = \frac{e A_0}{m_0} \boldsymbol{e} \cdot \boldsymbol{p}$$

Conduction electron $|c\boldsymbol{k}\rangle$, valence hole $|v\boldsymbol{k}'\rangle$
Transition probability is

$$W_\mathrm{vc} = \frac{2\pi e A_0^2}{\hbar m_0} |\langle c\boldsymbol{k}|\boldsymbol{e}\cdot\boldsymbol{p}|v\boldsymbol{k}'\rangle|^2 \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

$$= \frac{\pi e^2 A_0^2}{2\hbar m_0^2} |M|^2 \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

Optical absorption with transition from valence to conduction (2)

Bloch electrons

$$|c\boldsymbol{k}\rangle = u_{c\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}}, \quad |v\boldsymbol{k}\rangle = u_{v\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}}$$

$$\begin{aligned} M &= \int_V \frac{d^3 r}{V} e^{i(\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k})\cdot\boldsymbol{r}} u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot(\boldsymbol{p} + \hbar\boldsymbol{k}') u_{v\boldsymbol{k}'}(\boldsymbol{r}) \\ &= \frac{\sum_l e^{i(\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k})\cdot\boldsymbol{R}_l}}{V} \int_\Omega d^3 r u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot(\boldsymbol{p} + \hbar\boldsymbol{k}') u_{v\boldsymbol{k}'}(\boldsymbol{r}) \\ &= \frac{N}{V} \delta_{\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k}, \boldsymbol{K}} \int_\Omega d^3 r u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot(\boldsymbol{p} + \hbar\boldsymbol{k}') u_{v\boldsymbol{k}'}(\boldsymbol{r}) \end{aligned}$$

$$M = \int_\Omega \frac{d^3 r}{\Omega} u^*_{c\boldsymbol{k}}(\boldsymbol{r}) \boldsymbol{e}\cdot\boldsymbol{p} u_{v\boldsymbol{k}}(\boldsymbol{r})$$

Absorption coefficient for direct absorption

$$\alpha_{\mathrm{da}} = \frac{\pi e^2}{\bar{n}\epsilon_0 \omega c m_0^2} |M|^2 \underbrace{\sum_{\boldsymbol{k}} \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}) - \hbar\omega)}$$

joint density of states $\equiv J_{cv}(\hbar\omega)$

$$E_{cv}(\boldsymbol{k}) \equiv E_c(\boldsymbol{k}) - E_v(\boldsymbol{k})$$

Γ point $\quad E_{cv}(\vec{0}) = E_{\mathrm{g}}(\Gamma)$

$$J_{cv}(\hbar\omega) = \sum_{\boldsymbol{k}} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega) = 2\int \frac{d^3 k}{(2\pi)^3} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega)$$

Optical absorption with transition from valence to conduction (3)

$$d^3k = dS dk_\perp = dS \frac{dk_\perp}{dE_{cv}} dE_{cv} = dS |\boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv}|^{-1} dE_{cv}$$

$$\therefore J_{cv}(\hbar\omega) = \frac{2}{(2\pi)^3} \int \frac{dS}{|\boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv}(\boldsymbol{k})|_{E_{cv}=\hbar\omega}}$$

Minimum at $\boldsymbol{k}_0$

$$E_{cv}(\boldsymbol{k}_0) = E_{\mathrm{g}}, \quad \boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv} = \mathbf{0}$$

$$E_{cv}(\boldsymbol{k}) = E_{\mathrm{g}} + \sum_i \frac{\hbar^2}{2\xi_i}(k_i - k_{i0})^2, \quad \xi_i > 0 (i = 1, 2, 3) \text{ for simplicity.}$$

Change of variables

$$(\hbar/(2\xi_i)^{1/2})(k_i - k_{i0}) = s_i$$

$$E_{cv} = E_{\mathrm{g}} + \sum_i s_i^2 \equiv E_{\mathrm{g}} + s^2, \quad d^3k = \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} ds_1 ds_2 ds_3$$

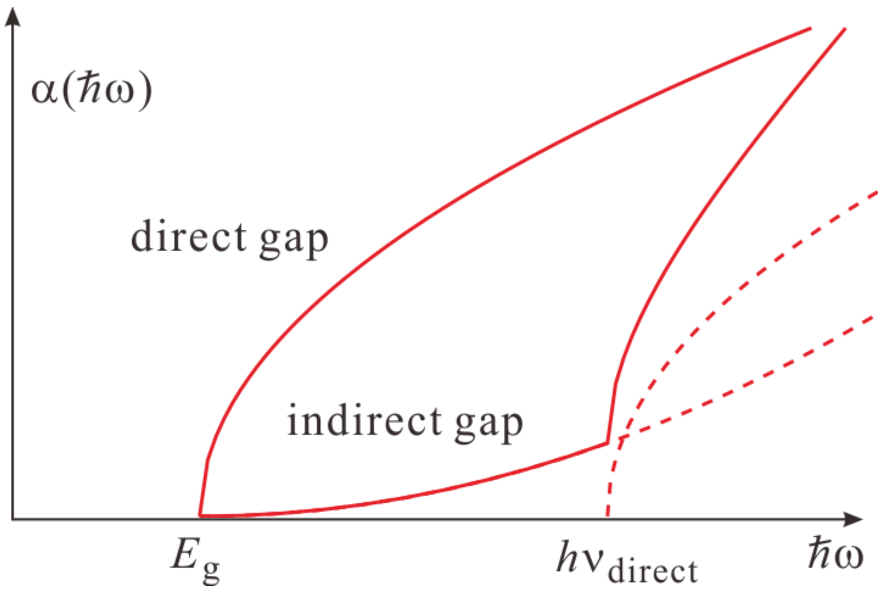
$$|\boldsymbol{\nabla}_{\boldsymbol{s}} E_{cv}| = 2s$$

$$J_{cv} = \frac{2}{(2\pi)^3} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \int \frac{dS}{2s} = \frac{1}{2\pi^2} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \sqrt{\hbar\omega - E_{\mathrm{g}}}$$

$$= \frac{\sqrt{2}}{\pi^2} \frac{m_r^{3/2}}{\hbar^3} \sqrt{\hbar\omega - E_{\mathrm{g}}}$$

$$\frac{1}{m_r} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Optical absorption with transition from valence to conduction (4)

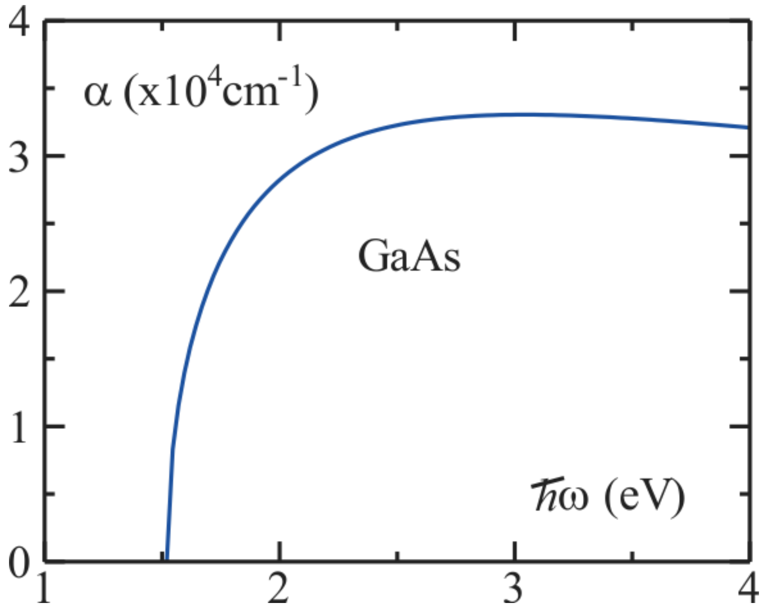


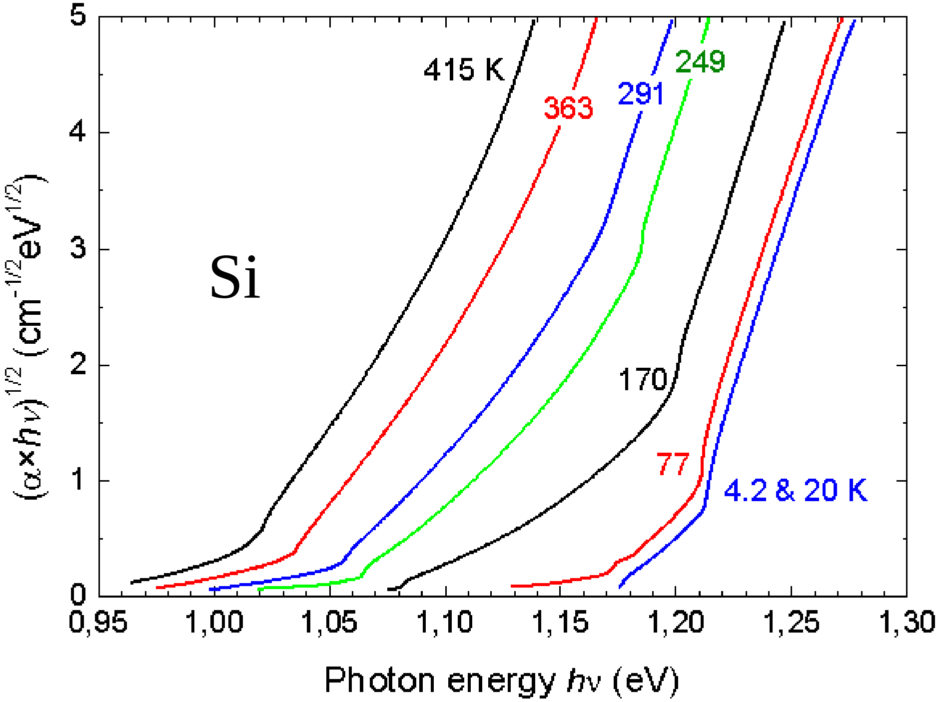
Absorption coefficient $\alpha(\hbar\omega) = \frac{e^2(2m_r)^{3/2}|M|^2}{2\pi\epsilon_0 m_0^2 \bar{n}\omega c\hbar^3}\sqrt{\hbar\omega - E_g}$

Oscillator strength $f_{vc} = \frac{2|M|^2}{m_0\hbar\omega}$

Indirect gap semiconductors $\alpha_{id}(\hbar\omega) \propto (\hbar\omega - E_g)^2$

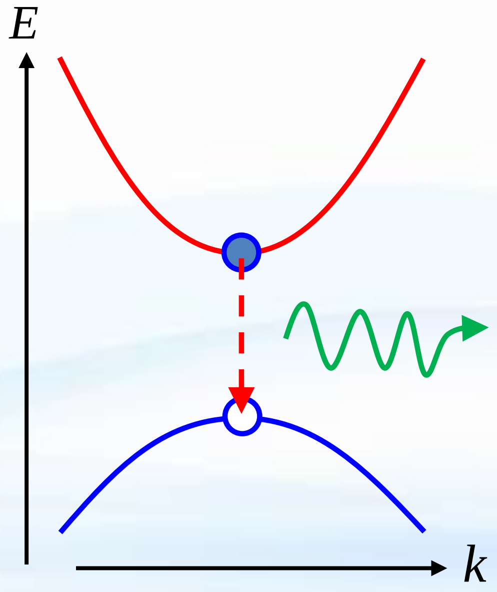
Example GaAs





Luminescence by inter-band transition

Electron-hole recombination:
- Radiative recombination
- Non-radiative recombination



Classification of luminescence with excitations

- Photoluminescence
- Electroluminescence
- Thermoluminescence
- Cathode luminescence
- Sonoluminescence
- Triboluminescence
- Chemiluminescence

Pseudo-Fermi level

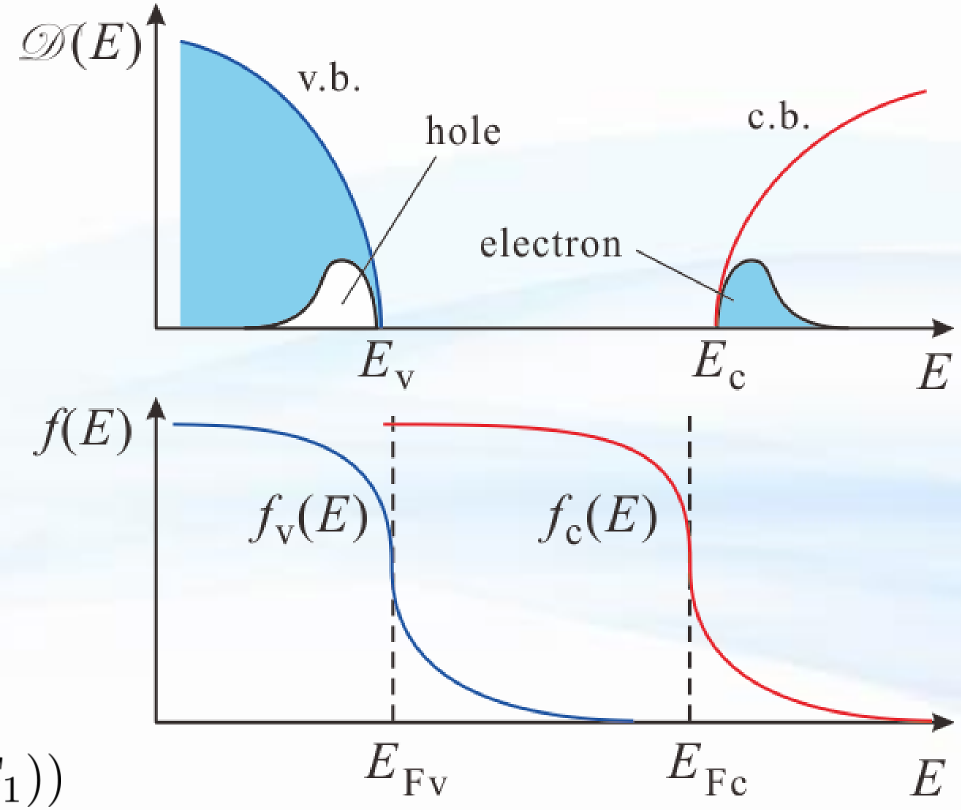
Planck distribution $$P(E) = \frac{8\pi\bar{n}^3E^3}{h^3c^3}\frac{1}{\exp(E/k_BT)-1}$$

Semiconductor under irradiation

Introduction of pseudo-Fermi levels: $E_{Fc}, \quad E_{Fv}$

Electron distribution function in conduction band $$f_c(E) = \left[\exp\left(\frac{E-E_{Fc}}{k_BT}\right)+1\right]^{-1},$$

Electron distribution function in valence band $$f_v(E) = \left[\exp\left(\frac{E-E_{Fv}}{k_BT}\right)+1\right]^{-1}.$$



optical absorption $$R(1\to 2) = B_{12}f_v(1-f_c)P(\hbar\omega)$$

spontaneous emission $$R(sp, 2\to 1) = A_{21}f_c(E_2)(1-f_v(E_1))$$

stimulated emission $$R(st, 2\to 1) = B_{21}f_c(E_2)(1-f_v(E_1))P(\hbar\omega)$$

balance equation $$R(1\to 2) = R(sp, 2\to 1) + R(st, 2\to 1)$$

Einstein relation $$A_{21} = \frac{8\pi\bar{n}^3E_{21}^3}{h^3c^3}B_{21}, \quad B_{12} = B_{21}$$

Relation with phenomenological approach

So far: Optical response of two-level system → Extended states → Inter-band absorption

Other effects : refractive index

? ⇕

Macroscopic phenomenological approach

Starting point:
Maxwell equation

$$\mathrm{div}\boldsymbol{D} = \rho, \quad \mathrm{div}\boldsymbol{B} = 0,$$
$$\mathrm{rot}\boldsymbol{E} = \frac{\partial \boldsymbol{B}}{\partial t}, \quad \mathrm{rot}\boldsymbol{H} = \boldsymbol{j} + \frac{\partial \boldsymbol{D}}{\partial t},$$
$$\boldsymbol{D} = \epsilon_0 \boldsymbol{E} + \boldsymbol{P}, \quad \boldsymbol{B} = \mu_0 \boldsymbol{H} + \boldsymbol{M}$$

Non-magnetic dielectric $\boldsymbol{M} = \vec{0} \qquad \boldsymbol{j} = \vec{0}$

Wave equation $$\Delta \boldsymbol{E} - \epsilon_0 \mu_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \mu_0 \frac{\partial^2 \boldsymbol{P}}{\partial t^2}$$

Effect of polarization $\boldsymbol{P} = \sum_i \boldsymbol{p}_i$

Relation with phenomenological approach (2)

Linear response approximation $\boldsymbol{P} = \epsilon_0 \chi \boldsymbol{E}$ χ : susceptibility

Relative dielectric function ε_r $\boldsymbol{D} = \epsilon_0 \boldsymbol{\epsilon}_{\rm r} \boldsymbol{E}, \quad \boldsymbol{\epsilon}_{\rm r} = 1 + \chi$

Below we consider isotropic crystal: response function tensor → scalar

The effect of polarization is normalized into the term of time-derivative

$$\Delta \boldsymbol{E} - \epsilon_0 \mu_0 \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \epsilon_0 \mu_0 (\epsilon_{\rm r} - 1) \frac{\partial^2 \boldsymbol{E}}{\partial t^2} \quad \rightarrow \quad \Delta \boldsymbol{E} - \frac{\epsilon_{\rm r}}{c^2} \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = 0$$

Polariton equation $c^2 \boldsymbol{k}^2 = \omega^2 \epsilon_{\rm r}(\omega, \boldsymbol{k})$

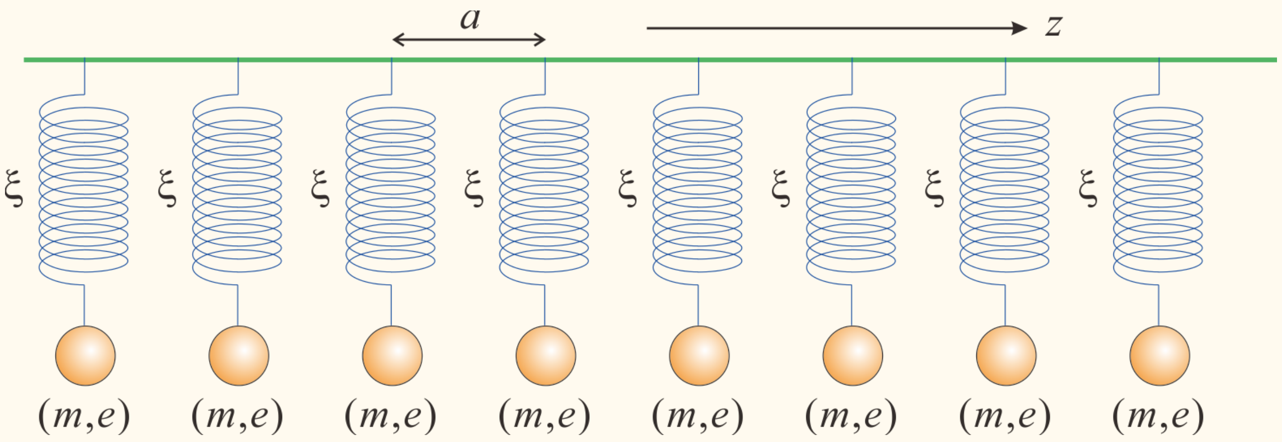
Absorption: imaginary part of response function: complex dielectric function, or

complex refractive index $\tilde{n}(\omega, \boldsymbol{k}) = n(\omega, \boldsymbol{k}) + i\kappa(\omega, \boldsymbol{k})$

absorption coefficient $\alpha = \dfrac{2\omega}{c} \kappa(\omega, \boldsymbol{k})$

Phenomenological approach: Lorentz model

Electromagnetic field in Materials:
set harmonic oscillators (m, e, ξ)



$$m\frac{d^2x}{dt^2} + \Gamma m \frac{dx}{dt} + \xi x = eE_0 \exp(-i\omega t)$$

energy dissipation

oscillator concentration N

eigenfrequency $\omega_{\mathrm{h}} = \sqrt{\frac{\xi}{m}}$

long term stable solution $x(t) = x_{\mathrm{p}} \exp(-i\omega t)$

$$P = N(ex_{\mathrm{p}}(\omega)) = \frac{Ne^2}{m}\frac{1}{\omega_{\mathrm{h}}^2 - \omega^2 - i\omega\Gamma}E_0$$

χ susceptibility

relative dielectric function

$$\epsilon_{\mathrm{r}}(\omega) = 1 + \frac{Ne^2}{\epsilon_0 m}\frac{1}{\omega_{\mathrm{h}}^2 - \omega^2 - i\omega\Gamma}$$

Multimode:
ration of mode j
$\rightarrow f_j$

$$\epsilon_{\mathrm{r}}(\omega) = 1 + \frac{Ne^2}{\epsilon_0 m}\sum_j \frac{f_j}{\omega_{\mathrm{h}}^2 - \omega^2 - i\omega\Gamma_j}$$

f_j: oscillator strength

Optical absorption by excitons

Exciton wavefunction (effective mass approximation)

$$\Phi_{n\boldsymbol{K}}(\boldsymbol{r},\boldsymbol{R}) = \frac{1}{\sqrt{V}}\exp(i\boldsymbol{K}\cdot\boldsymbol{R})\phi_n(\boldsymbol{r})$$

exciton local wavefunction

$\boldsymbol{r}$: electron-hole relative coordinate

$\boldsymbol{R}$: center of mass coordinate

Fourier transform

$$F_{n\boldsymbol{K}}(\boldsymbol{k}_\mathrm{e},\boldsymbol{k}_\mathrm{h}) = \frac{1}{V}\int d^3\boldsymbol{r}_\mathrm{e} d^3\boldsymbol{r}_\mathrm{h} e^{-i\boldsymbol{k}_\mathrm{e}\cdot\boldsymbol{r}_\mathrm{e}} e^{-i\boldsymbol{k}_\mathrm{h}\cdot\boldsymbol{r}_\mathrm{h}} \Phi_{n\boldsymbol{K}}(\boldsymbol{r},\boldsymbol{R})$$

$$= \frac{1}{\sqrt{V}}\int d^3\boldsymbol{r} d^3\boldsymbol{R} e^{-i\boldsymbol{R}\cdot(\boldsymbol{k}_\mathrm{e}+\boldsymbol{k}_\mathrm{h}-\boldsymbol{K})}\phi_n(\boldsymbol{r})e^{-i\boldsymbol{k}^*\cdot\boldsymbol{r}}$$

$$= \frac{1}{\sqrt{V}}\int d^3\boldsymbol{r} e^{-i\boldsymbol{k}^*\cdot\boldsymbol{r}}\phi_n(\boldsymbol{r})\delta_{\boldsymbol{K},\boldsymbol{k}_\mathrm{e}+\boldsymbol{k}_\mathrm{h}}, \quad \boldsymbol{k}^* \equiv \frac{m_\mathrm{h}\boldsymbol{k}_\mathrm{e} - m_\mathrm{e}\boldsymbol{k}_\mathrm{h}}{m_\mathrm{e}+m_\mathrm{h}}.$$

exciton total wavelength $\boldsymbol{K} = \boldsymbol{k}_\mathrm{e} + \boldsymbol{k}_\mathrm{h}$

ground state $\Phi_0 = \phi_{\mathrm{c}\boldsymbol{k}_\mathrm{e}}\phi_{\mathrm{v}\boldsymbol{k}_\mathrm{e}}$ $\xrightarrow{\text{excitation}}$ $\Phi_{n\boldsymbol{K}}(\boldsymbol{r},\boldsymbol{R})$

Transition probability

$$w_\mathrm{if} = \frac{2\pi}{\hbar}\frac{e^2}{m^2}|A_0|^2\frac{1}{V}\sum_\lambda |\langle\Phi_{\lambda\boldsymbol{K}}|\exp(i\boldsymbol{k}_\mathrm{p}\cdot\boldsymbol{r})\boldsymbol{e}\cdot\boldsymbol{p}|\Phi_0\rangle|^2\delta(E_\mathrm{g}+E_\lambda-\hbar\omega)$$

$$= \frac{2\pi}{\hbar}\frac{e^2}{m^2}|A_0|^2\frac{1}{V}\sum_{\boldsymbol{k}_\mathrm{e}\lambda} |F_{\lambda\boldsymbol{K}}(\boldsymbol{k}_\mathrm{e},-\boldsymbol{k}_\mathrm{e})\langle\phi_{\mathrm{c}\boldsymbol{k}_\mathrm{e}}|\boldsymbol{e}\cdot\boldsymbol{p}|\phi_{\mathrm{v}\boldsymbol{k}_\mathrm{e}}\rangle|^2\delta(E_\mathrm{g}+E_\lambda-\hbar\omega).$$

Optical absorption by excitons (2)

Because $\boldsymbol{k}_{\rm e} = -\boldsymbol{k}_{\rm h}$ $\quad F_{n\boldsymbol{K}}(\boldsymbol{k}_{\rm e}, -\boldsymbol{k}_{\rm h}) = \frac{1}{V}\int d^3\boldsymbol{r}_{\rm e} d^3\boldsymbol{r}_{\rm h} \exp[-i\boldsymbol{k}_{\rm e}\cdot(\boldsymbol{r}_{\rm e}-\boldsymbol{r}_{\rm h})]\Phi_{\lambda\boldsymbol{K}}(\boldsymbol{r}_{\rm e},\boldsymbol{r}_{\rm h})$

Because the sum will be taken over $\boldsymbol{k}_{\rm e}$ $\quad \boldsymbol{r}_{\rm e} = \boldsymbol{r}_{\rm h}$

$F_{n\boldsymbol{K}}$ is large only for $\boldsymbol{k}_{\rm e} \approx \vec{0}$ while $\langle \phi_{c\boldsymbol{k}_{\rm e}} | \boldsymbol{e}\cdot\boldsymbol{p} | \phi_{v\boldsymbol{k}_{\rm e}}\rangle$ is almost constant

which is $M = \int_\Omega \frac{d^3r}{\Omega} u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot\boldsymbol{p}u_{v\boldsymbol{k}}(\boldsymbol{r})$

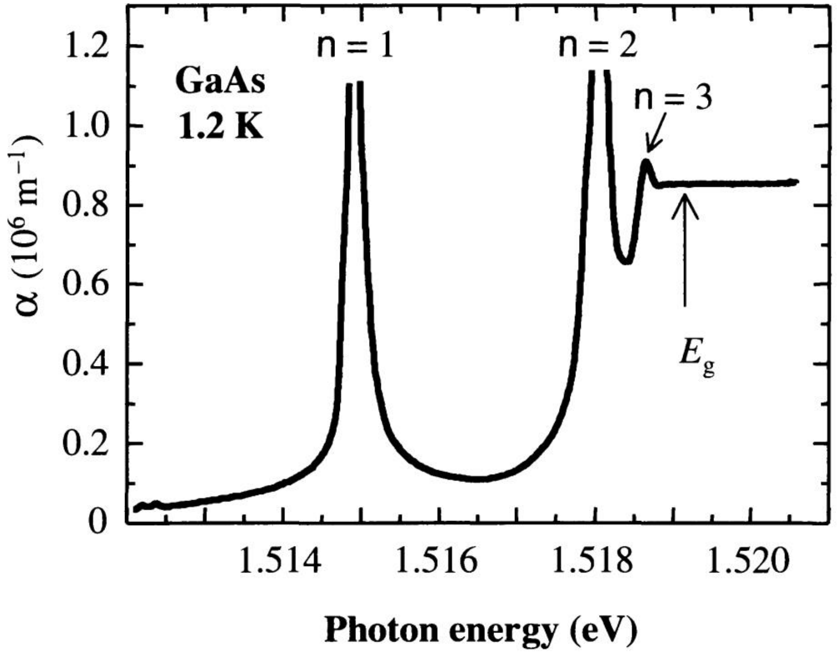
Fermi's golden rule: $w_{\rm if} = \frac{2\pi}{\hbar}\frac{e^2}{m^2}|A_0|^2\sum_\lambda |M|^2|\phi_\lambda(0)|^2\delta(E_{\rm g}+E_\lambda-\hbar\omega)$

For $\phi(0)$ not to be 0, ϕ must be an *s*-state $\quad |\phi_n(0)|^2 = \frac{1}{\pi a_{\rm ex}^3 n^3}, \quad E_n = -\frac{E_{\rm ex}}{n^2}$

Imaginary part of the complex relative dielectric function $\quad \epsilon_{\rm r2}(\omega) = \frac{\pi e^2}{\epsilon_0 m^2\omega^2}|M|^2\frac{1}{\pi a_{\rm ex}^3}\sum_n \frac{1}{n^3}\delta\left(E_{\rm g}-\frac{E_{\rm ex}}{n^2}-\hbar\omega\right)$

(spin degree of freedom: factor of 2)

Optical absorption by excitons (3)



Exciton absorption peaks in GaAs.

Fehrenbach *et al.*, J. Luminescence **30**, 154 (1985).

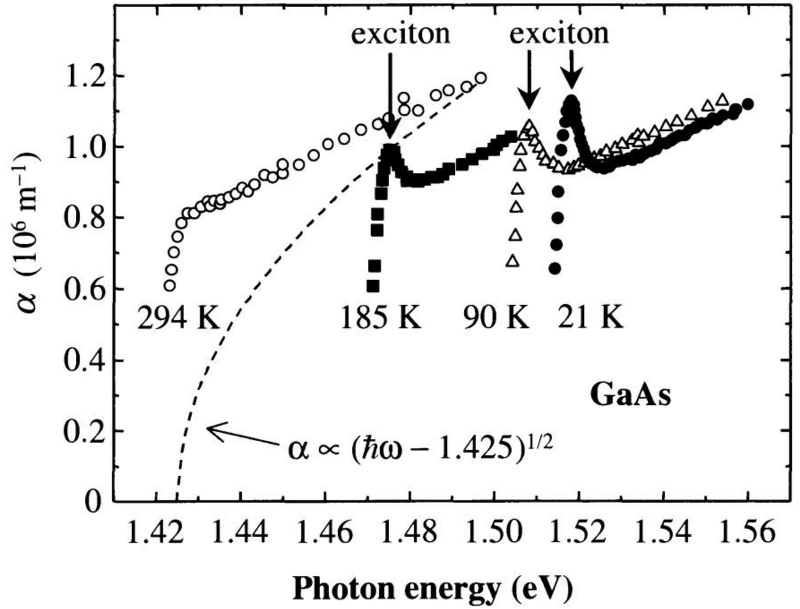
in simplest form $$\epsilon_{r2} = C\delta\left(E_g - \frac{E_{ex}}{n^2} - \hbar\omega\right)$$

identity $$\lim_{\Gamma\to+0}\frac{1}{x_0 - x - i\Gamma} = \mathcal{P}\frac{1}{x_0 - x} + i\pi\delta(x_0 - x)$$

comparison gives $$\epsilon_{r2} = \mathrm{Im}\left\{\frac{C/\pi}{E_g - \frac{E_{ex}}{n^2} - (\hbar\omega + i\delta)}\right\}$$

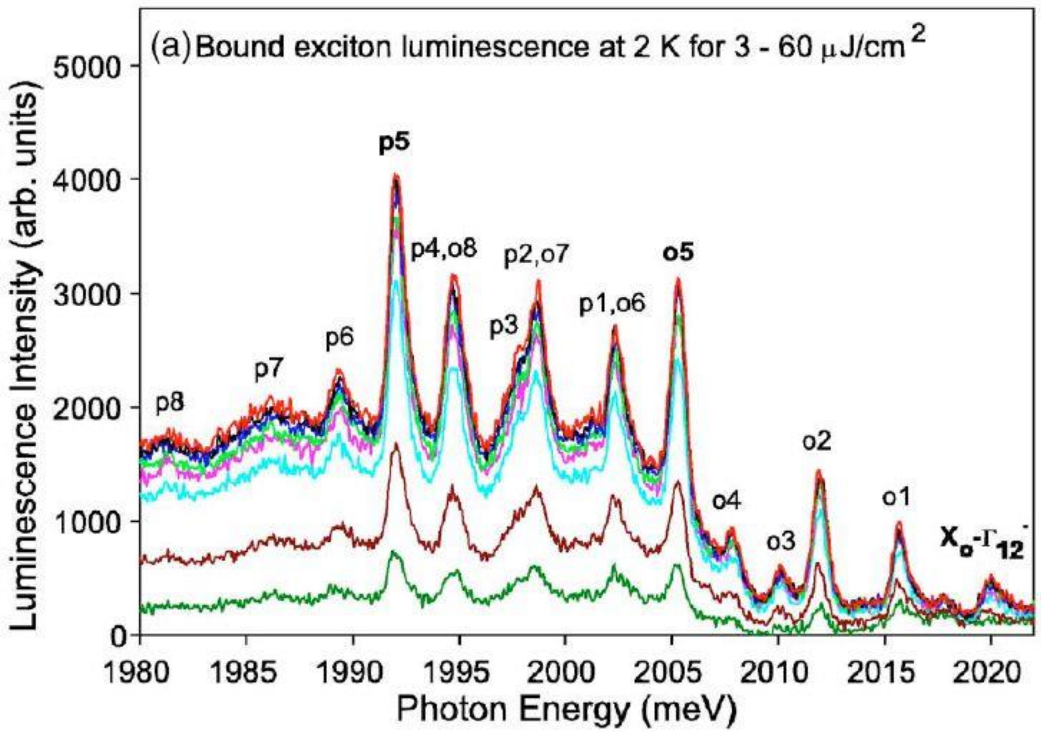
Kramers-Kronig relation $$\chi_1(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\chi_2(\omega')}{\omega' - \omega}d\omega'$$

$$\epsilon_r = \frac{C/\pi}{E_g - \frac{E_{ex}}{n^2} - (\hbar\omega + i\Gamma)}$$



Sturge, Phys. Rev. **127**, 768 (1962)

Photoemission by exitons



Jang *et al.*, Phys. Rev. B **74**, 235204 (2006)

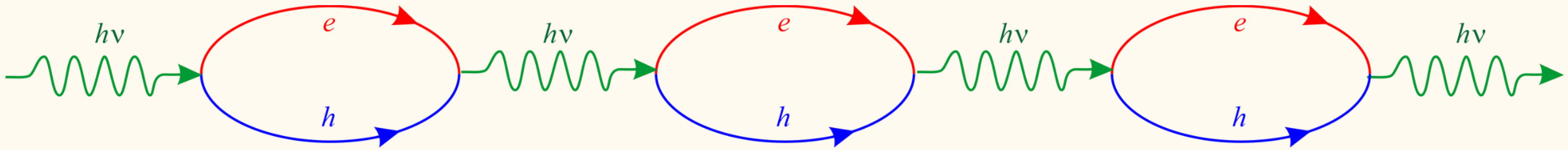
Photoemission: reversal process

Bound exciton emission peaks in Cu_2O

Exciton-polariton

Concept of exciton-polariton

Chain of photon-exciton



1 cycle $\sim$ few fs

coherent propagation in solids

ϵ_{s}: contributions other than from excitons
$$\epsilon_{\mathrm{r}}(\omega) = \epsilon_{\mathrm{s}}\left(1 + \frac{\Delta_{\mathrm{ex}}}{\omega_0 - \omega - i\gamma}\right)$$

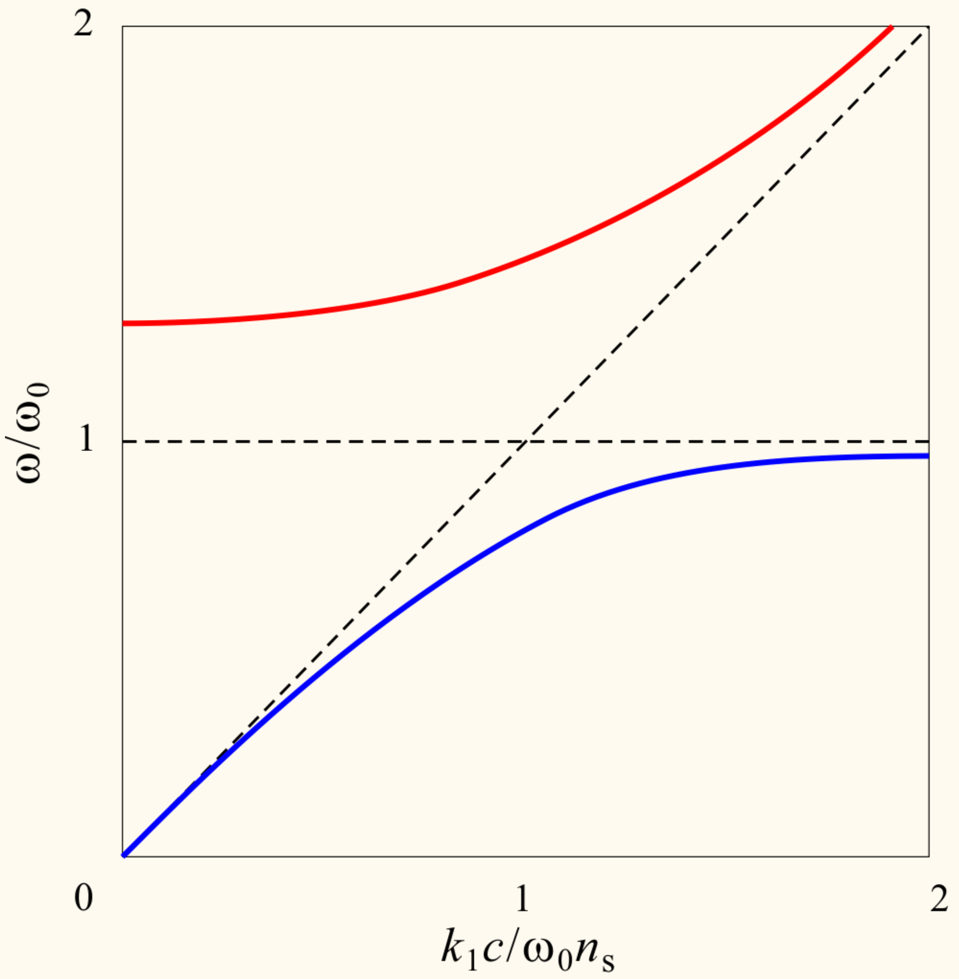
transverse wave:
$$\left.\begin{aligned} \boldsymbol{k}\cdot\boldsymbol{E} &= 0 \\ \omega_{\mathrm{t}} &= \omega_0 \end{aligned}\right\}$$

polariton equation
$$c^2\boldsymbol{k}^2 = \omega_0^2\epsilon_{\mathrm{r}}(\omega_0, \boldsymbol{k})$$

Longitudinal wave:
$$\omega_{\mathrm{l}} = \omega_0 + \Delta_{\mathrm{ex}} = \omega_{\mathrm{t}} + \Delta_{\mathrm{ex}}$$

Δ_{ex} : longitudinal-transverse splitting

Exciton-polariton (2)



$$k = k_1 + ik_2$$

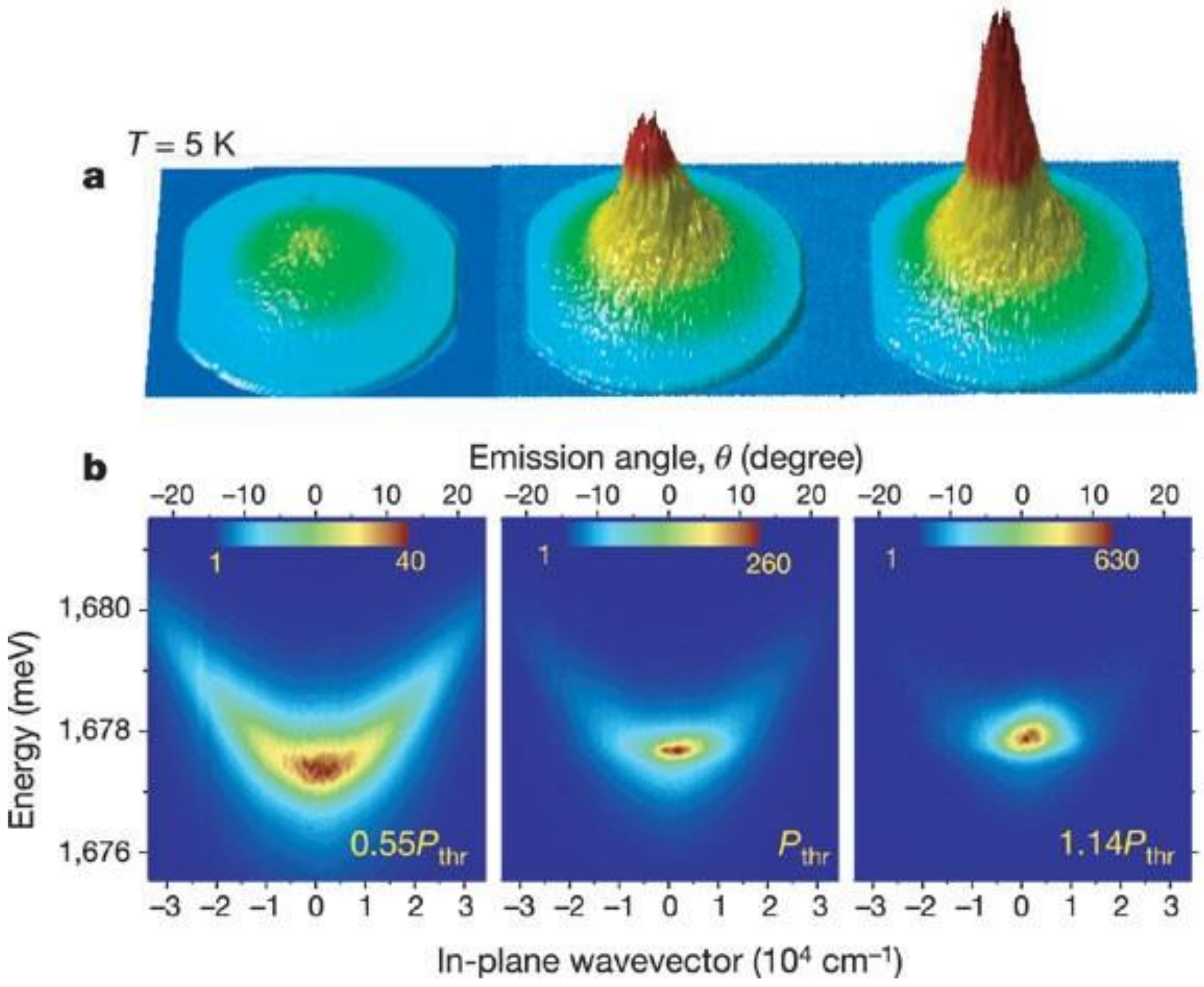
$$\begin{cases} \frac{\omega^2\epsilon_s}{c^2}\left(1 + \frac{\Delta_{ex}}{\omega_0 - \omega}\right) = k_1^2 - k_2^2, \\ \pi\delta(\omega - \omega_0)\frac{\omega_0^2\epsilon_s}{c^2} = 2k_1k_2 \end{cases}$$

Resonance

Dispersion relation

$$\omega\sqrt{\frac{\omega - \omega_{-}\Delta_{ex}}{\omega - \omega_0}} = \frac{ek_1}{\sqrt{\epsilon_s}}$$

Bose-Einstein condensation of exciton-polaritons



J. Kasprzak *et al*., Nature **443**, 409 (2006).

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.5.19 Lecture 06

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Review of lecture in the last week

- Optical absorption with inter-band transition
- Photon emission from inter-band transition
- Optical absorption with exciton formation
- Photon emission from exciton recombination
- Concept of exciton-polariton

Contents today

Concept of exciton-polariton (continued)

Chapter 5 Semi-classical treatment of transport

Transport coefficient

Classical transport: Boltzmann equation

Currents: particle flows

Drude formula, Diffusion current, Hall effect

Various scatterings

Heat transport, Thermoelectric effect

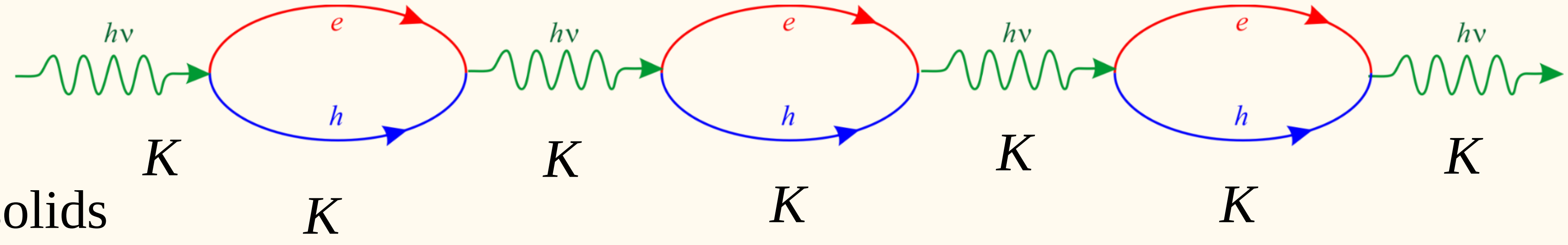
Exciton-polariton

Concept of exciton-polariton

Chain of photon-exciton

1 cycle $\sim$ few fs

coherent propagation in solids

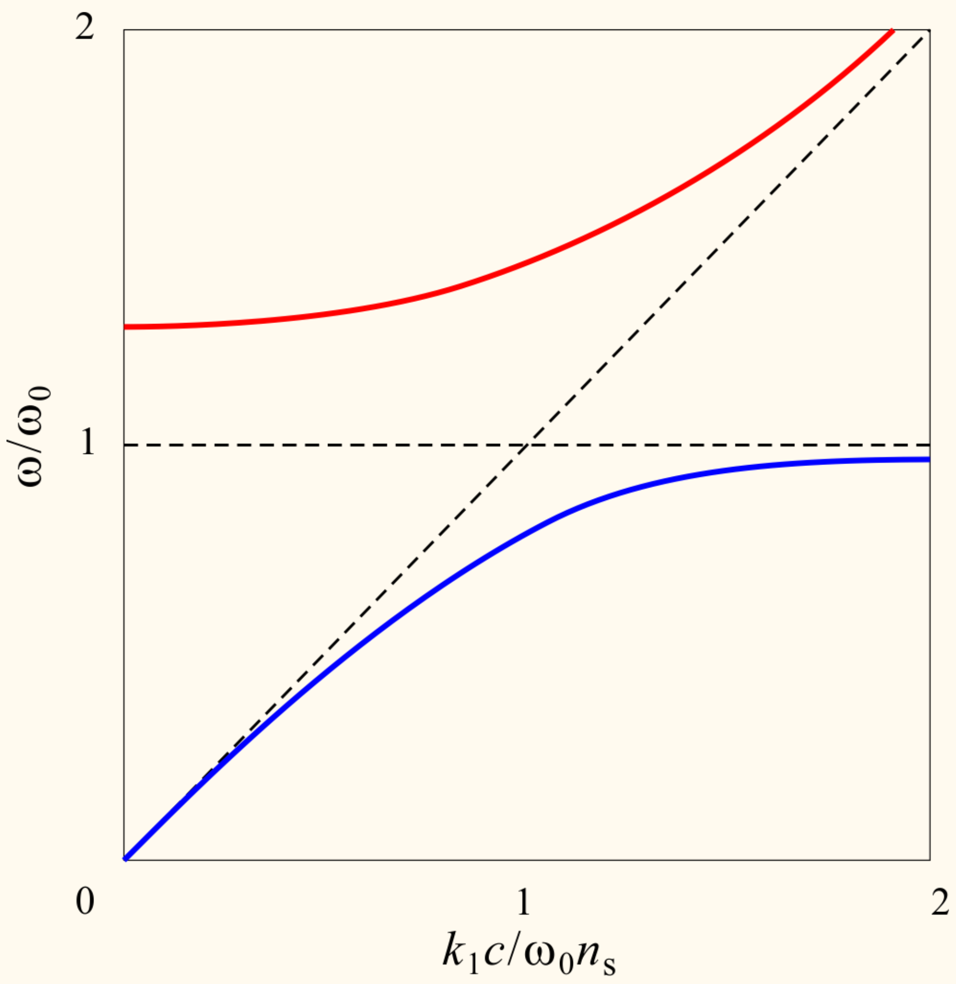


$\epsilon_{\rm s}$: contributions other than from excitons $\quad \epsilon_{\rm r}(\omega) = \epsilon_{\rm s}\left(1 + \dfrac{\Delta_{\rm ex}}{\omega_0 - \omega - i\gamma}\right)$

transverse wave: $\left.\begin{array}{l} \boldsymbol{k}\cdot\boldsymbol{E} = 0 \\ \omega_{\rm t} = \omega_0 \end{array}\right\}$ polariton equation $\quad c^2\boldsymbol{k}^2 = \omega_0^2\epsilon_{\rm r}(\omega_0, \boldsymbol{k})$

Longitudinal wave: $\quad \omega_{\rm l} = \omega_0 + \Delta_{\rm ex} = \omega_{\rm t} + \Delta_{\rm ex}$

$\Delta_{\rm ex}$: longitudinal-transverse splitting



For transverse wave

$$k = k_1 + ik_2$$

Real-imaginary comparison

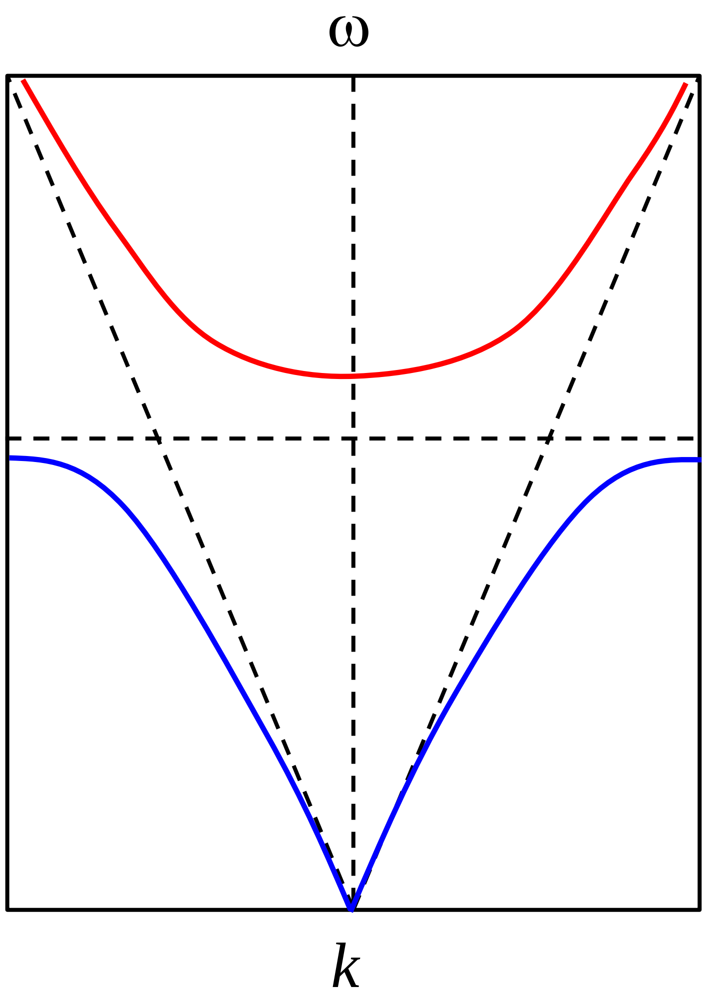
$$\begin{cases} \dfrac{\omega^2 \epsilon_{\mathrm{s}}}{c^2}\left(1 + \dfrac{\Delta_{\mathrm{ex}}}{\omega_0 - \omega}\right) = k_1^2 - k_2^2, \\ \pi\delta(\omega - \omega_0)\dfrac{\omega_0^2 \epsilon_{\mathrm{s}}}{c^2} = 2k_1 k_2 \end{cases}$$

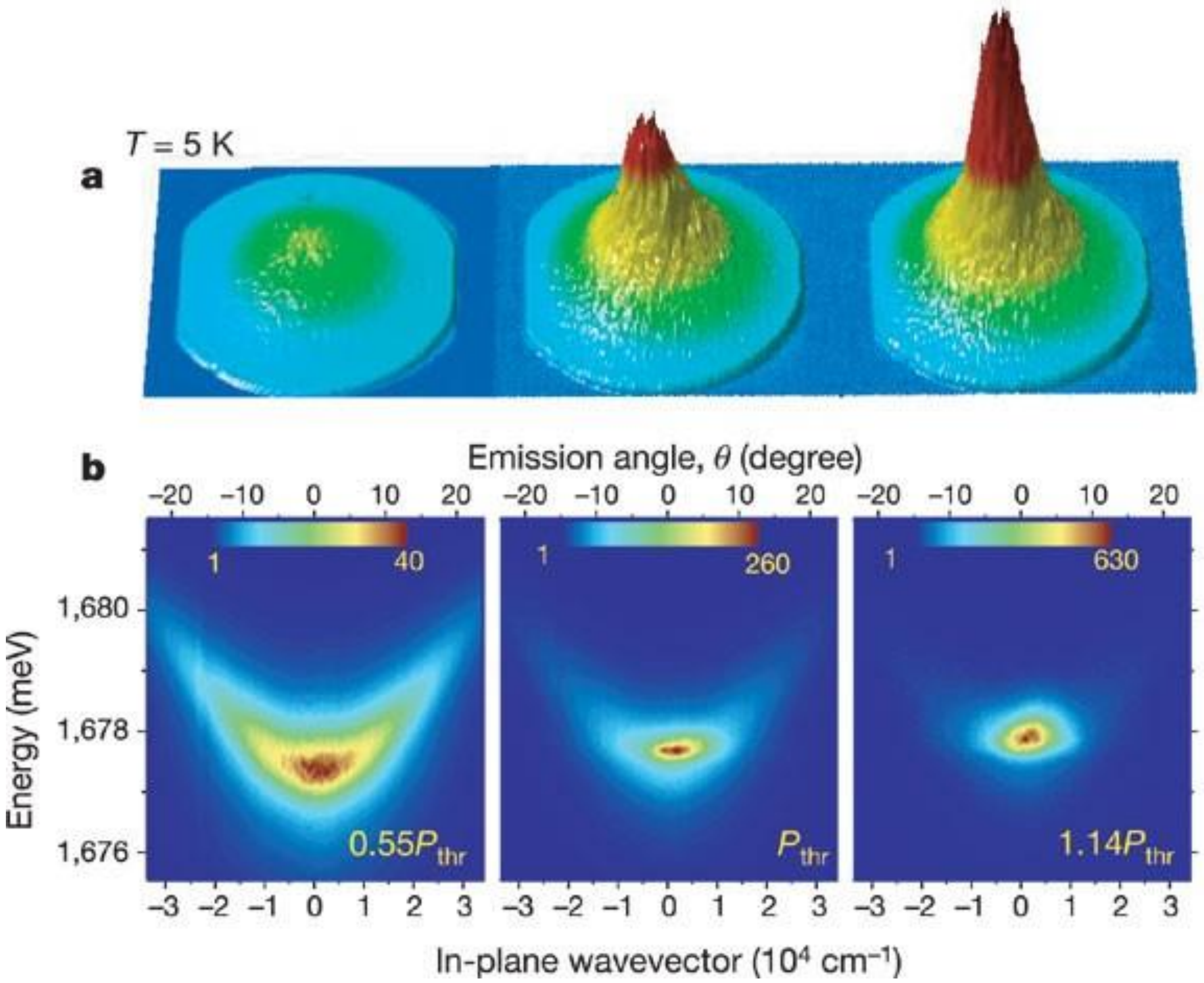
Resonance

Dispersion relation

$$\omega\sqrt{\frac{\omega - \omega_{-}\Delta_{\mathrm{ex}}}{\omega - \omega_0}} = \frac{ek_1}{\sqrt{\epsilon_{\mathrm{s}}}}$$

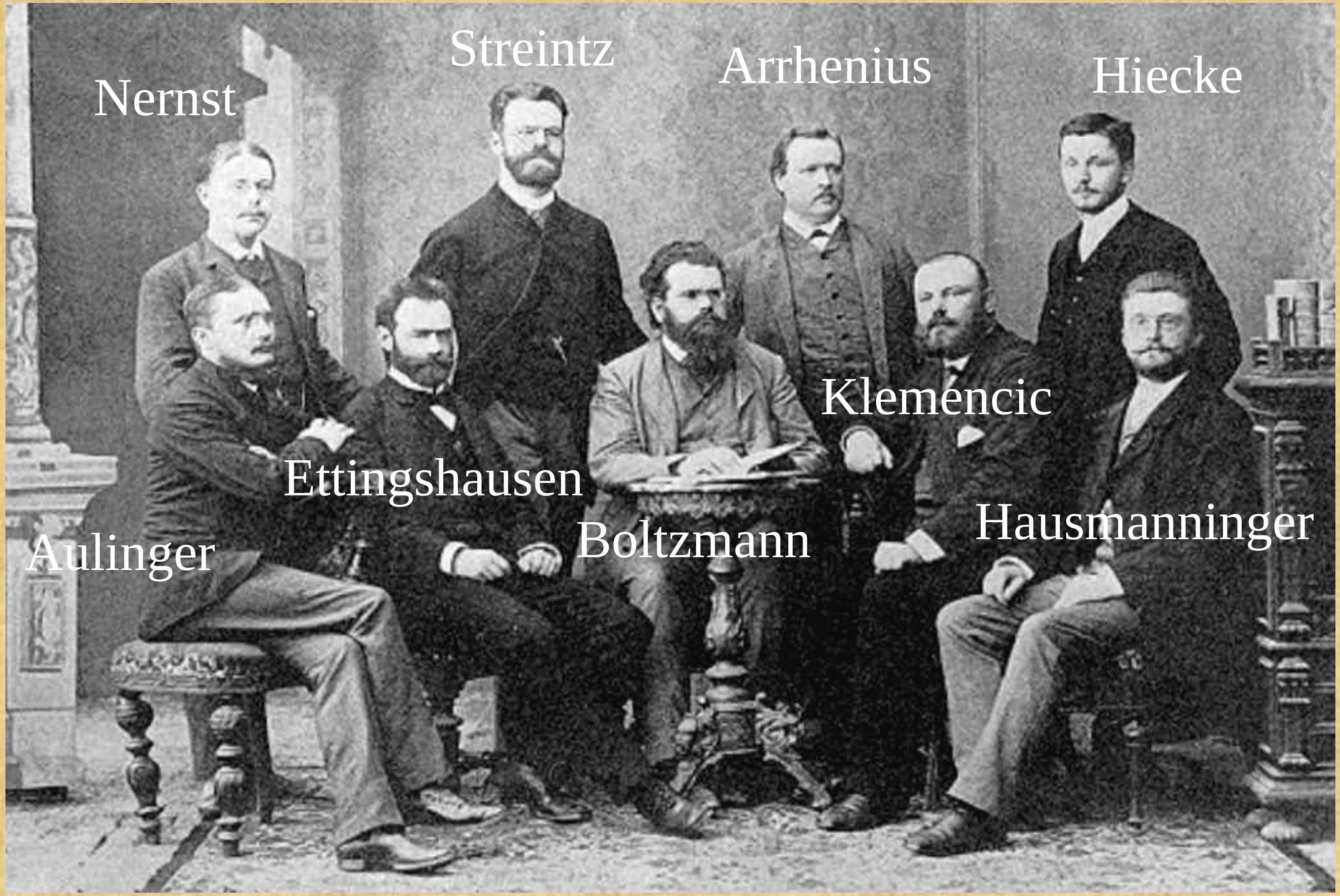
Bose-Einstein condensation of exciton-polaritons





J. Kasprzak *et al.*, Nature **443**, 409 (2006).

Chapter 5 Semi-classical treatment of transport



Ludwig Boltzmann
1844 - 1906

From Wikipedia

Classical, semi-classical transport, transport coefficient

Transport in condensed matter: Charge, heat, spin carriers $\begin{cases} \text{electrons : most electric devices} \\ \text{ions : batteries, sensors} \end{cases}$

Classical, semi-classical transport ⟷ (quantum mechanical nature in transport) Quantum transport

Semi-classical: quantum mechanics affects energy distribution function

Classical semi-classical boundary Fermi degenerate temperature

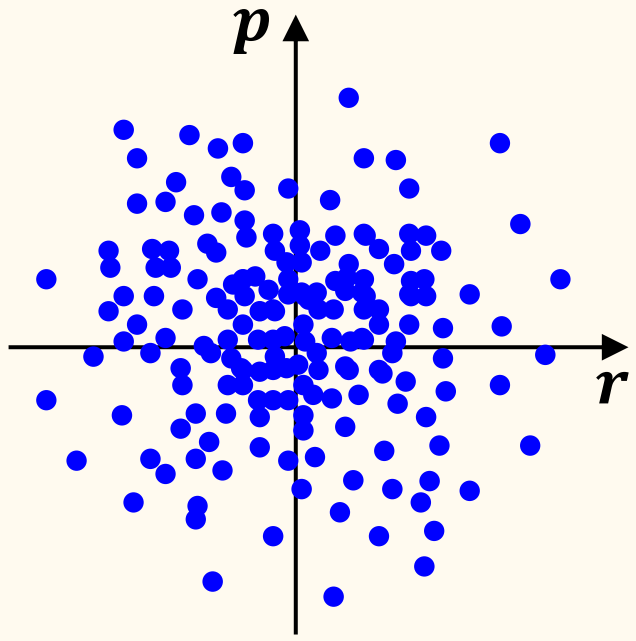
$$\begin{cases} T_{\mathrm{F}} = \dfrac{\hbar^2}{2mk_{\mathrm{B}}}(3\pi^2 n)^{2/3} & \text{for 3-dimensional systems} \\ T_{\mathrm{F}} = \dfrac{\hbar^2}{16\pi m k_{\mathrm{B}}} n & \text{for 2-dimensional systems} \end{cases}$$

External perturbation → Linear response: Transport coefficient Conductance, Resistance

current density $\boldsymbol{j} = \boldsymbol{\sigma}\mathbf{E}$ electric field $\mathbf{E} = \boldsymbol{\rho}\boldsymbol{j} = \boldsymbol{\sigma}^{-1}\boldsymbol{j}$

conductivity tensor resistivity tensor

Classical transport: Boltzmann equation



$(\boldsymbol{r}, \boldsymbol{p})$ 6-dimensional phase space

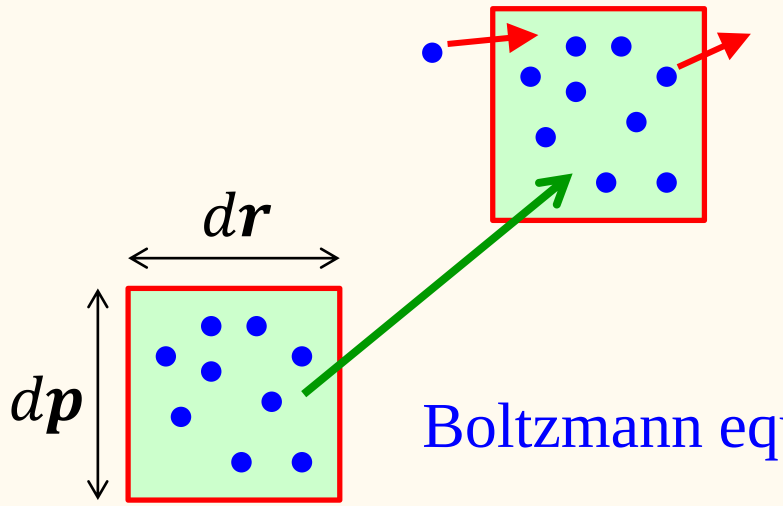
Distribution function $f(\boldsymbol{r}, \boldsymbol{p}, t)$ $\quad \dfrac{d\boldsymbol{r}}{dt} = \boldsymbol{v} = \dfrac{\boldsymbol{p}}{m}, \quad \dfrac{d\boldsymbol{p}}{dt} = \boldsymbol{F}$

No collision: $f(\boldsymbol{r} + \boldsymbol{v}dt, \boldsymbol{p} + \boldsymbol{F}dt, t + dt) = f(\boldsymbol{r}, \boldsymbol{p}, t)$

Introduction of collision: $(\partial f / \partial t)_c$

$$f\left(\boldsymbol{r} + \frac{\boldsymbol{p}}{m^*}dt, \boldsymbol{p} + \boldsymbol{F}dt, t + dt\right) + \left(\frac{\partial f}{\partial t}\right)_c dt = f(\boldsymbol{r}, \boldsymbol{p}, t)$$

$$\rightarrow f(\boldsymbol{r}, \boldsymbol{p}, t) + \left[\frac{\partial f}{\partial \boldsymbol{r}}\frac{d\boldsymbol{r}}{dt} + \frac{\partial f}{\partial \boldsymbol{p}}\frac{d\boldsymbol{p}}{dt} + \frac{\partial f}{\partial t}\right] dt$$



Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = -\left(\frac{\partial f}{\partial t}\right)_c$$

Currents: Particle flows

Boltzmann equation $$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = -\left(\frac{\partial f}{\partial t}\right)_c$$

Relaxation time approximation: $$-\left(\frac{\partial f}{\partial t}\right)_c = -\frac{f - f_0}{\tau}$$

$\boldsymbol{p}$: Anisotropic distribution = Current

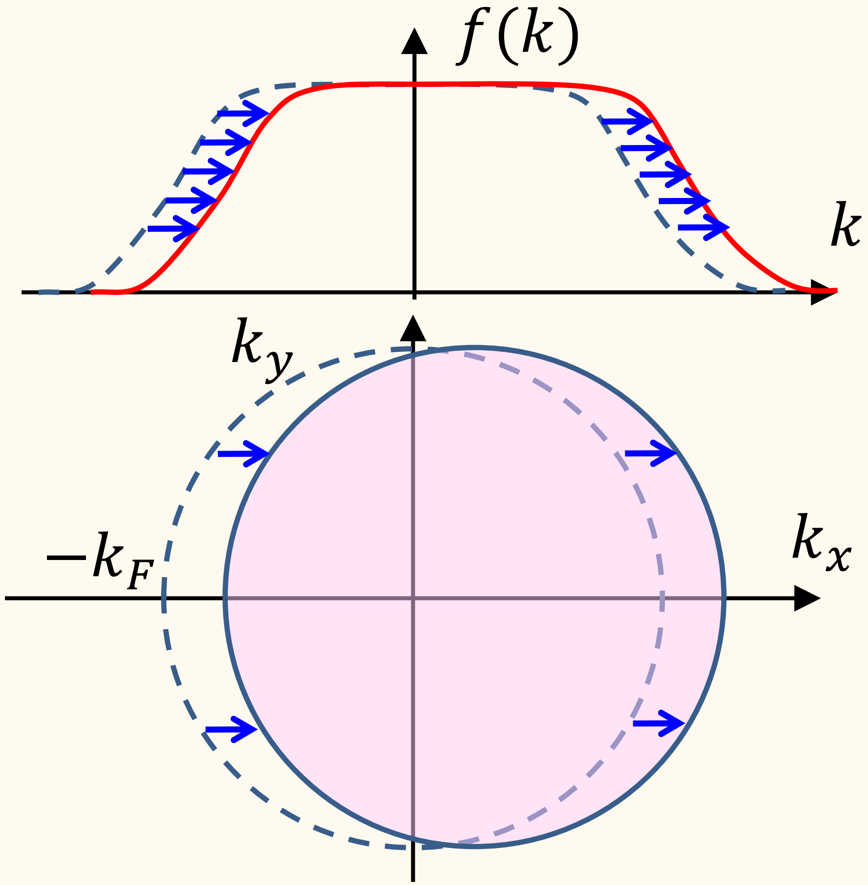
f_0: isotropic in $\boldsymbol{p}$-space → the collision term leads to current

$\frac{\partial f}{\partial t}$: time derivative of the distribution, zero for steady states

$\frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}}$: velocity times spatial gradient in the particle density → Diffusion current

$\boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}}$: force on the particles times gradient of f in $\boldsymbol{p}$-space → Drift current

Drift current by electric field



$$-e\mathbf{E}\cdot\frac{\partial f}{\partial \boldsymbol{p}} = -\frac{f-f_0}{\tau(\boldsymbol{p})}$$

$$\therefore f(\boldsymbol{p}) = f_0(\boldsymbol{p}) + e\tau(\boldsymbol{p})\mathbf{E}\cdot\frac{\partial f}{\partial \boldsymbol{p}} \approx f_0(\boldsymbol{p}) + e\tau(\boldsymbol{p})\mathbf{E}\cdot\frac{\partial f_0}{\partial \boldsymbol{p}} \approx f_0(\boldsymbol{p}+e\tau\mathbf{E})$$

$$\mathbf{E} = (\mathcal{E}_x, 0, 0)$$

$$\langle v\rangle = \int \frac{d^3k}{(2\pi)^3}\boldsymbol{v}(\boldsymbol{k})\left(f_0 + e\tau\mathbf{E}\cdot\frac{\partial f_0}{\hbar\partial \boldsymbol{k}}\right) = \int \frac{d^3k}{(2\pi)^3}\frac{\hbar k_x}{m}e\tau\mathcal{E}_x\frac{\partial f_0}{\hbar\partial k_x}$$
$$= \frac{e\mathcal{E}_x}{m}\int \mathscr{D}(E)\tau(E)\frac{\hbar^2k_x^2}{m}\frac{\partial f_0}{\partial E}dE$$

Density of states: $\mathscr{D}(E) \propto \sqrt{E}(=A\sqrt{E})$

Kinetic energy: $\dfrac{\hbar^2k_x^2}{m} \to 2\cdot\dfrac{E}{3}$

law of equipartition of energy

Drude formula

Paul Drude (1863 – 1906)

For metals ($T_F \gg 300$ K) Low temperature approximation: $\frac{\partial f_0}{\partial E} \approx -\delta(E - E_\mathrm{F})$

$$\langle v_x \rangle = -A \frac{e\mathcal{E}_x}{m} \frac{2\tau(E_\mathrm{F})}{3} E_\mathrm{F}^{3/2} \qquad n = \int_0^{E_\mathrm{F}} \mathscr{D}(E) dE = A \frac{2}{3} E_\mathrm{F}^{3/2}$$

$$\sigma = -e \frac{\langle v_x \rangle}{\mathcal{E}_x} = \frac{e^2 n \tau(E_\mathrm{F})}{m}$$

Drude formula for metals

For Maxwell distribution $(f_0 \approx A_\mathrm{F} \exp(-E/k_\mathrm{B}T))$

$$-\frac{\partial f_0}{\partial E} = -\frac{A_\mathrm{F}}{k_\mathrm{B}T} \exp\left[-\frac{E}{k_\mathrm{B}T}\right] = -\frac{f_0}{k_\mathrm{B}T} = -\frac{f_0}{(2\langle E \rangle / 3n)}$$

$$\sigma = e^2 \int \tau(E) \mathscr{D}(E) \frac{2E}{3m} \frac{3nf_0}{2\langle E \rangle} dE = \frac{ne^2 \langle \tau \rangle_E}{m}$$

Drude-like formula

$$\langle \tau \rangle_E \equiv \frac{\langle \tau E \rangle}{\langle E \rangle} = \int_0^\infty \tau(E) E^{3/2} f_0 dE \Big/ \int_0^\infty E^{3/2} f_0 dE$$

Diffusion current

No external force: $\boldsymbol{F} = \vec{0}, \quad f = f_0 + f_1$

Relaxation time approximation: $\boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} = -\frac{f_1}{\tau} \quad f_1 \approx \tau \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}}$

$$\boldsymbol{J} = (-e) \int_V \tau \boldsymbol{v}(\boldsymbol{v} \cdot \boldsymbol{\nabla} f) d\boldsymbol{r}$$

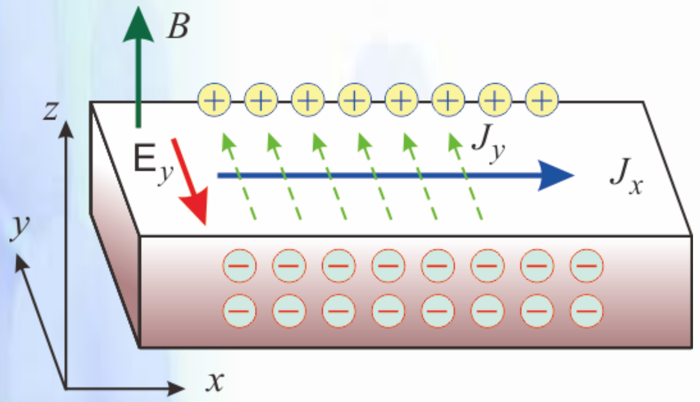
Take the x-direction to that of ∇f: $j_x = -e \int_{\text{uv}} \tau v_x^2 \frac{\partial f}{\partial x} d\boldsymbol{r} = -e \left\langle \frac{\tau v^2}{3} \right\rangle \frac{\partial n}{\partial x}$

$$\boldsymbol{j} = (-e) D \boldsymbol{\nabla} n, \quad D = \left\langle \frac{\tau v^2}{3} \right\rangle$$

Einstein relation: $D = \frac{\tau}{3} \langle v^2 \rangle = \frac{\tau k_{\rm B} T}{m^*} = \frac{\mu}{e} k_{\rm B} T$

$\mu = \frac{e\tau}{m^*}$: mobility

The Hall effect



Galvanomagnetic effect: Force on electrons ← Lorentz force

$\boldsymbol{B} \parallel z$-axis

$$\boldsymbol{j} = \frac{ne^2}{m^*}\left(\begin{array}{cc|c} A_l & -A_t & 0 \\ A_t & A_i & 0 \\ \hline 0 & 0 & A_z \end{array}\right)\mathbf{E}$$

A_t term creates j_y hence E_y : Hall voltage (electric field)

The Hall coefficient is defined as $R_{\mathrm{H}} = \dfrac{\mathcal{E}_y}{J_x B_z}$ $\quad \mathcal{E}_y = -\dfrac{A_t}{A_l}\mathcal{E}_x$

With cyclotron frequency $\omega_c = \dfrac{eB}{m^*}$ $\quad \sigma_{xx} = \dfrac{ne^2}{m^*}A_l = \dfrac{ne^2}{m^*}\left\langle \dfrac{\tau}{1+(\omega_c\tau)^2}\right\rangle_E, \ \sigma_{xy} = \dfrac{ne^2}{m^*}\left\langle \dfrac{\omega_c\tau^2}{1+(\omega_c\tau)^2}\right\rangle_E$

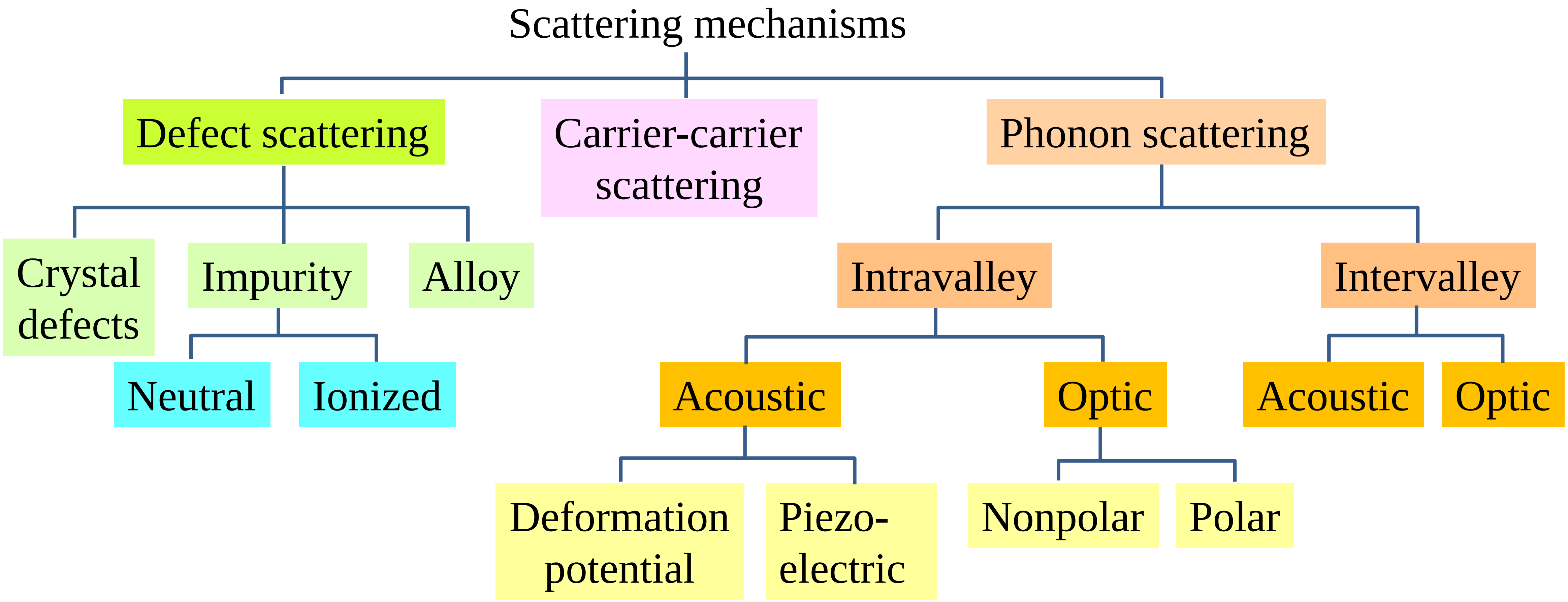
In case $\omega_c\tau \ll 1$

$$R_{\mathrm{H}} = -\frac{1}{ne}\frac{\langle\tau^2\rangle_E}{\langle\tau\rangle_E^2} = \frac{1}{n(-e)}\frac{\Gamma(2s+5/2)\Gamma(5/2)}{(\Gamma(s+5/2))^2} = \frac{r_{\mathrm{H}}}{n(-e)}$$

$r_{\mathrm{H}} \sim 1$ is called Hall factor

Mobility is defined and expressed as $\mu = \dfrac{v}{|\mathcal{E}|} = \dfrac{nev}{ne|\mathcal{E}|} = \dfrac{j}{ne|\mathcal{E}|} = \dfrac{\sigma}{ne} = \sigma|R_{\mathrm{H}}| = \dfrac{e\tau}{m^*}$

Carrier scattering mechanisms



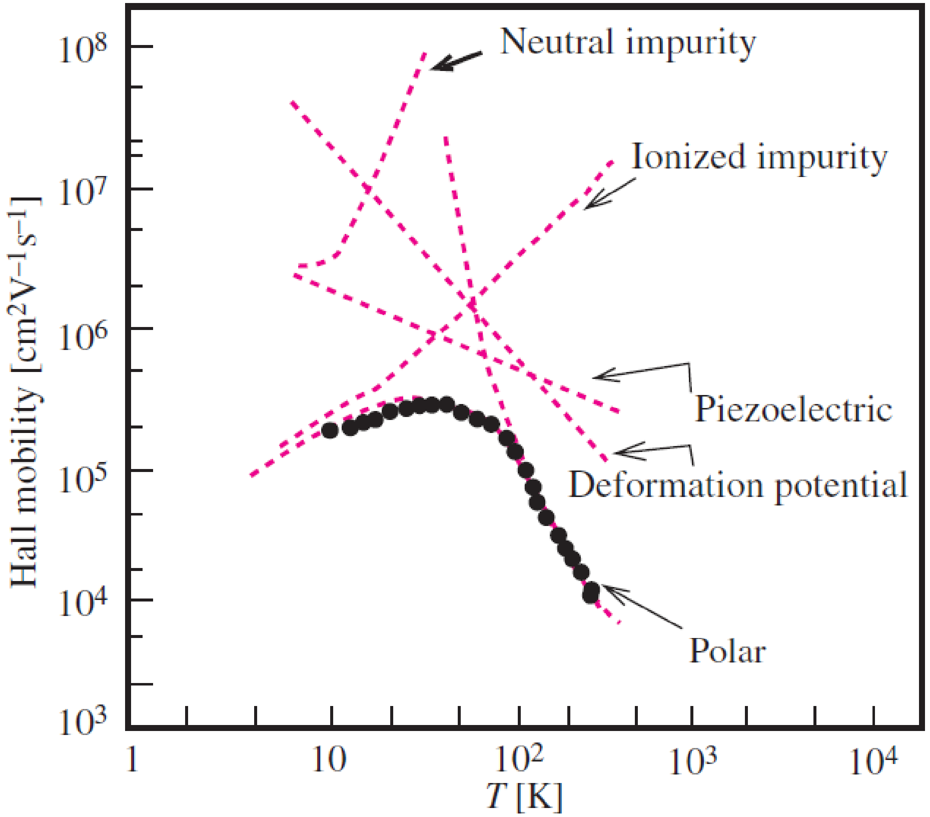
The parameter which represents the scattering mechanism
= averaged time interval of scattering

Scattering time: τ_β β : scattering mechanism

Matthiessen's rule and effect of scattering on the electric transport

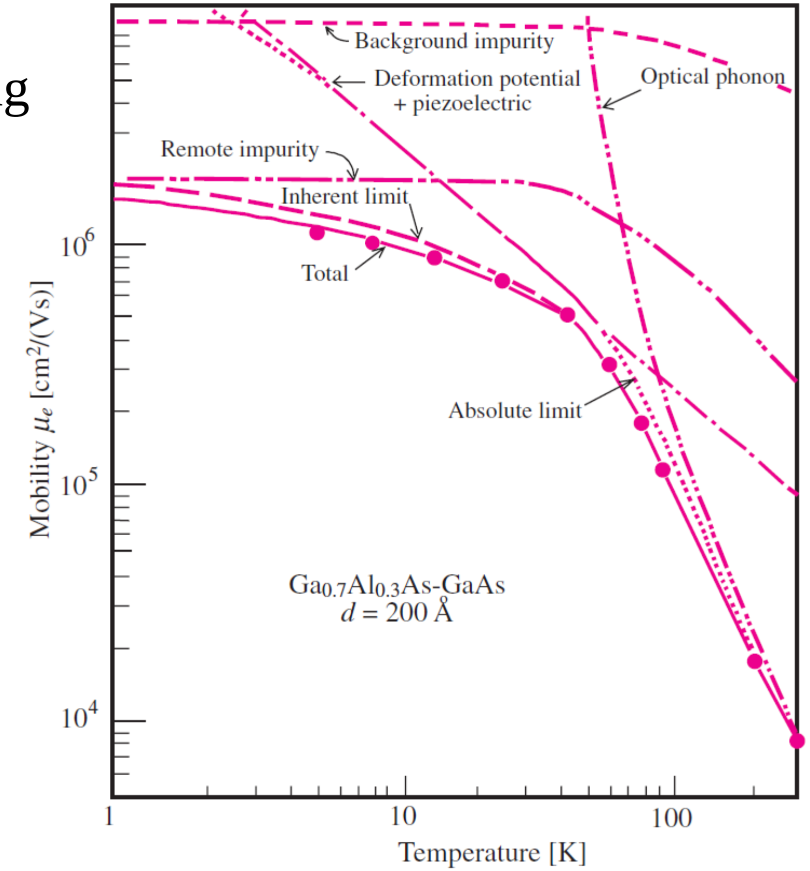
Matthiessen's rule (series connection of scattering)

$$\frac{1}{\tau_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\tau_{\beta}} = \frac{1}{\tau_{\mathrm{defects}}} + \frac{1}{\tau_{\mathrm{cattier}}} + \frac{1}{\tau_{\mathrm{lattice}}} + \cdots \qquad \frac{1}{\mu_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\mu_{\beta}} = \frac{1}{\mu_{\mathrm{defects}}} + \frac{1}{\mu_{\mathrm{cattier}}} + \frac{1}{\mu_{\mathrm{lattice}}} + \cdots$$



Fletcher *et al.*, J. Phys. C **5**, 212 (1972)

Reduction of impurity scattering by modulation doping structure



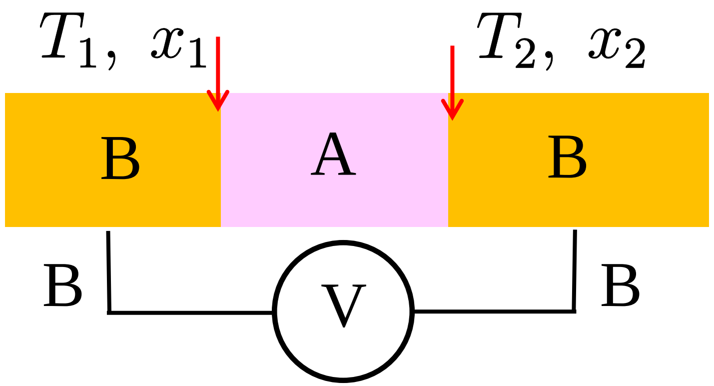
Walukiewicz *et al.* Phys. Rev. B **30**, 4571 (1984).

Heat transport, thermoelectric effect

Heat flux density: $j_{qx} = \langle n v_x (E-\mu) \rangle = \int_0^\infty v_x (E-\mu) f(E) \mathscr{D}(E) dE$

Temperature gradient ∇T Carrier thermal conductivity $\kappa_n = -\dfrac{j_{qx}}{\partial T/\partial x}$ $(\boldsymbol{j}_q = -\hat{\kappa}\nabla T)$

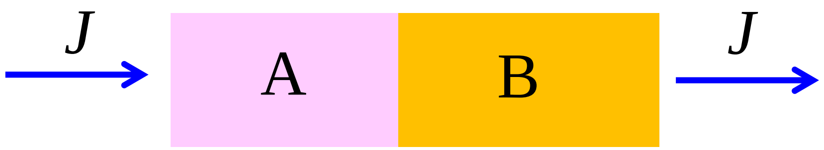
Seebeck effect



J: current, *V*: voltage, *T*: temperature, *Q*: heat flow

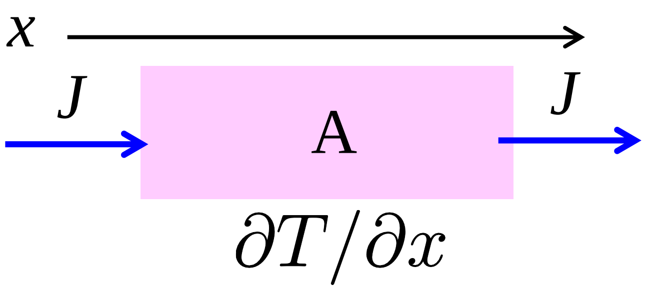
$S_{\mathrm{AB}} = \dfrac{V_{\mathrm{AB}}}{\Delta T}$ Seebeck coefficient

Peltier effect



$\Pi_{\mathrm{AB}} = \dfrac{Q_{\mathrm{AB}}}{J}$ Peltier coefficient

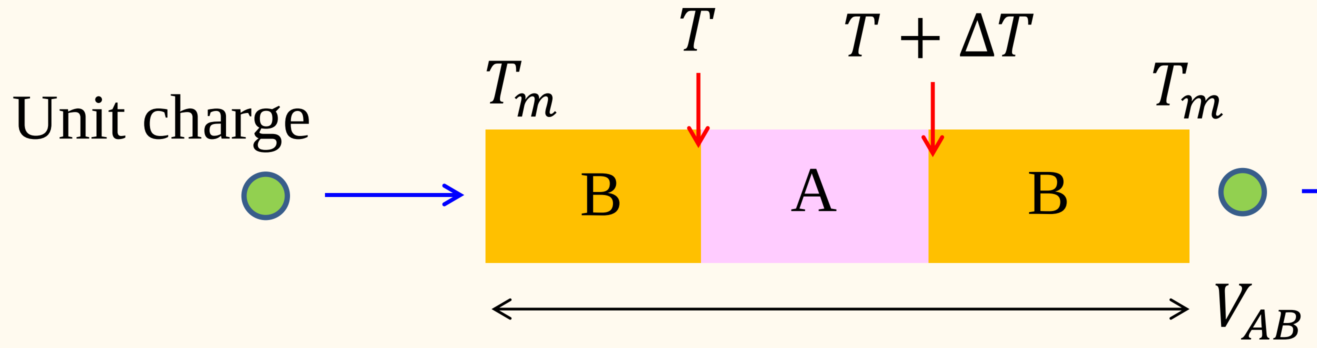
Thomson effect



$\tau = \dfrac{\partial Q/\partial x}{J(\partial T/\partial x)}$ Thomson coefficient

can be obtained from single material

The Kelvin relations



Quasi-static process → Thermodynamics can be applied

First law of thermodynamics $$V_{\mathrm{BA}} + \Pi_{\mathrm{BA}}(T) - \Pi_{\mathrm{BA}}(T + \Delta T) + (\tau_{\mathrm{B}} - \tau_{\mathrm{A}})\Delta T = 0$$

Second law of thermodynamics $$\frac{\Pi_{\mathrm{BA}}(T)}{T} - \frac{\Pi_{\mathrm{BA}}(T+\Delta T)}{T+\Delta T} + \frac{\tau_{\mathrm{B}} - \tau_{\mathrm{A}}}{T}\Delta T = 0$$

Taking $\Delta T \to 0$, these two become $$\frac{dV_{\mathrm{BA}}}{dT} - \frac{d\Pi_{\mathrm{BA}}}{dT} + \tau_{\mathrm{B}} - \tau_{\mathrm{A}} = 0, \quad \frac{d}{dT}\left(\frac{\Pi_{\mathrm{BA}}}{T}\right) = \frac{\tau_{\mathrm{B}} - \tau_{\mathrm{A}}}{T}$$

The second equation becomes $$\tau_{\mathrm{B}} - \tau_{\mathrm{A}} = T\frac{d}{dT}\left(\frac{\Pi_{\mathrm{BA}}}{T}\right) = \frac{d\Pi_{\mathrm{BA}}}{dT} - \frac{\Pi_{\mathrm{BA}}}{T}$$

The Kelvin relations are obtained as $$\therefore S_{\mathrm{AB}} = \frac{\Pi_{\mathrm{AB}}}{T}, \quad \frac{dS_{\mathrm{AB}}}{dT} = \frac{\tau_{\mathrm{A}} - \tau_{\mathrm{B}}}{T}$$

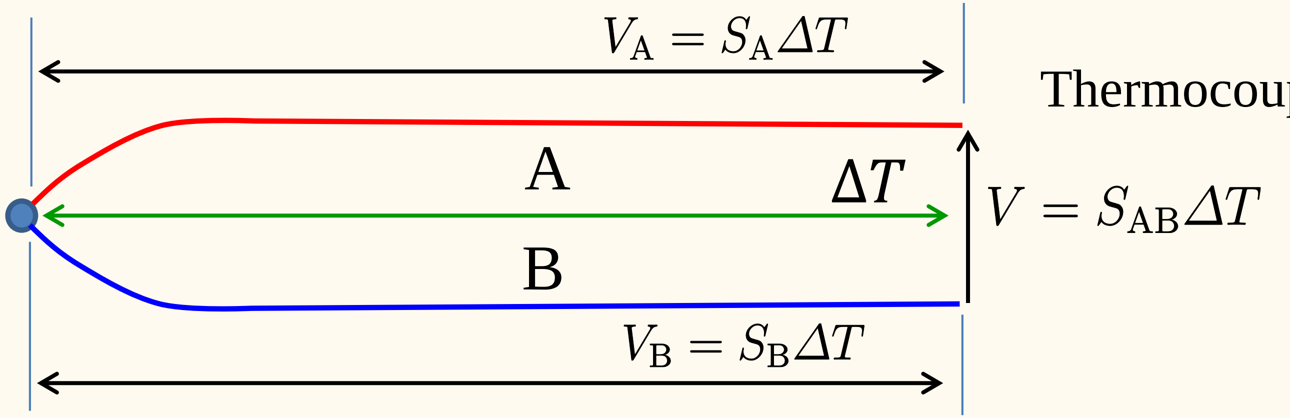
The absolute Seebeck, Peltier coefficients can be obtained from the relations.

Seebeck coefficient as material constant

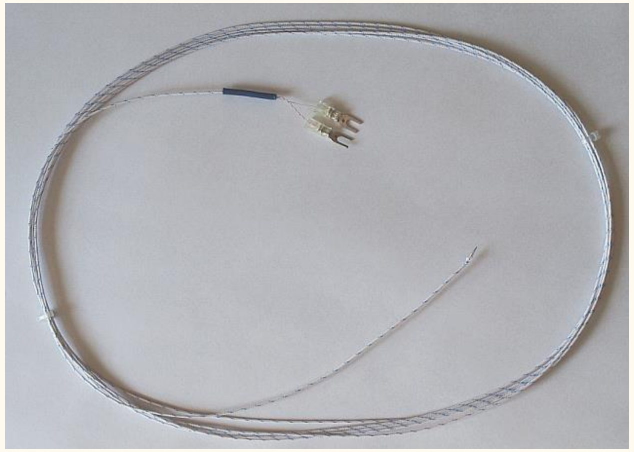
Material specific (absolute) constant can be experimentally obtained from

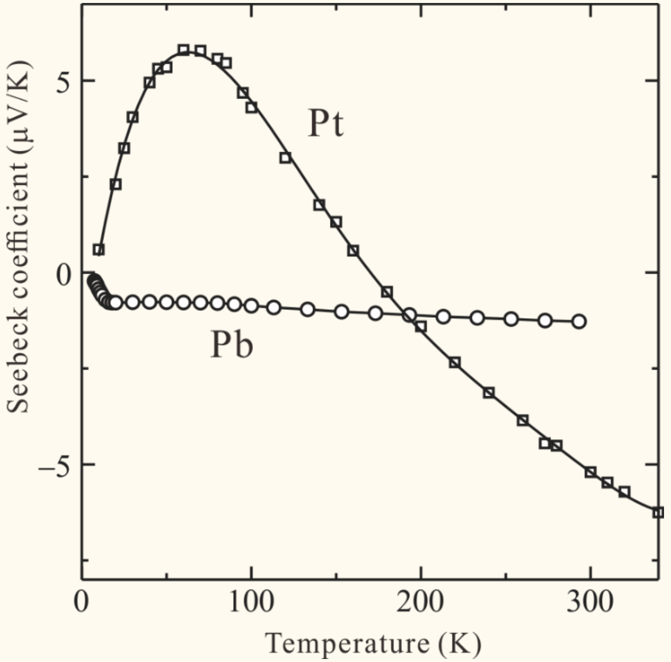
$$S_{\mathrm{A}}(T) \equiv \int_0^T \frac{\tau_{\mathrm{A}}(T')}{T'} dT'$$

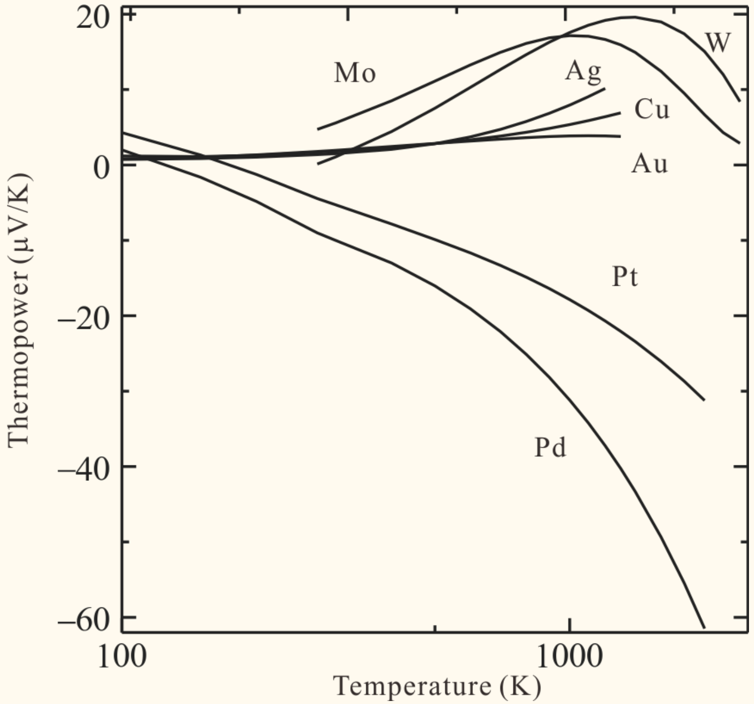
Then for other materials $S_{\mathrm{AB}} = S_{\mathrm{A}} - S_{\mathrm{B}}$



Thermocouple







Boltzmann equation and thermoelectric constants

For the thermoelectric effect, we need to consider (only) ∇T

The distribution function in lhs is replaced with unperturbed one.

$$\boldsymbol{v}\cdot\nabla f+\frac{\boldsymbol{F}}{m^*}\nabla_v f=-\frac{f-f_0}{\tau(E)}\approx\left[\boldsymbol{v}\cdot\nabla+\frac{\boldsymbol{F}}{m^*}\nabla_{\boldsymbol{v}}\right]f_0$$

With $a\equiv-\dfrac{E-E_{\rm F}}{k_{\rm B}T}$

$$\frac{\partial f_0}{\partial T}=\frac{\partial f_0}{\partial E}\frac{\partial E}{\partial a}\frac{\partial a}{\partial T}=\frac{\partial f_0}{\partial E}(-k_{\rm B}T)\left(\frac{E-E_{\rm F}}{k_{\rm B}T^2}\right)=\frac{\partial f_0}{\partial E}\frac{E_{\rm F}-E}{T}$$

From the above we can rewrite

$$\nabla f_0=\nabla T\frac{E_{\rm F}-E}{T}\frac{\partial f_0}{\partial E},\qquad \nabla_v f_0=\nabla_v E\frac{\partial f_0}{\partial E}=m\boldsymbol{v}\frac{\partial f_0}{\partial E}$$

Then the Boltzmann equation gives

$$f=f_0-\tau(E)\boldsymbol{v}\cdot\left[-e\mathbf{E}+\frac{E_{\rm F}-E}{T}\nabla T\right]\frac{\partial f_0}{\partial E}$$

Substituting the above and $\mathbf{E}=(\mathcal{E}_x,0,0)$ into the current expression

$$j_x=-e\langle nv_x\rangle=-e\int_0^\infty v_x f(E)\mathscr{D}(E)dE$$

$$=e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x+\frac{E_{\rm F}-E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE$$

Boltzmann equation and thermoelectric constants (2)

$$j_x = e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x + \frac{E_F - E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE = 0$$

$j_x = 0$ means the balancing of the drift current and the diffusion current

Then the Seebeck coefficient is calculated as

$$S = \frac{\mathcal{E}_x}{\partial T/\partial x} = \int_0^\infty v_x^2\tau\frac{E_F - E}{eT}\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE \Bigg/ \int_0^\infty v_x^2\tau\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE$$

$$= \frac{1}{eT}\left[E_F - \int_0^\infty \tau E^2\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE \Bigg/ \int_0^\infty \tau E\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE\right]$$

$$= \langle\tau E\rangle_E/\langle\tau\rangle_E$$

Maxwell approximation
$$\frac{\partial f_0}{\partial E} = -\frac{f_0}{k_B T}$$

Energy dependence of relaxation time
$$\tau \propto E^s$$

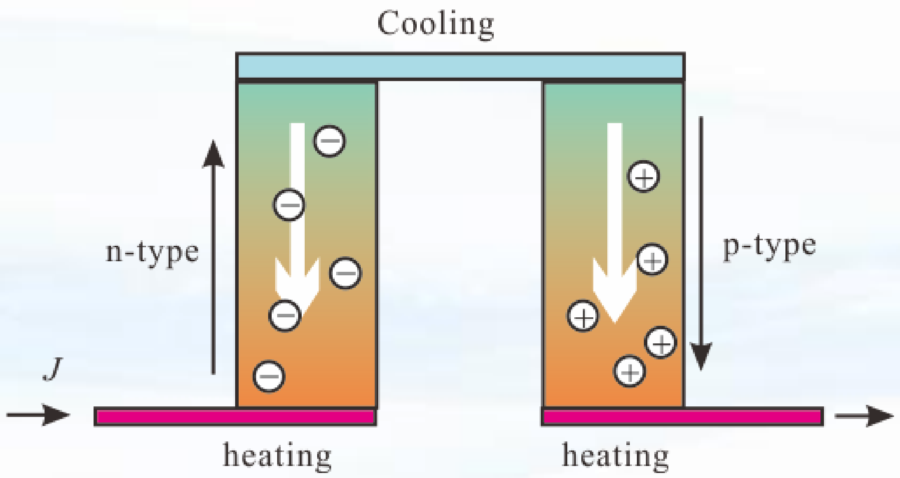
$$S = -\frac{1}{eT}\left[\frac{\langle\tau E\rangle_E}{\langle\tau\rangle_E} - E_F\right] = -\frac{1}{eT}\left[\left(\frac{5}{2}+s\right)k_B T - E_F\right]$$

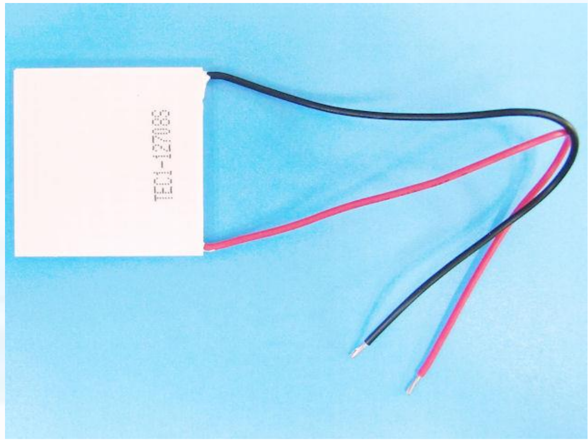
Seebeck measurement provides information on E_F and scattering mechanisms

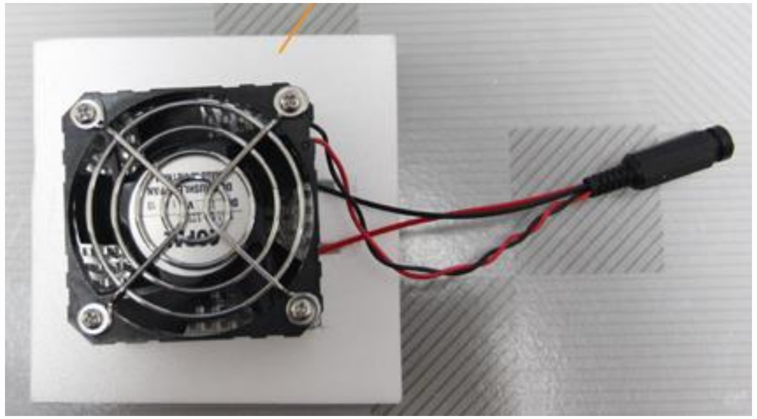
Peltier device

$$S = \frac{1}{qT}\left[\left(\frac{5}{2}+s\right)k_{\mathrm{B}}T - E_{\mathrm{F}}\right] \qquad \Pi = ST$$

Sign of the coefficient changes with carrier charge







Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.5.26 Lecture 07

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Review of last week

Concept of exciton-polariton (continued)

Chapter 5 Semi-classical treatment of transport

Transport coefficient

Classical transport: Boltzmann equation

Currents: particle flows

Drude formula, Diffusion current, Hall effect

Various scatterings

Heat transport, Thermoelectric effect

Boltzmann equation and thermoelectric constants

For the thermoelectric effect, we need to consider (only) ∇T

The distribution function in lhs is replaced with unperturbed one.

$$\boldsymbol{v}\cdot\nabla f + \frac{\boldsymbol{F}}{m^*}\nabla_v f = -\frac{f-f_0}{\tau(E)} \approx \left[\boldsymbol{v}\cdot\nabla + \frac{\boldsymbol{F}}{m^*}\nabla_{\boldsymbol{v}}\right] f_0$$

With $a \equiv -\dfrac{E-E_{\rm F}}{k_{\rm B}T}$

$$\frac{\partial f_0}{\partial T} = \frac{\partial f_0}{\partial E}\frac{\partial E}{\partial a}\frac{\partial a}{\partial T} = \frac{\partial f_0}{\partial E}(-k_{\rm B}T)\left(\frac{E-E_{\rm F}}{k_{\rm B}T^2}\right) = \frac{\partial f_0}{\partial E}\frac{E_{\rm F}-E}{T}$$

From the above we can rewrite

$$\nabla f_0 = \nabla T\frac{E_{\rm F}-E}{T}\frac{\partial f_0}{\partial E}, \quad \nabla_v f_0 = \nabla_v E\frac{\partial f_0}{\partial E} = m\boldsymbol{v}\frac{\partial f_0}{\partial E}$$

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$$f = f_0 - \tau(E)\boldsymbol{v}\cdot\left[-e\mathbf{E} + \frac{E_{\rm F}-E}{T}\nabla T\right]\frac{\partial f_0}{\partial E}$$

Substituting the above and $\mathbf{E} = (\mathcal{E}_x, 0, 0)$ into the current expression

$$j_x = -e\langle nv_x\rangle = -e\int_0^\infty v_x f(E)\mathscr{D}(E)dE$$

$$= e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x + \frac{E_{\rm F}-E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE$$

Boltzmann equation and thermoelectric constants (2)

$$j_x = e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x + \frac{E_F - E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE = 0$$

$j_x = 0$ means the balancing of the drift current and the diffusion current

Then the Seebeck coefficient is calculated as

$$S = \frac{\mathcal{E}_x}{\partial T/\partial x} = \int_0^\infty v_x^2\tau\frac{E_F - E}{eT}\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE \Big/ \int_0^\infty v_x^2\tau\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE$$

$$= \frac{1}{eT}\left[E_F - \int_0^\infty \tau E^2\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE \Big/ \int_0^\infty \tau E\frac{\partial f_0}{\partial E}\mathscr{D}(E)dE\right]$$

$$= \langle\tau E\rangle_E / \langle\tau\rangle_E$$

Maxwell approximation

$$\frac{\partial f_0}{\partial E} = -\frac{f_0}{k_B T}$$

Energy dependence of relaxation time

$$\tau \propto E^s$$

$$S = -\frac{1}{eT}\left[\frac{\langle\tau E\rangle_E}{\langle\tau\rangle_E} - E_F\right] = -\frac{1}{eT}\left[\left(\frac{5}{2}+s\right)k_B T - E_F\right]$$

Seebeck measurement provides information on E_F and scattering mechanisms

Peltier device

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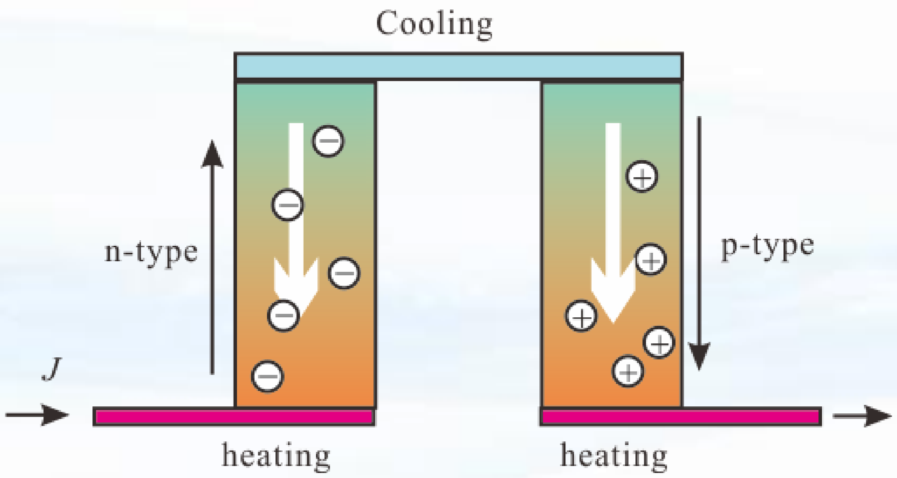
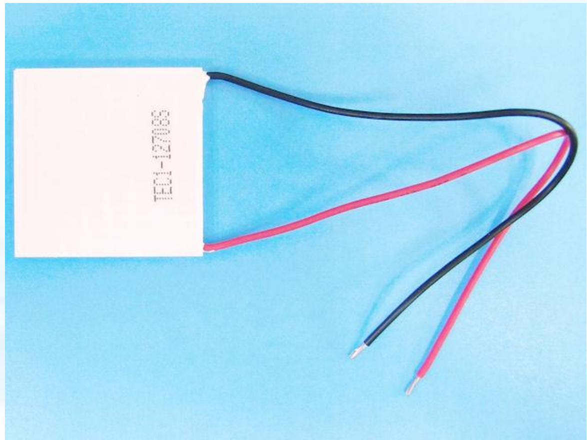
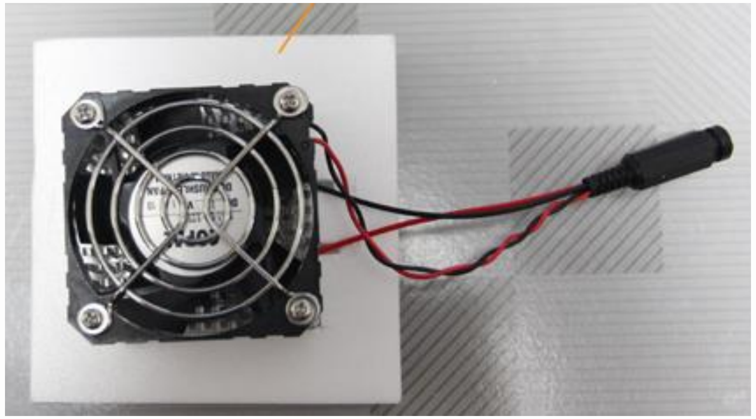
Sign of the coefficient changes with carrier charge







Physics in spatially structured semiconductors

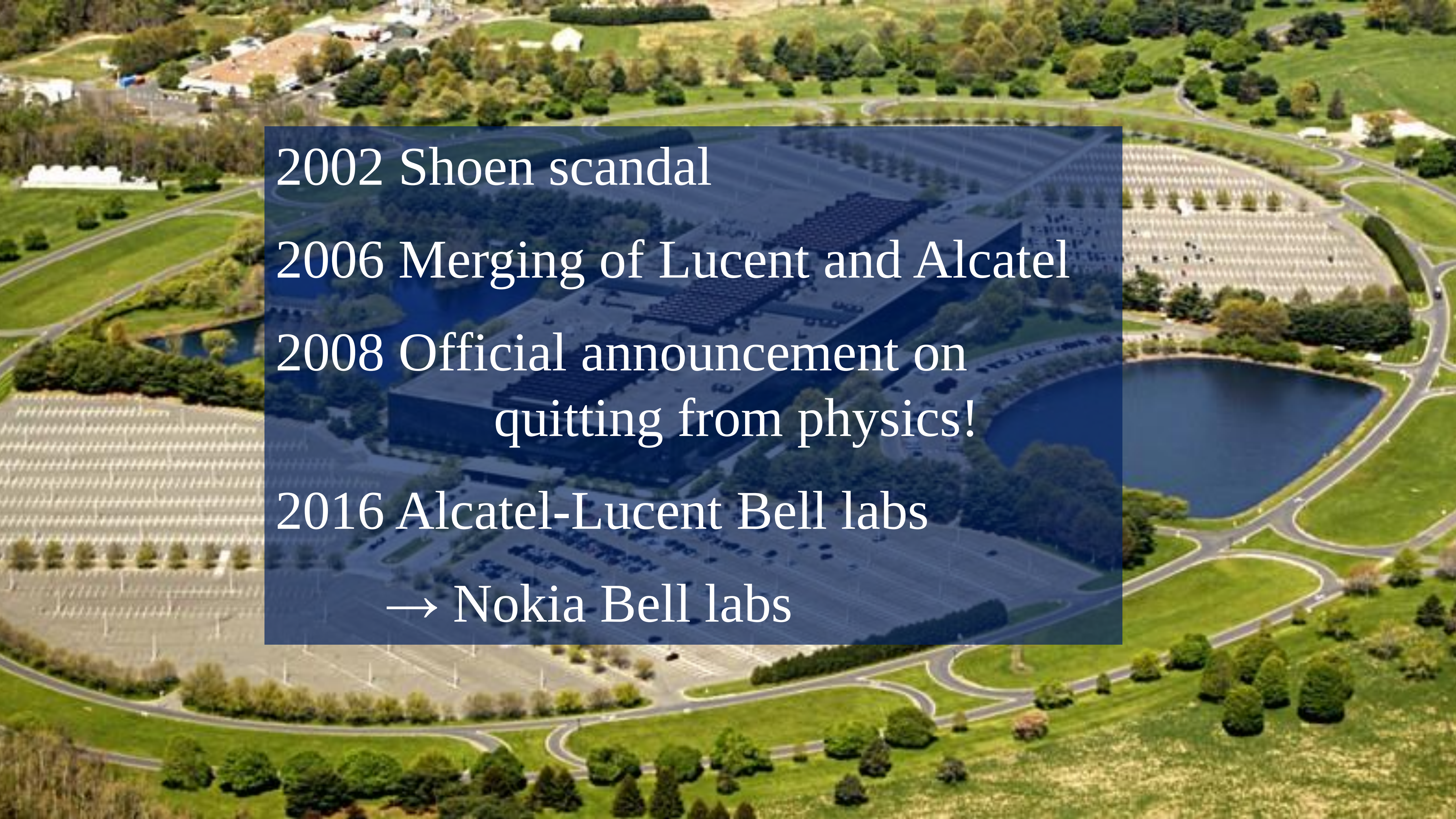
Our apparatus:

- Band structure
- Effective mass approximation
- Carrier statistics
- Electron-photon couplings
- Thermodynamics
- Semi-classical transport (Boltzmann equation)

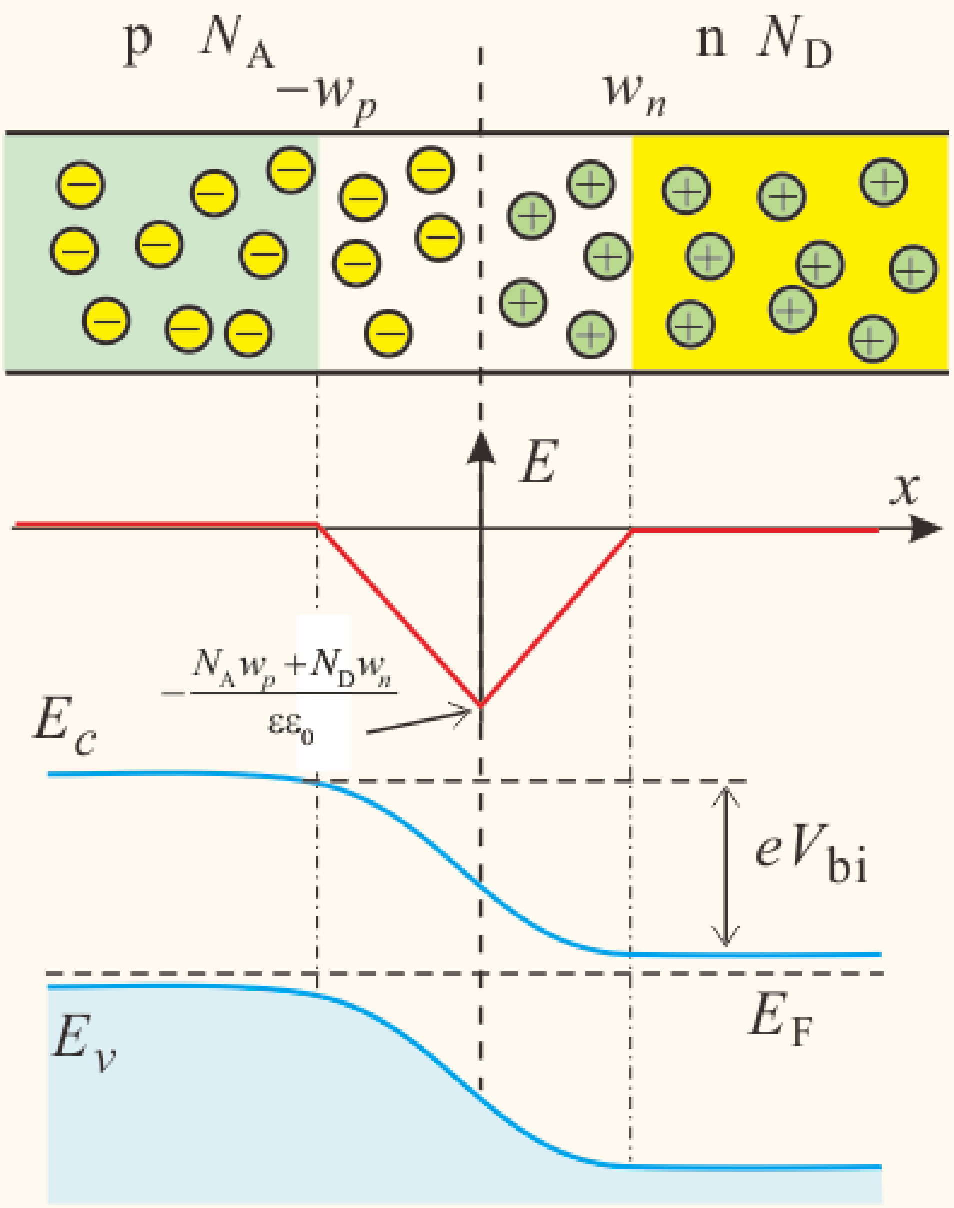
Chapter 6 Homo and hetero junctions

Bell laboratories ～1984


Bell laboratories 90’s
Lucent Technologies


2002 Shoen scandal
2006 Merging of Lucent and Alcatel
2008 Official announcement on
quitting from physics!
2016 Alcatel-Lucent Bell labs
→ Nokia Bell labs

pn homo junctions



Fabrication of pn junctions:
- Epitaxial growth
- Counter doping
- Masked, focused doping

Equilibrium

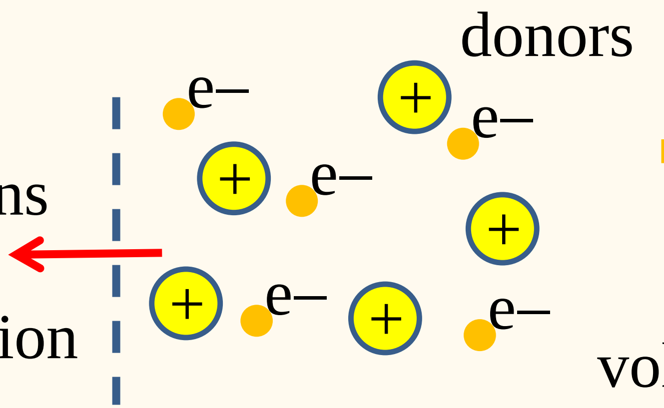
Diffusion current:
Entropy increase

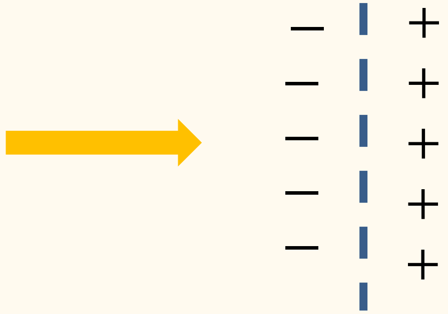
Balance:
Minimize Free energy

Drift current:
Internal energy decrease

- ➢ Carrier depletion layer (space charge layer)
- ➢ Built-in potential

Consider electrons attached to a vacuum without work function





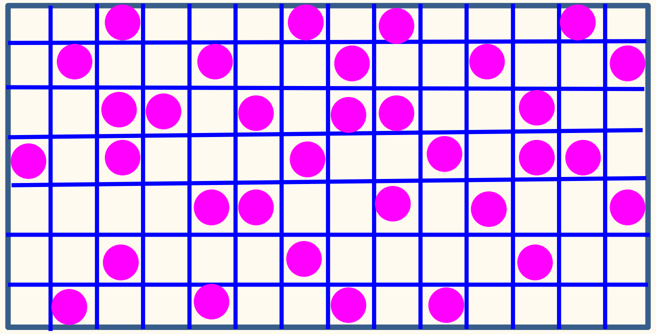
voltage (polarization) → energy cost

$F = \underline{U} - T\underline{S}$ Minimization of F → Built-in (diffusion) voltage V_{bi}

Voltage (internal energy cost)

Diffusion (entropy)

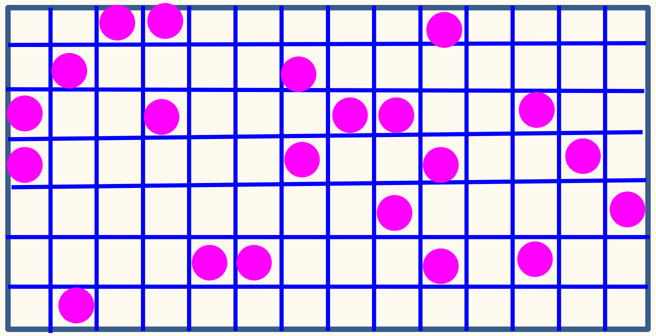
number of sites: N



particle number: N_1

$$dN_1 = -dN_2$$

number of sites: N



particle number: N_2

Estimation of built-in potential

Notation of carrier concentration

	electrons	holes
n-layer	n_n	p_n
p-layer	n_p	p_p

$$n_n \sim N_\mathrm{D},\ p_p \sim N_\mathrm{A} \quad n_p = \frac{n_i^2}{p_p} \sim \frac{n_i^2}{N_\mathrm{A}}$$

Number of cases: $W = {}_N\mathrm{C}_{N_1}\,{}_N\mathrm{C}_{N_2}$

$N \gg N_1, N_2$ Stirling approximation: $\ln N! \approx N\ln N - N$

$$\ln W = \ln \frac{N!}{(N-N_1)!N_1!}\frac{N!}{(N-N_2)!N_2!} \qquad \frac{d\ln W}{dN_1} \approx \ln\frac{N_2}{N_1}\frac{N-N_1}{N-N_2} \approx \ln\frac{N_2}{N_1}$$

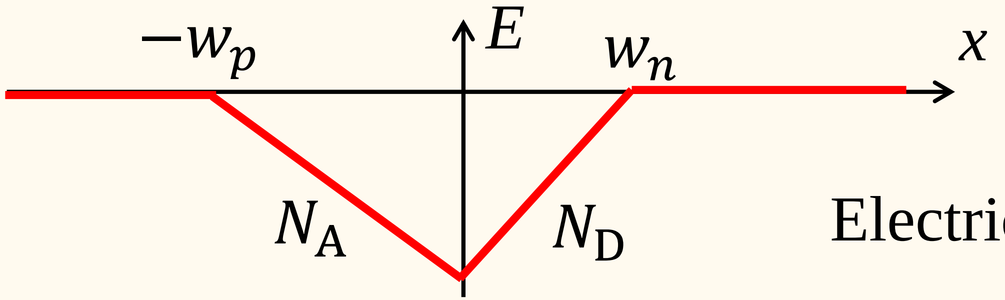
:Mixing entropy

$$N_1 = n_n, \quad N_2 = n_p, \qquad F = U - TS = U - Tk_\mathrm{B}\ln W$$

$$\frac{dF}{dn_n} = 0 \ \rightarrow \ \frac{dU}{dn_n} = eV_\mathrm{bi} = k_\mathrm{B}T\frac{d\ln W}{dn_n} = k_\mathrm{B}T\ln\frac{n_n}{n_p}$$

$$np = n_i^2 = N_\mathrm{c}N_\mathrm{v}\exp\left(-\frac{E_\mathrm{g}}{k_\mathrm{B}T}\right) \ \rightarrow \qquad \approx k_\mathrm{B}T\ln\frac{N_\mathrm{D}N_\mathrm{A}}{n_i^2} = E_\mathrm{g} - k_\mathrm{B}T\ln\frac{N_\mathrm{c}N_\mathrm{v}}{N_\mathrm{D}N_\mathrm{A}}$$

Estimation of depletion layer width



Charge neutrality: $w_n N_D = w_p N_A$

Electric field:
$$-\epsilon\epsilon_0 E(x) = e[N_A(2x + w_p) + N_D w_n] \quad (x < 0)$$
$$= e[N_A w_p + N_D(w_n - 2x)] \quad (x \geq 0)$$

Built-in potential is $V_{bi} = \int_{-w_p}^{w_n} (-E(x))dx = \frac{e}{\epsilon\epsilon_0}(N_D + N_A)w_n w_p = \frac{e}{\epsilon\epsilon_0}(N_D + N_A)\frac{N_D}{N_A}w_n^2$

$$V_{bi} = \frac{1}{e}\left(E_g - k_B T \ln \frac{N_c N_v}{N_D N_A}\right)$$

$$\therefore \ w_n = \frac{1}{e}\sqrt{\frac{\epsilon\epsilon_0 N_A}{(N_D + N_A)N_D}\left(E_g - k_B T \ln \frac{N_c N_v}{N_A N_D}\right)}$$

$$w_p = \frac{1}{e}\sqrt{\frac{\epsilon\epsilon_0 N_D}{(N_D + N_A)N_A}\left(E_g - k_B T \ln \frac{N_c N_v}{N_A N_D}\right)}$$

Current-voltage characteristics

Electrons

Equilibrium
$$n_n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right),$$
$$n_p = N_c \exp\left(\frac{E_F - E_c - eV_{bi}}{k_B T}\right) = n_n \exp\left(-\frac{eV_{bi}}{k_B T}\right)$$

Current balance $J_{pn} = ev_n n_p \qquad J_{np} = ev_n n_n \exp\left(-\frac{eV_{bi}}{k_B T}\right)$

External voltage V

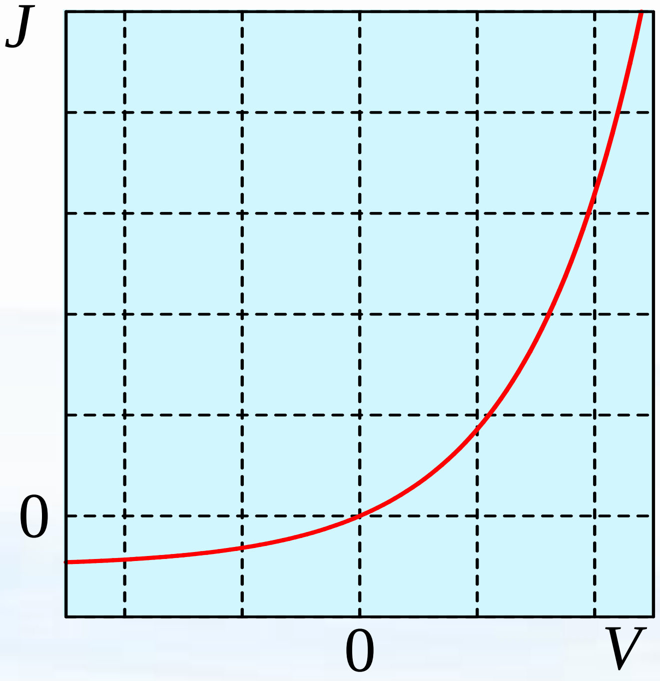
Forward bias (against V_{bi}) : lowers barrier for diffusion current n_n

$$V_{bi} \to V_{bi} - V \qquad J_{np} = ev_n n_n \exp\left(-\frac{e(V_{bi} - V)}{k_B T}\right) = ev_n n_p \exp\left(\frac{eV}{k_B T}\right)$$

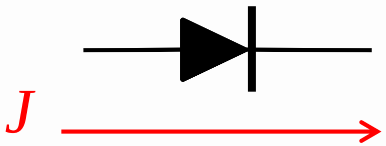
$$J_e = J_{np} - J_{pn} = ev_n n_p \exp\frac{eV}{k_B T} - ev_n n_p = ev_n n_p \left[\exp\frac{eV}{k_B T} - 1\right]$$

Electron, hole summation
$$J = e(v_n n_p + v_p p_n)\left[\exp\frac{eV}{k_B T} - 1\right]$$

Injection of minority carriers



pn junction circuit symbol



$$J = \underbrace{e(v_n n_p + v_p p_n)}_{\text{minority carrier current}} \underbrace{\left[\exp\frac{eV}{k_\mathrm{B}T} - 1\right]}_{\text{barrier overflow}}$$

minority carrier current   barrier overflow

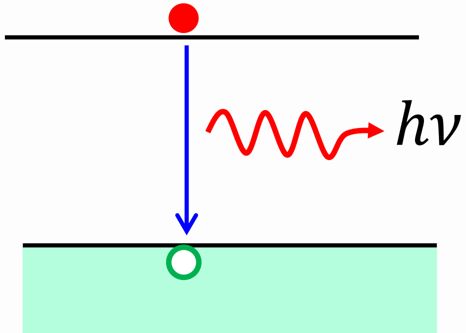
Forward bias region: minority carrier injection

Diffusion equation: $$D_e \frac{d^2 n_p}{dx^2} = \frac{n_p - n_{p0}}{\tau_e}$$

Minority carrier diffusion length: $$L_e = \sqrt{D_e \tau_e},\ L_h = \sqrt{D_h \tau_h}$$

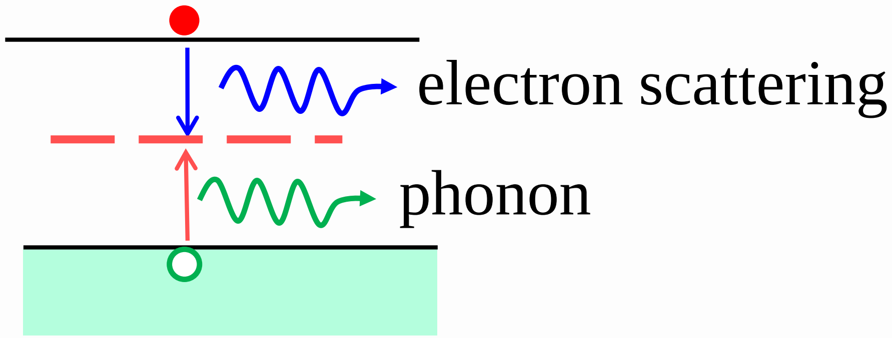
Fate of injected minority carriers

Radiative recombination

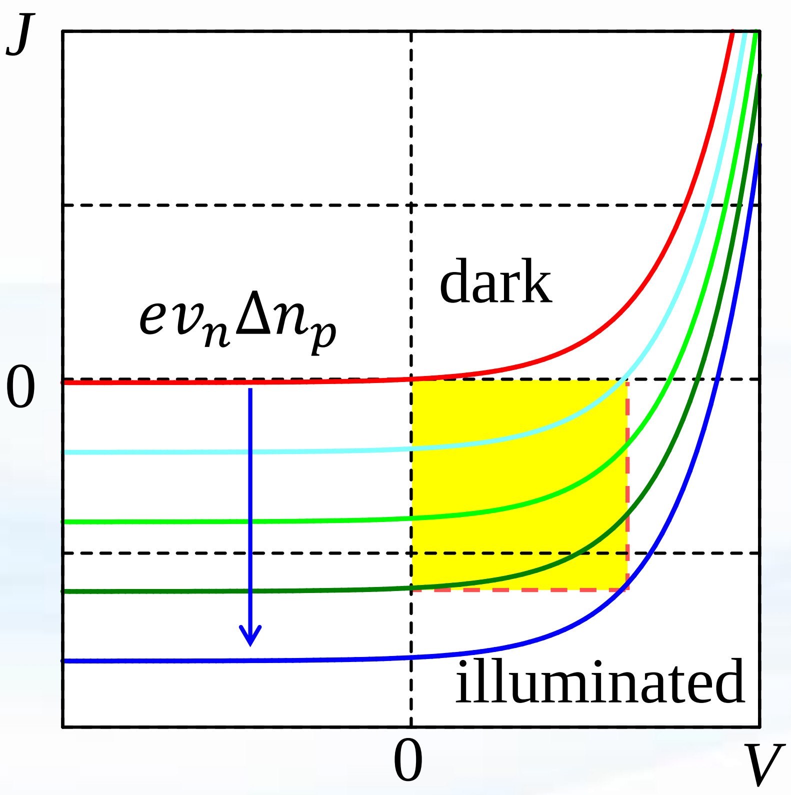


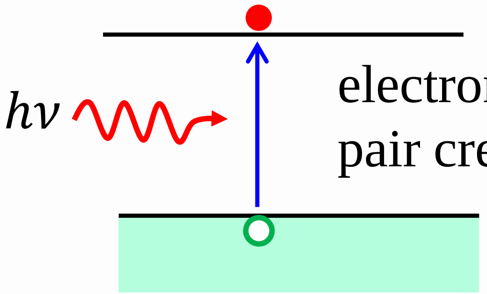
light emitting diode

Non-radiative recombination



Solar cells (external injection of minority carriers)





$$J_{e0} = ev_n n_p \left[\exp\frac{eV}{k_{gB}T} - 1\right]$$

$$J_e = ev_n n_p \exp\frac{eV}{k_B T} - ev_n(n_p + \Delta n_p)$$

$$= J_{n0} - ev_n\Delta n_p$$

external injection

Voltage for $J = 0$ V_{oc}

Current for $V = 0$ J_{sc}

Minority carriers which diffuse to the junction region are swept out to the other side.

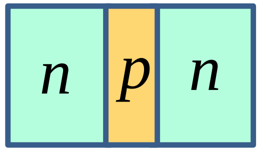
$$\text{Filling factor (FF)} = \frac{P_{max}}{J_{sc}V_{oc}}$$

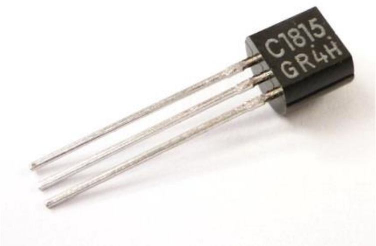
Gerald Pearson, Daryl Chapin
and Calvin Fuller at Bell labs. 1954

pn junction (bipolar) transistors

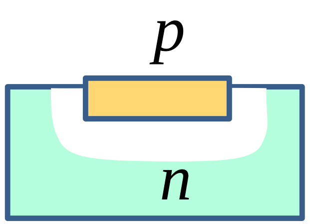
John Bardeen, William Shockley, Walter Brattain 1948 Bell Labs.

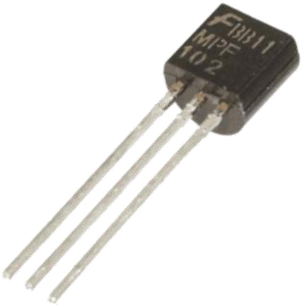
Bipolar junction transistor



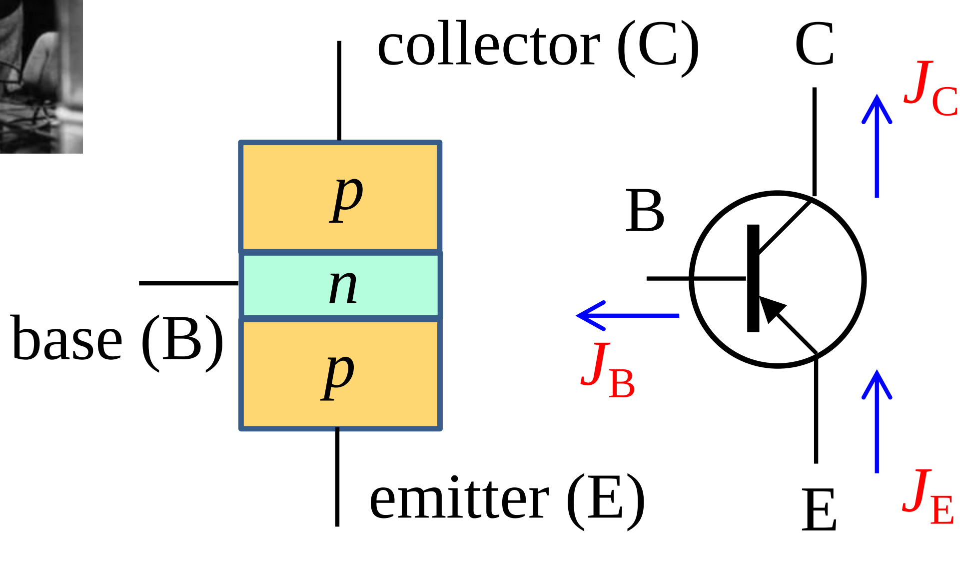


Field effect transistor

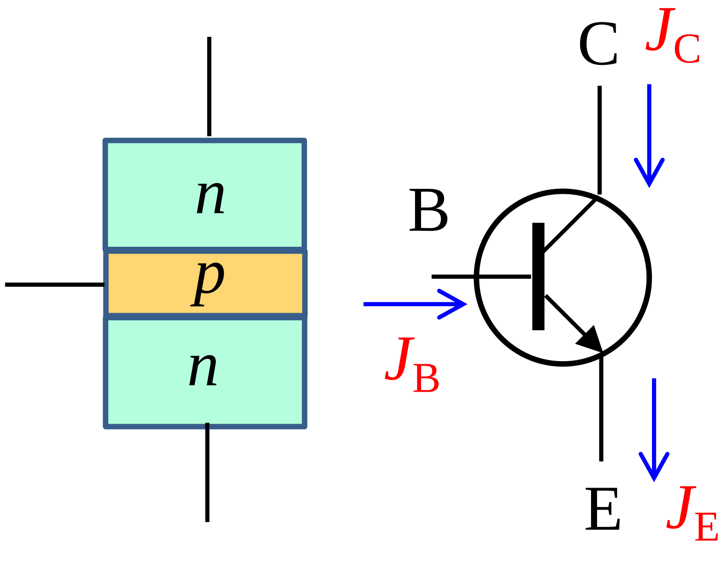




Bipolar transistor structures and symbols



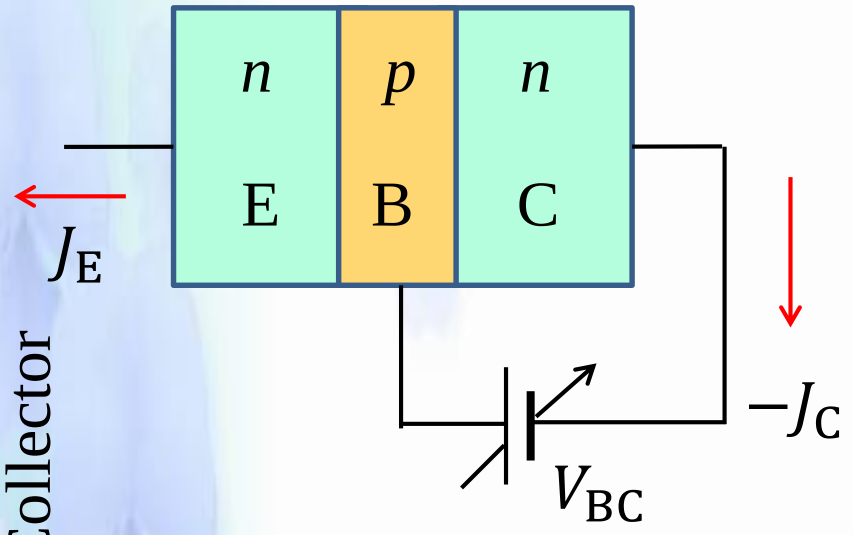
PNP type

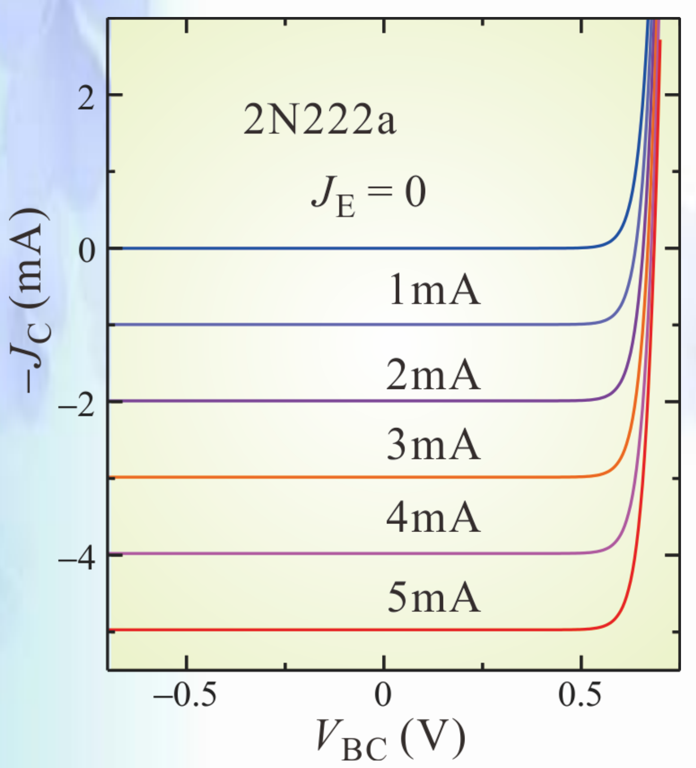


NPN type

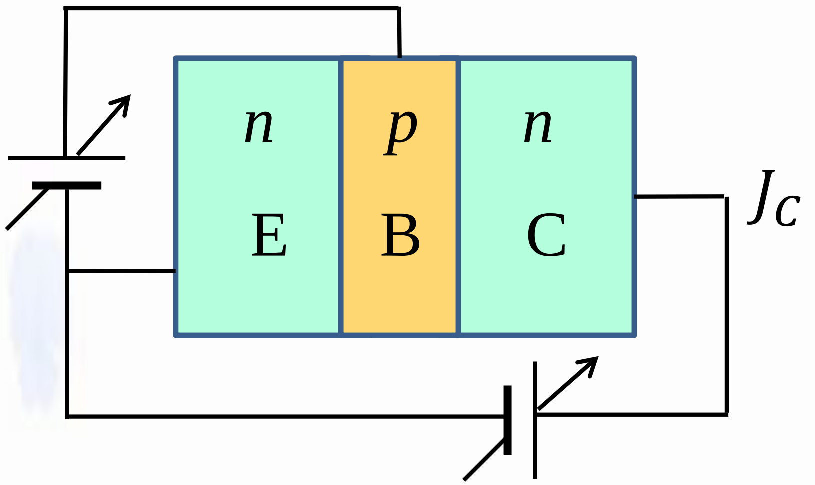
Base-Collector, Collector-Emitter characteristics

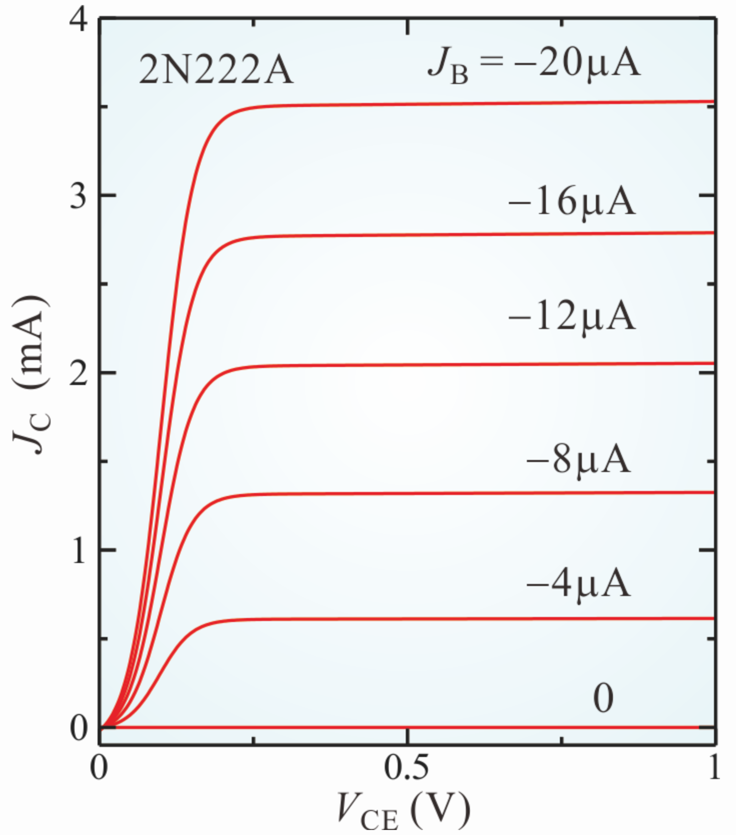
Base-Collector

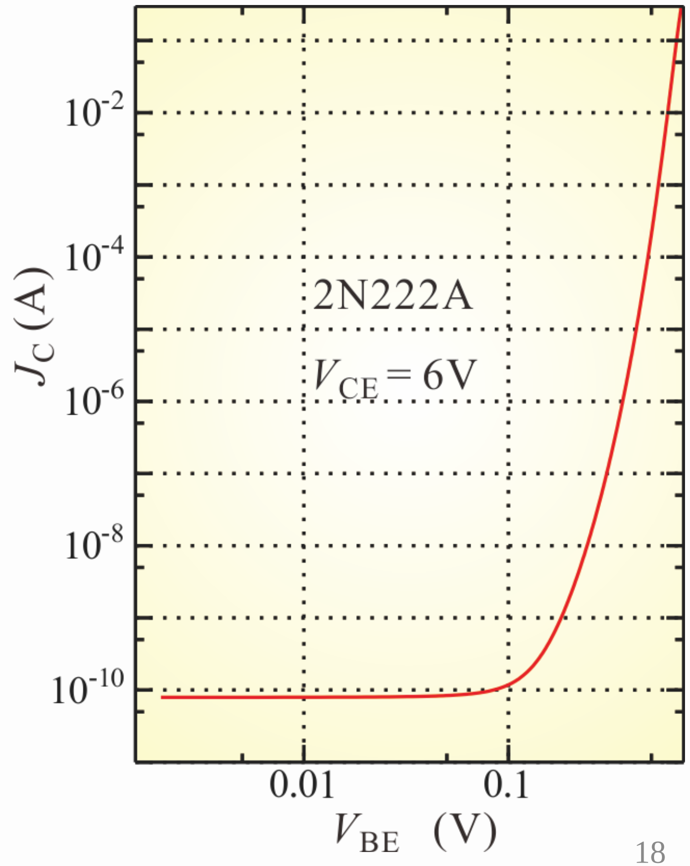




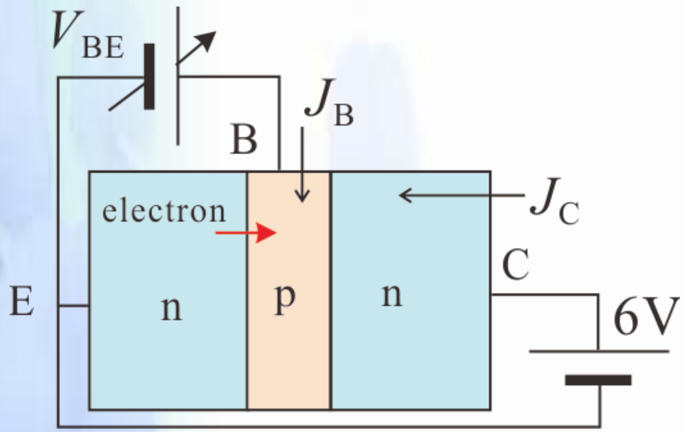
Collector-Emitter

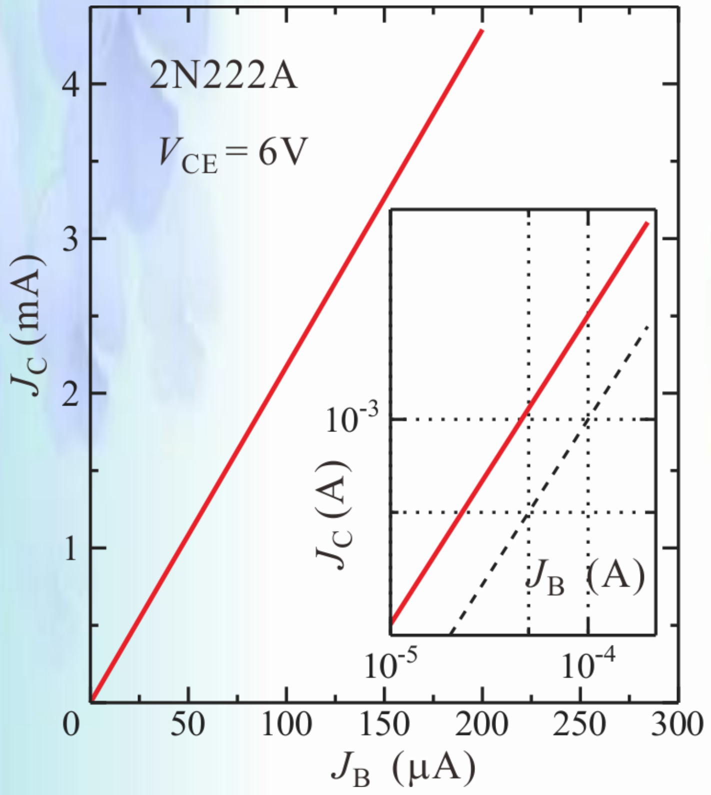






Current amplification: Linearization with quantity selection

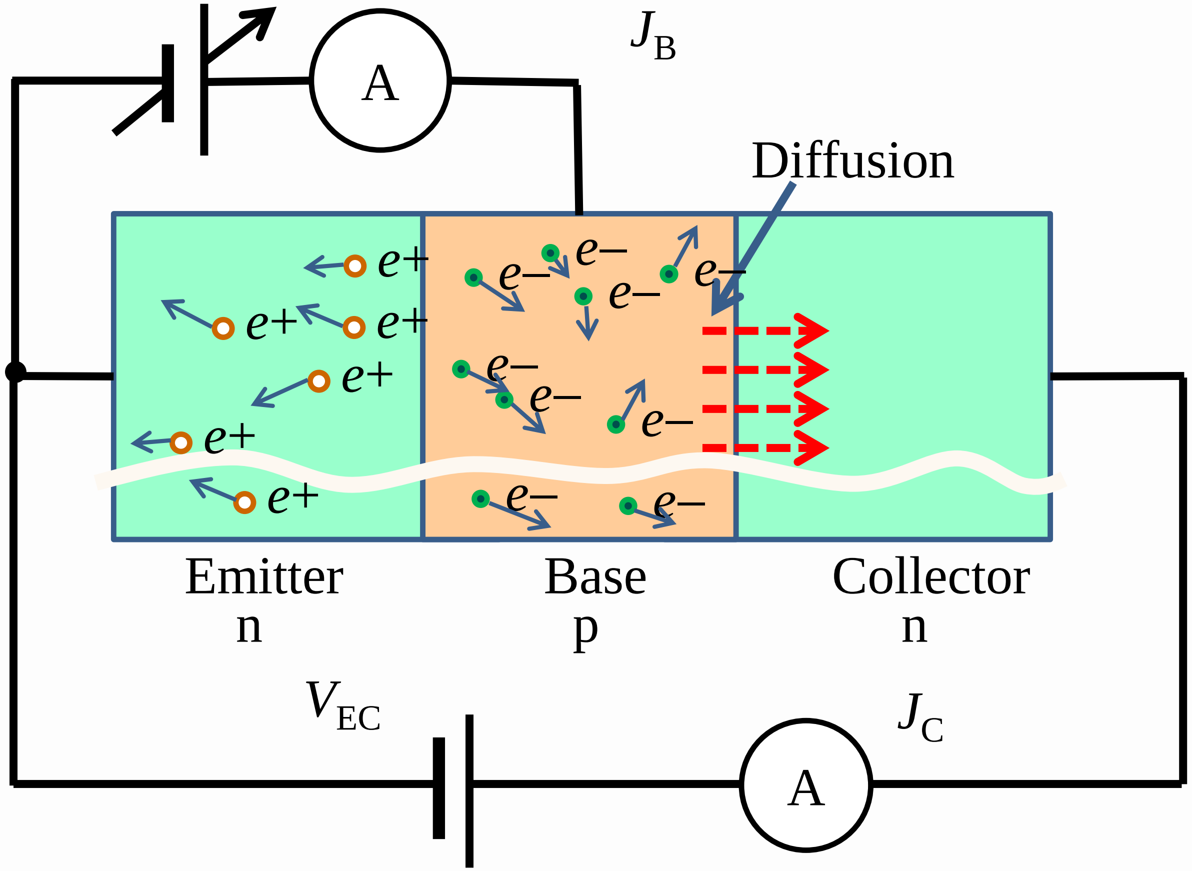




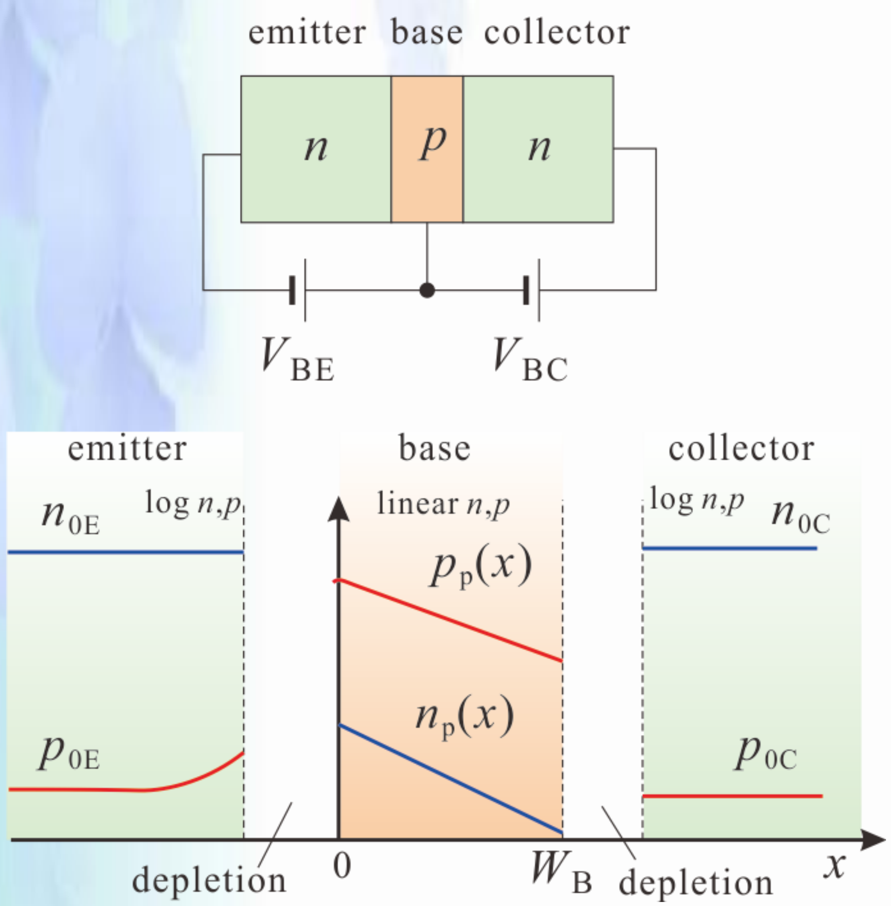
$$J_C = h_{FE} \, J_B$$

Emitter-common current gain

How a bipolar transistor amplifies signal?



Expression of h_{FE}



Sweeping out of minority carriers at the depletion edge $\quad n_p(W_{\mathrm{B}}) = n_{p0}\exp\dfrac{-eV_{\mathrm{BC}}}{k_{\mathrm{B}}T} \approx 0$

Diffusion current in the base: constant $\quad \dfrac{dn_p}{dx}$: constant $\quad n_p(x)$: linear in x

Device cross section A $\quad j_{\mathrm{D}e} = -D_e\dfrac{dn_p}{dx} \approx eD_e\dfrac{n_p(0)}{W_{\mathrm{B}}} = \dfrac{J_{\mathrm{C}}}{A}$

The law of mass action $\quad n_{p0} \approx \dfrac{n_i^2}{N_{\mathrm{A}}}$

$$J_{\mathrm{C}} \approx \frac{eAD_e n_{p0}}{W_{\mathrm{B}}}\exp\frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T} \approx \frac{eAD_e n_i^2}{W_{\mathrm{B}}N_{\mathrm{A}}}\exp\frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T} \equiv J_{\mathrm{S}}\exp\frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T}$$

$$J_{\mathrm{B}h} = \frac{eAD_h}{L_h}p_{n\mathrm{E}}(0) = \frac{eAD_h}{L_h}p_{n\mathrm{E}0}\exp\frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T} = \frac{eAD_h}{L_h}\frac{n_i^2}{N_{\mathrm{D}}}\exp\frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T}$$

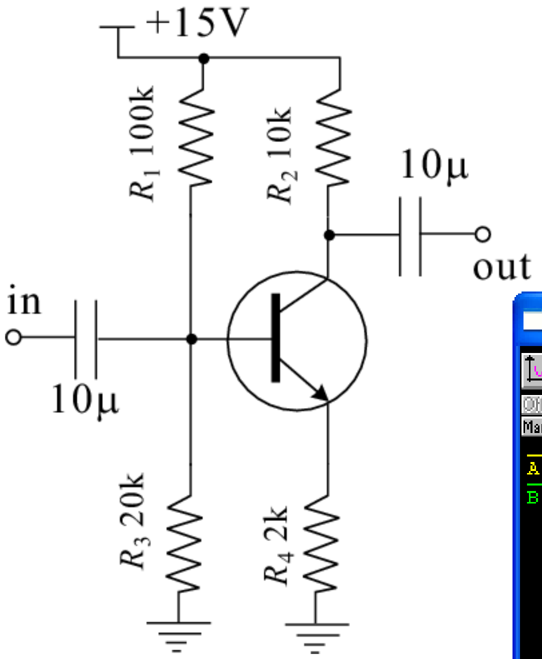
Recombination current: $\quad J_{\mathrm{Br}} = \dfrac{Q_e}{\tau_b} = \dfrac{en_p(0)AW_{\mathrm{B}}}{2\tau_b}\exp\dfrac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T}$

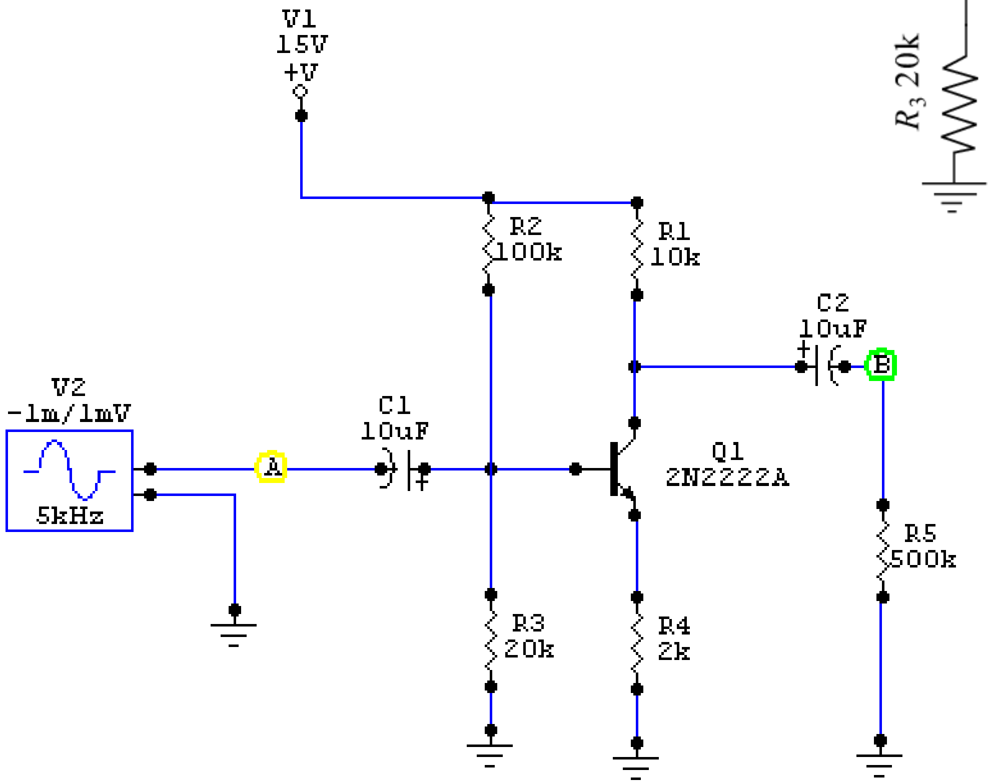
$$h_{\mathrm{FE}} = \left(\frac{D_h}{D_e}\frac{W_{\mathrm{B}}}{L_h}\frac{N_{\mathrm{A}}}{N_{\mathrm{B}}} + \frac{W_{\mathrm{B}}^2}{2\tau_b D_e}\right)^{-1}$$

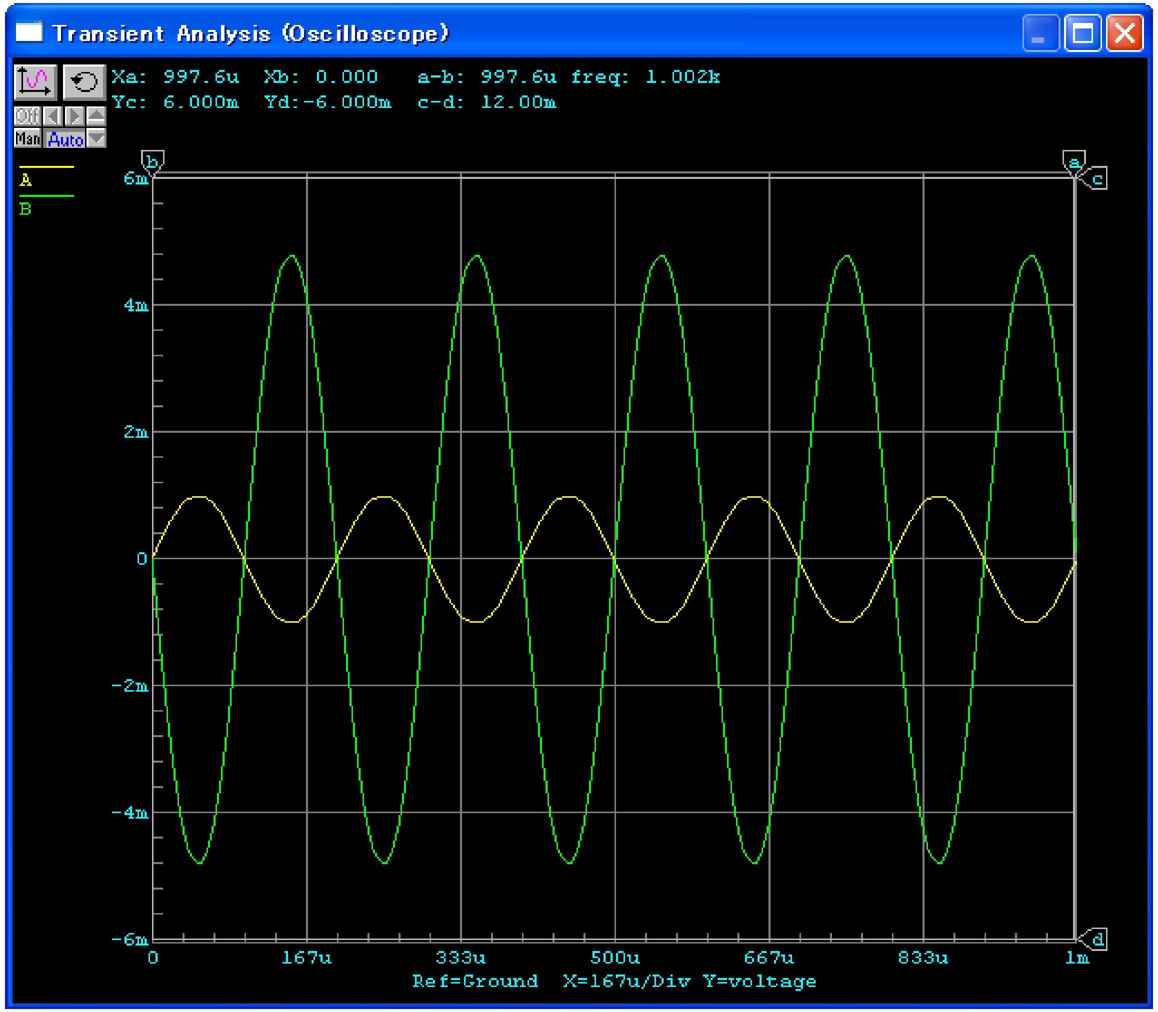
Example of an amplification circuit

$$\Delta V_{\mathrm{C}} = R_2 \Delta J_{\mathrm{C}} \approx R_2 \Delta J_{\mathrm{E}}$$

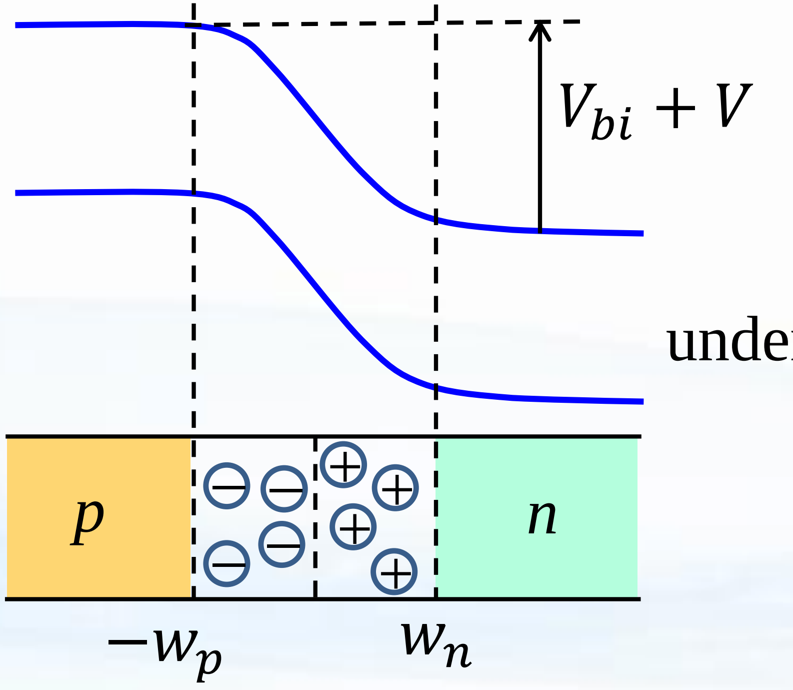
$$= R_2 \frac{\Delta V_{\mathrm{E}}}{R_4} = \frac{R_2}{R_4} \Delta V$$







Depletion layer width with reverse bias voltage



Poisson equation $\frac{d^2\phi}{dx^2} = -aq(x) \quad (a \equiv (\epsilon\epsilon_0)^{-1})$

charge: $\begin{cases} q = -eN_A & (-w_p \leq x \leq 0), \\ q = eN_D & (0 \leq x \leq w_n) \end{cases}$

under conditions

potential boundary: $\begin{cases} \phi(-\infty) = 0 \\ \phi(-w_p) = 0, \quad \left.\frac{d\phi}{dx}\right|_{-w_p} = 0, \\ \phi(w_n) = V + V_{\rm bi}, \quad \left.\frac{d\phi}{dx}\right|_{w_n} = 0 \end{cases}$

$\lim_{x\to+0} \phi = \lim_{x\to-0} \phi,$

$\lim_{x\to+0} (d\phi/dx) =$

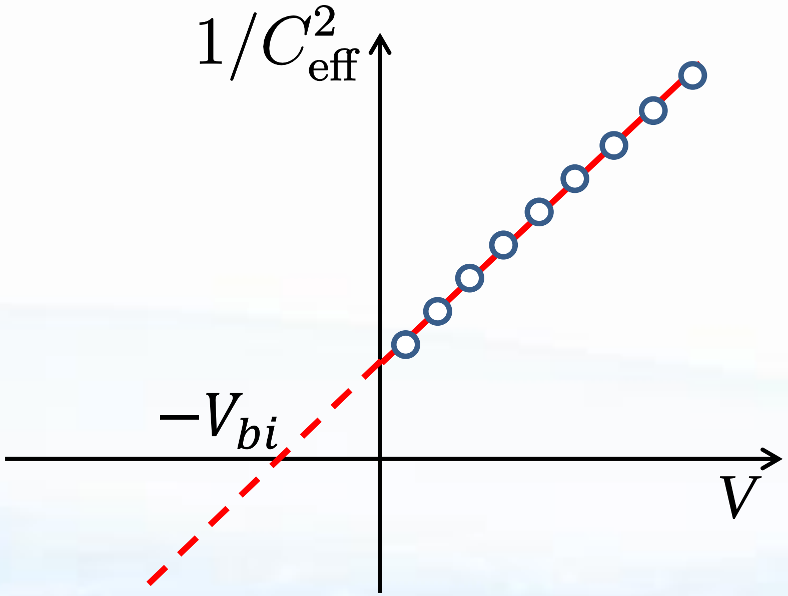
$\lim_{x\to-0} (d\phi/dx)$

The integration gives $\phi(x) = \begin{cases} \frac{aeN_A}{2}(x + w_p)^2 & (-w_p \leq x \leq 0), \\ V + V_{\rm bi} - \frac{aeN_D}{2}(x - w_n)^2 & (0 \leq x \leq w_n) \end{cases}$

$$w_p = \left[\frac{2\epsilon_0\epsilon(V + V_{\rm bi})}{eN_A} \cdot \frac{N_D}{N_D + N_A}\right]^{1/2}, \quad w_n = \left[\frac{2\epsilon_0\epsilon(V + V_{\rm bi})}{eN_D} \cdot \frac{N_A}{N_D + N_A}\right]^{1/2}$$

$$w_d = w_p + w_n = \left[\frac{2\epsilon_0\epsilon(V + V_{\rm bi})}{e} \cdot \frac{N_A + N_D}{N_A N_D}\right]^{1/2}.$$

Effective capacitance and reverse bias voltage



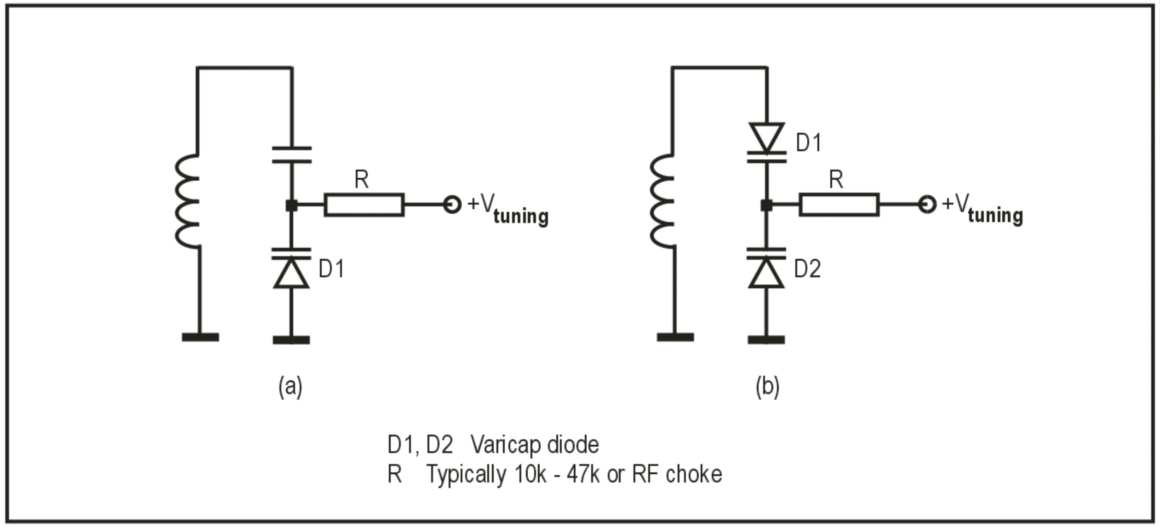
$$\frac{1}{C_{\rm eff}^2} = \frac{2}{\epsilon\epsilon_0 e N_{\rm D}}(V + V_{\rm bi})$$

This gives a way for the doping profiling.

Varicap diode

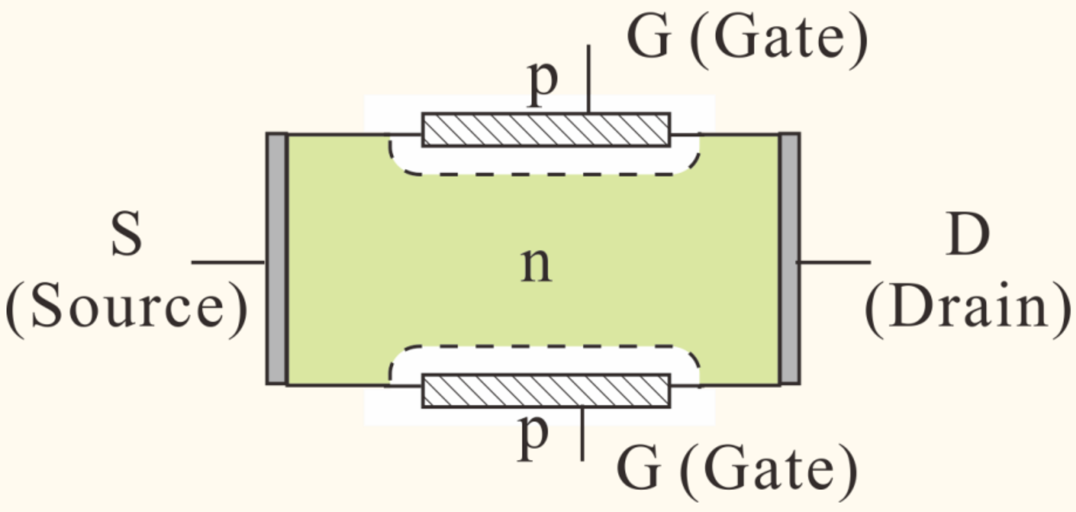
KB505

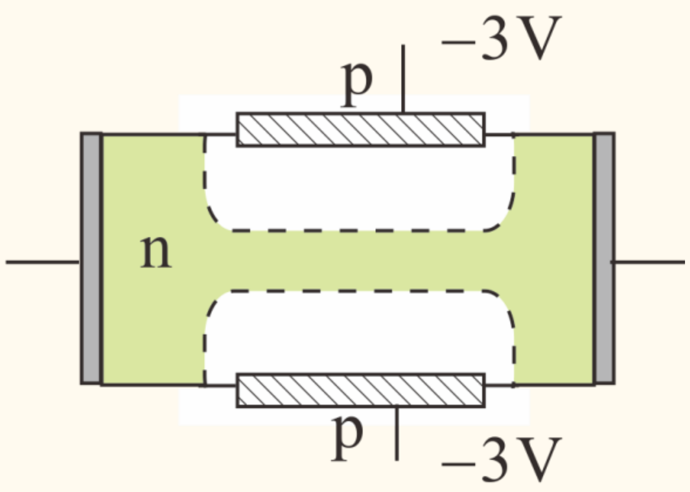
circuit example



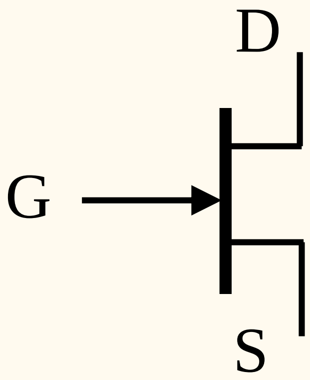
Frequency modulation
Phase lock loop

pn junction field effect transistor (JFET)

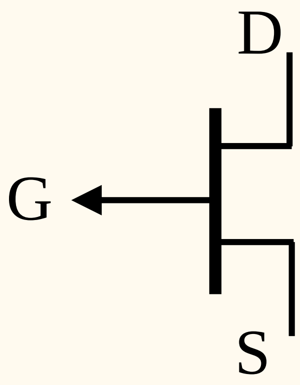




Circuit symbols

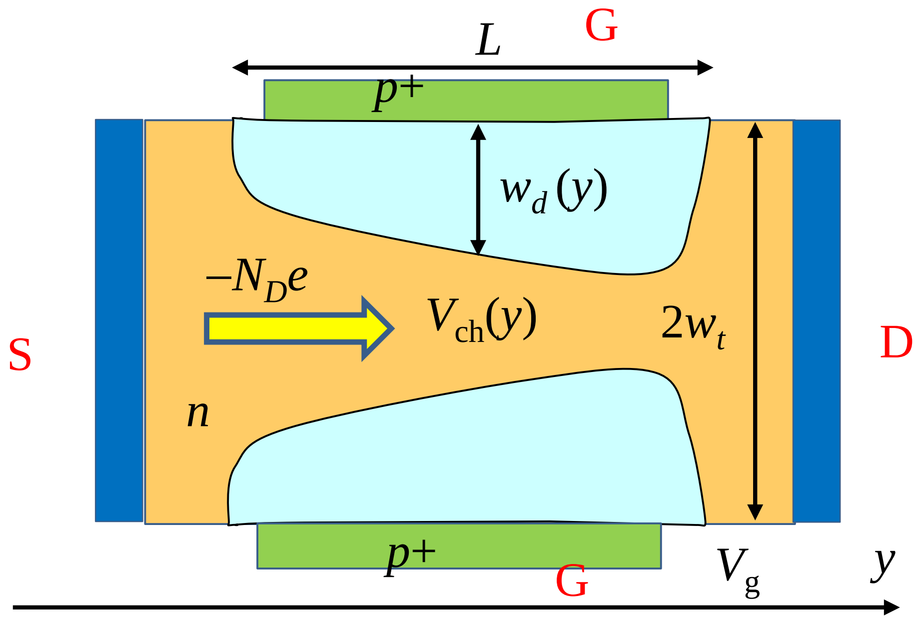


n-channel



p-channel

pn junction FET



$$V(y) = V_g + V_{bi} - V_{ch}(y)$$

$$w_d(y) = \sqrt{\frac{2\epsilon\epsilon_0 V(y)}{eN_D}}$$

$$J_{ch} = eN_D\mu_n \frac{dV_{ch}}{dy} \cdot 2[w_t - w_d(y)]W$$

conductivity — electric field — channel width

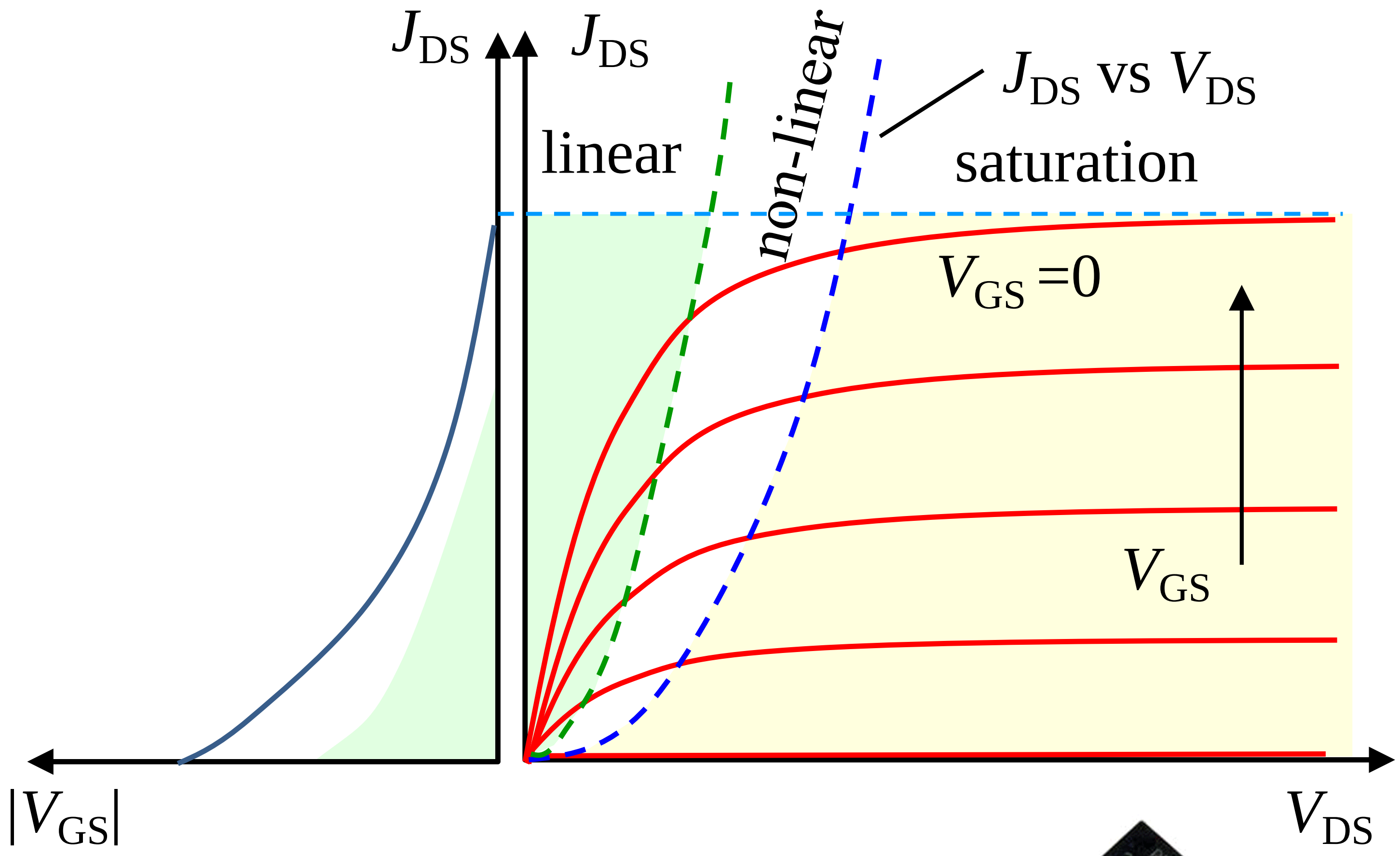
$$J_{ch}L = \int_0^L J_{ch}dy = 2eN_D\mu_n W \int_0^L (w_t - w_d)\frac{dV}{dy}dy = 2w_t eN_D\mu_n W \int_{V_0}^{V_L} \left(1 - \frac{w_d}{w_t}\right) dV$$

pinch off (internal) voltage: $w_d(V_c) = w_t \quad V_c = \frac{eN_D w_t^2}{2\epsilon\epsilon_0}$

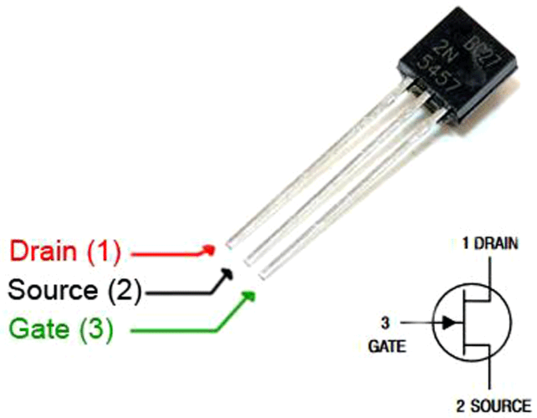
$$J_{ch} = \frac{2N_D e\mu_n W w_t}{L}\left[V_L - V_0 + \frac{2}{3\sqrt{V_c}}(V(V_0)^{3/2} - V(V_L)^{3/2})\right]$$

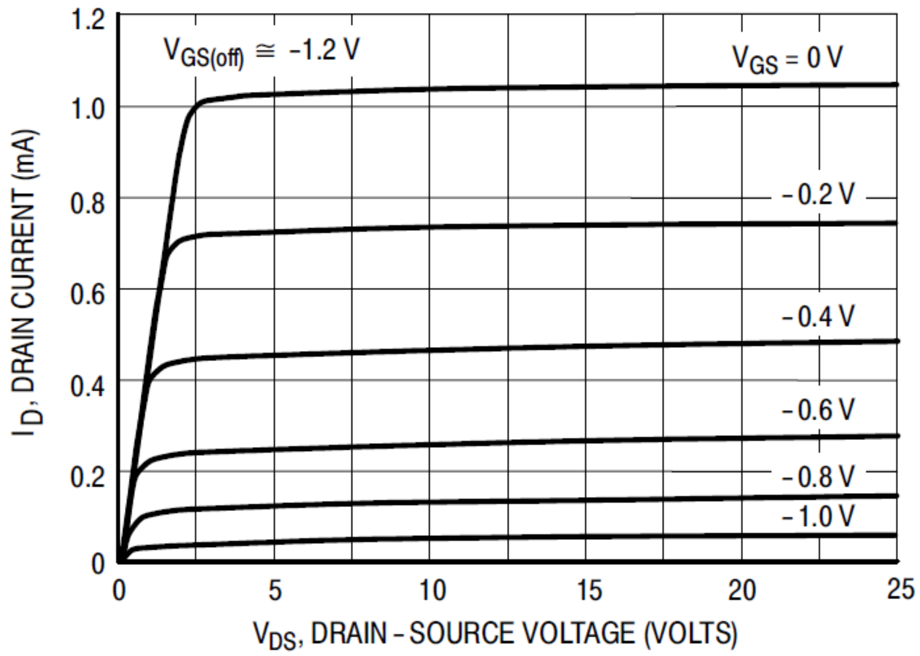
Only valid for $w_d < w_t/2$.

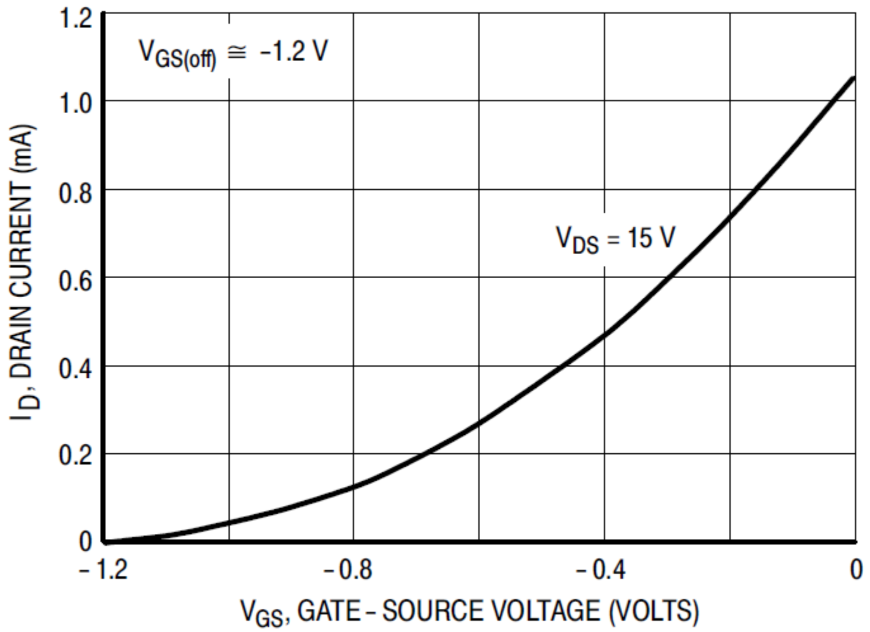
I-V characteristics of JFET



Example: 2N5457
n-channel
depletion-type





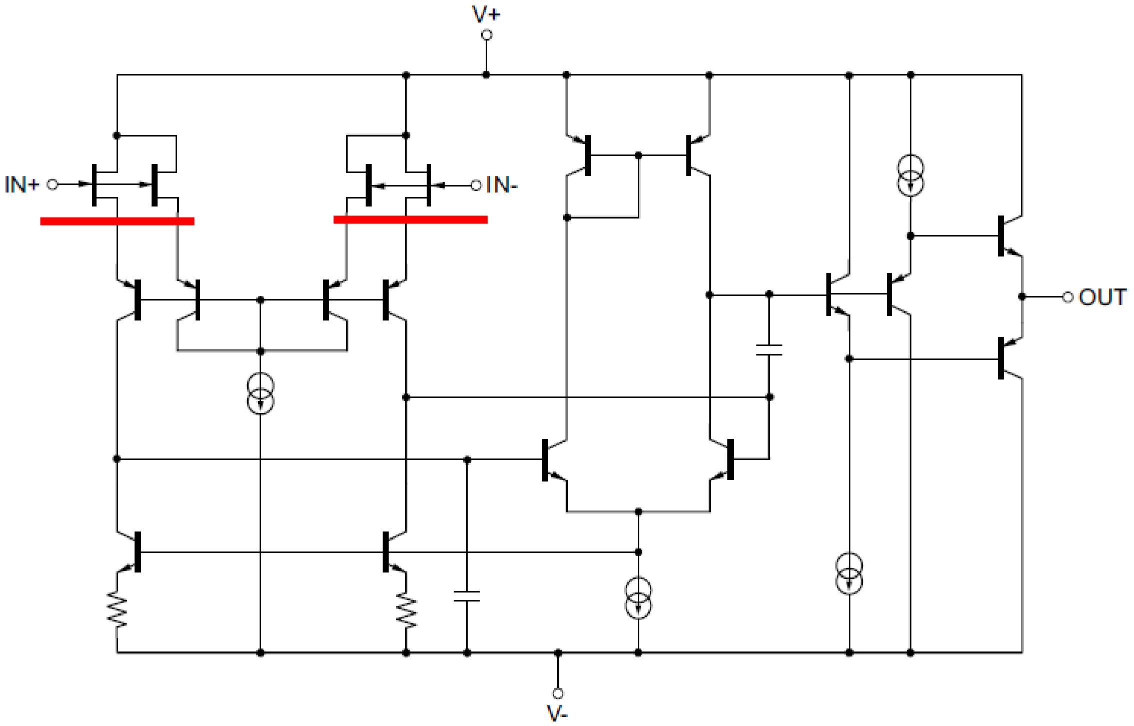


Low linearity → linearization with feedback with high gain

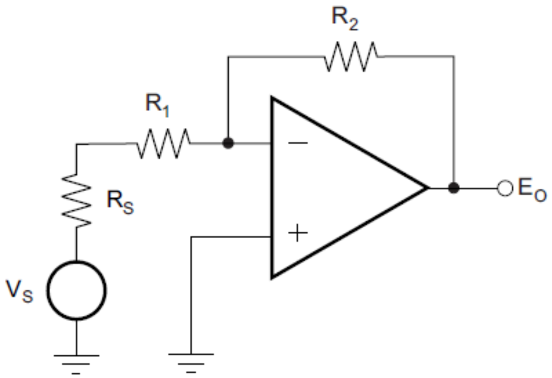
High input impedance, low bias current (operation at the reverse bias region)

: fit the input stage of operational amplifier

Example: OPA827



- Input voltage noise: 4 nV/$\sqrt{\text{Hz}}$ at 1 kHz
- Input bias current 10 pA max
- Input impedance 10^{13} Ω



Inverting amplifier

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.6.02 Lecture 08

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Chapter 6 Homo and hetero junctions

pn homo junctions

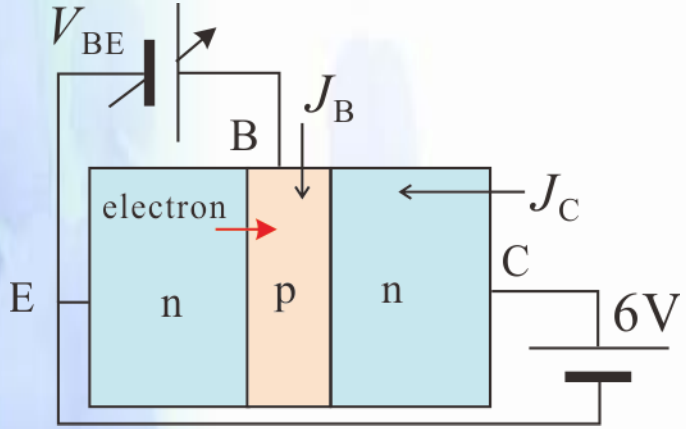
Solar cells

Bipolar transistors

John Bardeen, William Shockley, Walter Brattain 1948 Bell Labs.

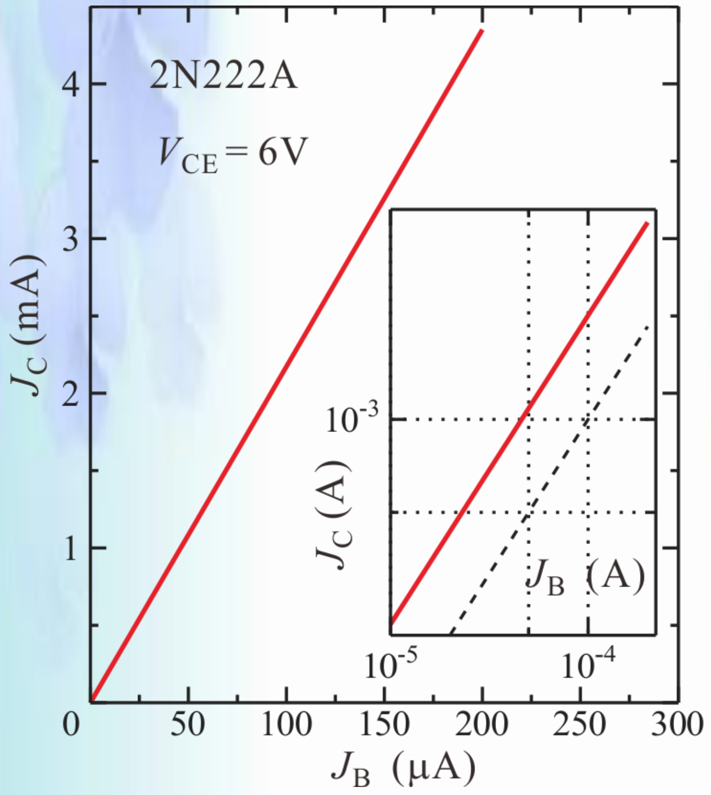
Gerald Pearson, Daryl Chapin and Calvin Fuller at Bell labs. 1954

Current amplification: Linearization with quantity selection

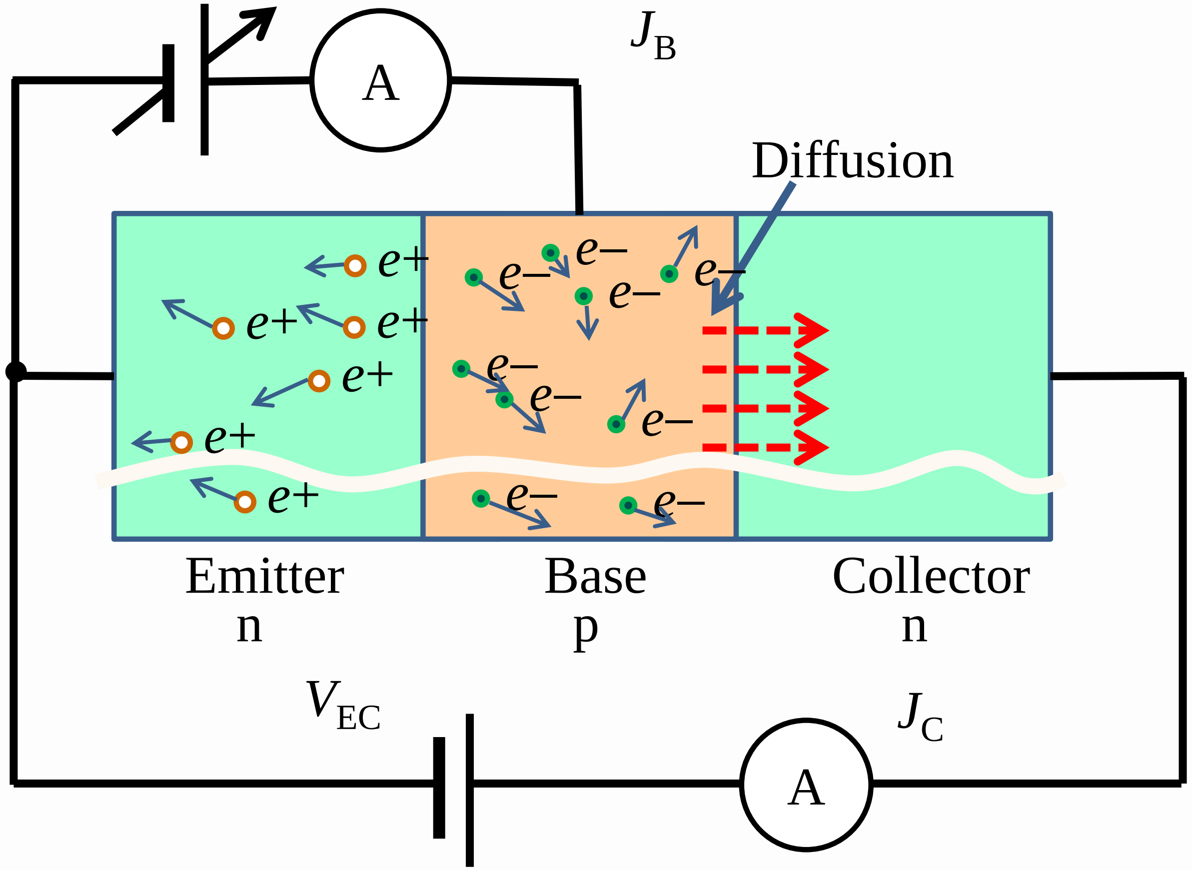


$$J_C = h_{FE}\,J_B$$

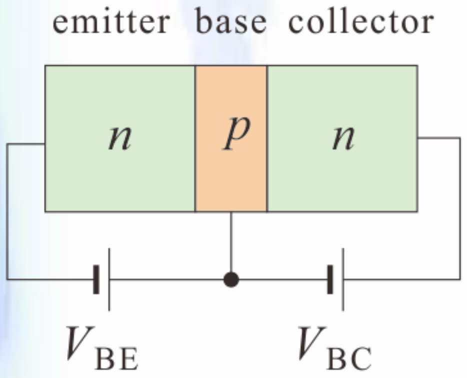
Emitter-common current gain

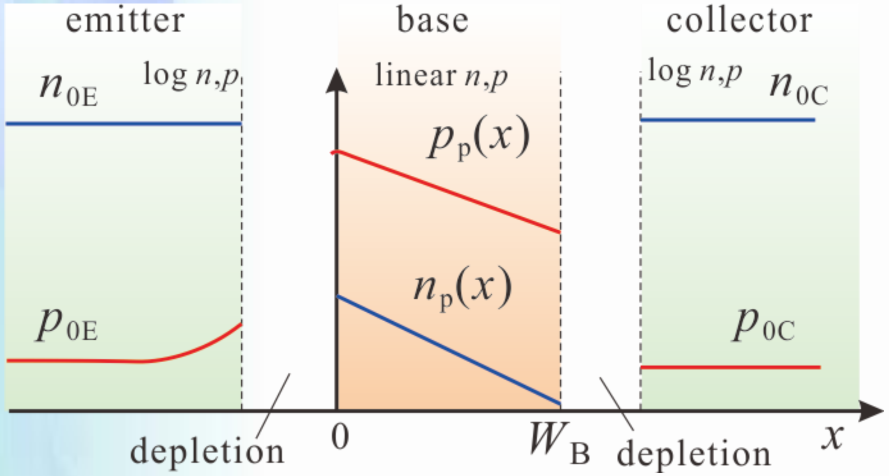


How a bipolar transistor amplifies signal?



Expression of h_{FE}





Sweeping out of minority carriers at the depletion edge $\quad n_p(W_{\mathrm{B}}) = n_{p0} \exp \frac{-eV_{\mathrm{BC}}}{k_{\mathrm{B}}T} \approx 0$

Diffusion current in the base: constant $\quad \frac{dn_p}{dx}$: constant $\quad n_p(x)$: linear in x

Device cross section A $\quad j_{\mathrm{D}e} = -D_e \frac{dn_p}{dx} \approx eD_e \frac{n_p(0)}{W_{\mathrm{B}}} = \frac{J_{\mathrm{C}}}{A}$

The law of mass action $\quad n_{p0} \approx \frac{n_i^2}{N_{\mathrm{A}}}$

$$J_{\mathrm{C}} \approx \frac{eAD_e n_{p0}}{W_{\mathrm{B}}} \exp \frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T} \approx \frac{eAD_e n_i^2}{W_{\mathrm{B}} N_{\mathrm{A}}} \exp \frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T} \equiv J_{\mathrm{S}} \exp \frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T}$$

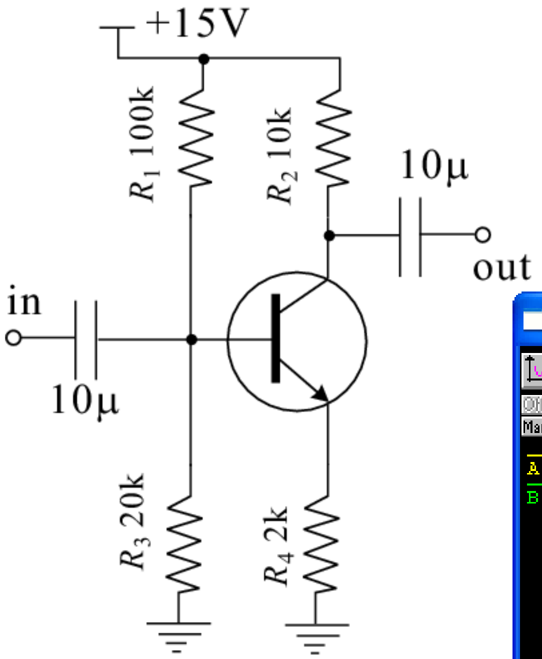
$$J_{\mathrm{B}h} = \frac{eAD_h}{L_h} p_{n\mathrm{E}}(0) = \frac{eAD_h}{L_h} p_{n\mathrm{E}0} \exp \frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T} = \frac{eAD_h}{L_h} \frac{n_i^2}{N_{\mathrm{D}}} \exp \frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T}$$

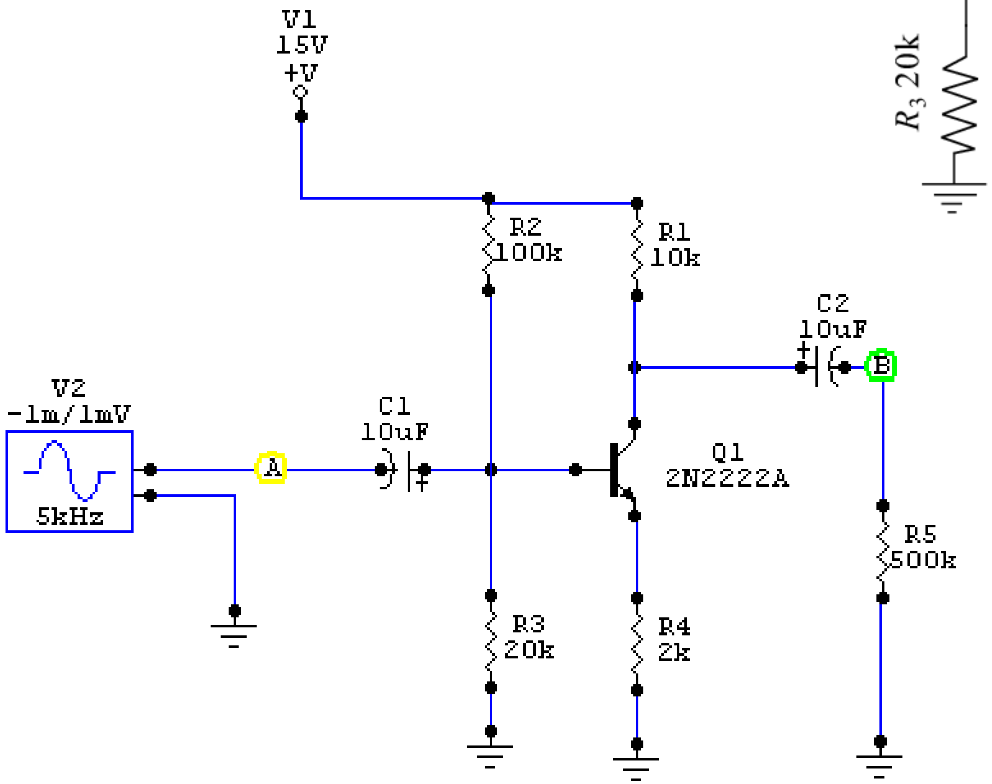
Recombination current: $\quad J_{\mathrm{Br}} = \frac{Q_e}{\tau_b} = \frac{en_p(0)AW_{\mathrm{B}}}{2\tau_b} \exp \frac{eV_{\mathrm{BE}}}{k_{\mathrm{B}}T}$

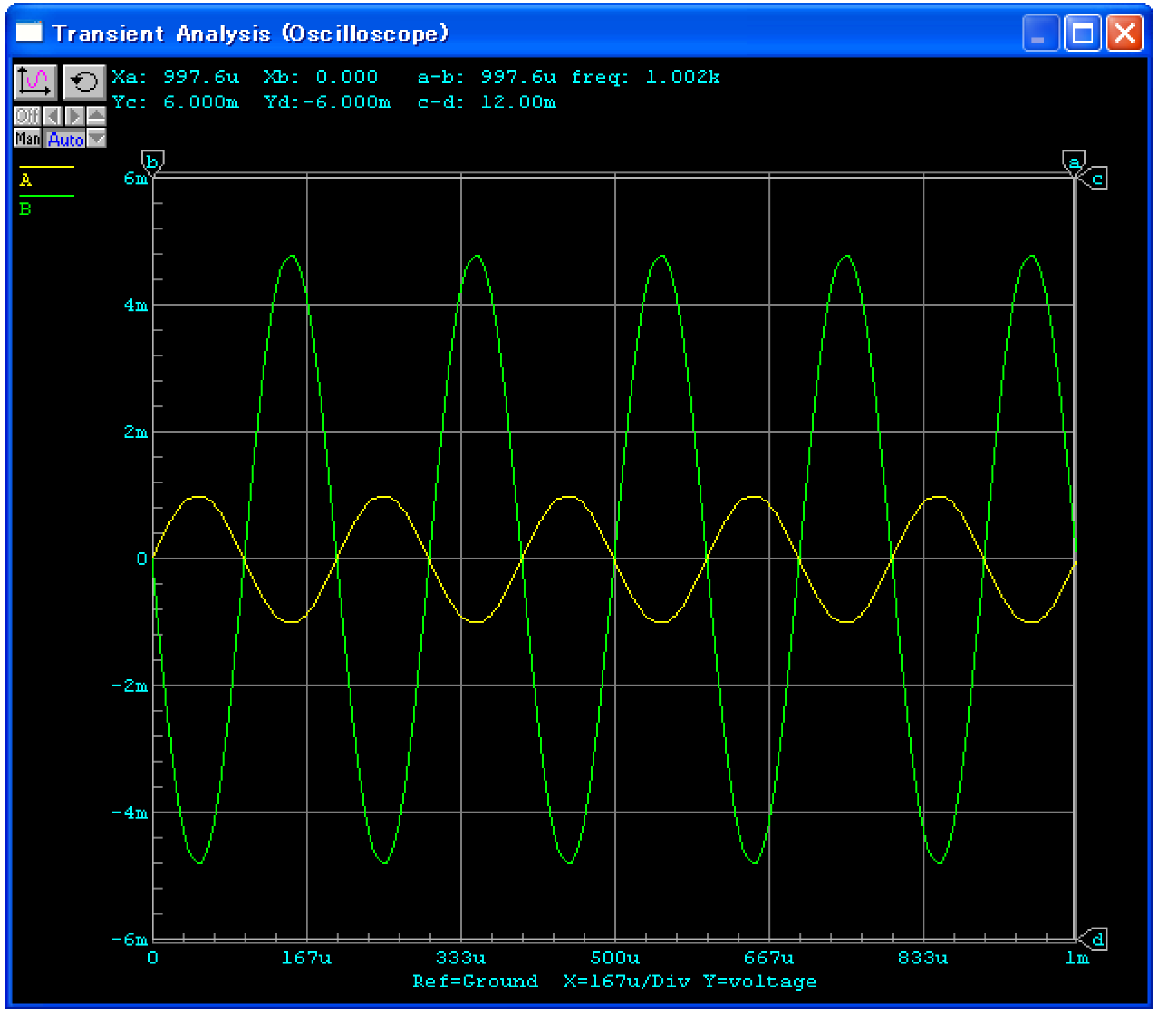
$$h_{\mathrm{FE}} = \left(\frac{D_h}{D_e} \frac{W_{\mathrm{B}}}{L_h} \frac{N_{\mathrm{A}}}{N_{\mathrm{B}}} + \frac{W_{\mathrm{B}}^2}{2\tau_b D_e} \right)^{-1}$$

Example of an amplification circuit

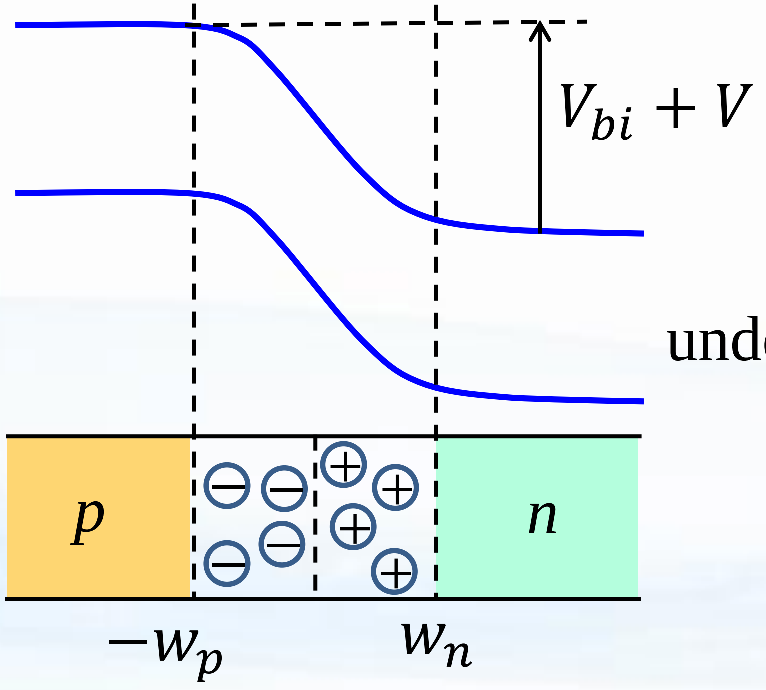
$$\Delta V_C = R_2 \Delta J_C \approx R_2 \Delta J_E$$
$$= R_2 \frac{\Delta V_E}{R_4} = \frac{R_2}{R_4} \Delta V$$







Depletion layer width with reverse bias voltage



Poisson equation $$\frac{d^2\phi}{dx^2}=-aq(x)\quad (a\equiv(\epsilon\epsilon_0)^{-1})$$

charge: $$\begin{cases} q=-eN_A & (-w_p\le x\le 0),\\ q=eN_D & (0\le x\le w_n) \end{cases}$$

under conditions

potential boundary: $$\begin{cases} \phi(-\infty)=0 \\ \phi(-w_p)=0, \quad \left.\dfrac{d\phi}{dx}\right|_{-w_p}=0, \\ \phi(w_n)=V+V_{\rm bi}, \quad \left.\dfrac{d\phi}{dx}\right|_{w_n}=0 \end{cases}$$

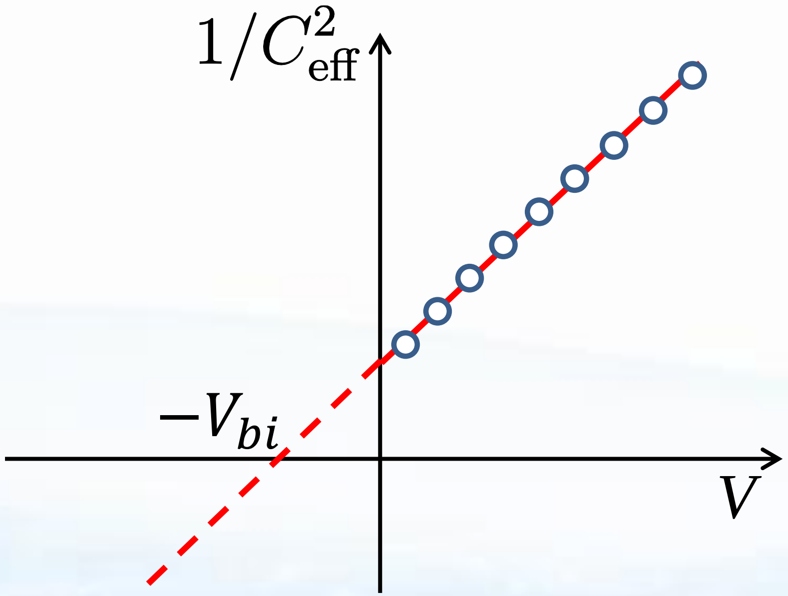
The integration gives $$\phi(x)=\begin{cases} \dfrac{aeN_A}{2}(x+w_p)^2 & (-w_p\le x\le 0),\\ V+V_{\rm bi}-\dfrac{aeN_D}{2}(x-w_n)^2 & (0\le x\le w_n) \end{cases}$$

$$\lim_{x\to+0}\phi=\lim_{x\to-0}\phi,$$
$$\lim_{x\to+0}(d\phi/dx)=$$
$$\lim_{x\to-0}(d\phi/dx)$$

$$w_p=\left[\frac{2\epsilon_0\epsilon(V+V_{\rm bi})}{eN_A}\cdot\frac{N_D}{N_D+N_A}\right]^{1/2},\quad w_n=\left[\frac{2\epsilon_0\epsilon(V+V_{\rm bi})}{eN_D}\cdot\frac{N_A}{N_D+N_A}\right]^{1/2}$$

$$w_d=w_p+w_n=\left[\frac{2\epsilon_0\epsilon(V+V_{\rm bi})}{e}\cdot\frac{N_A+N_D}{N_AN_D}\right]^{1/2}.$$

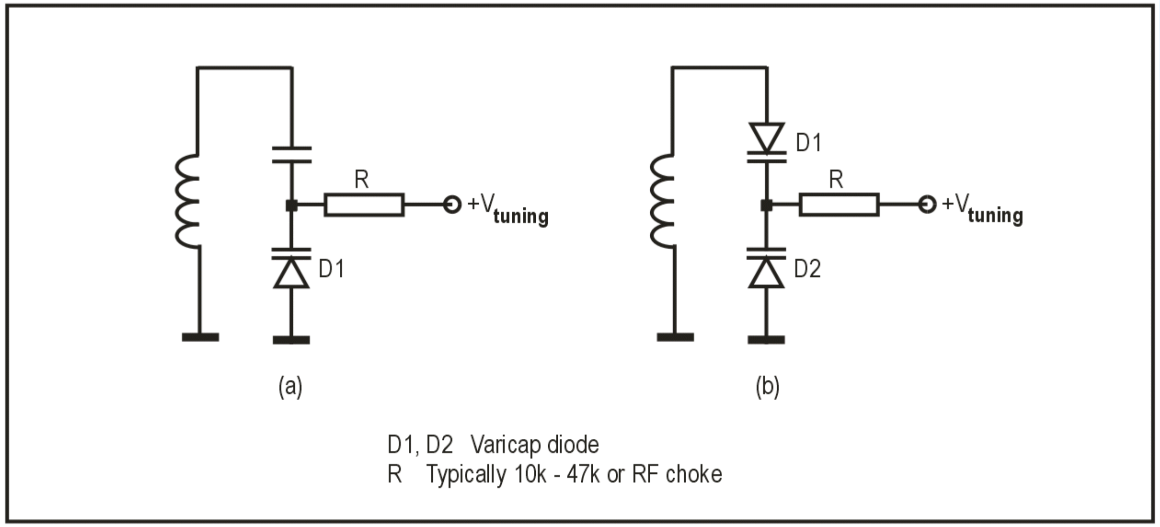
Effective capacitance and reverse bias voltage



$$\frac{1}{C_{\text{eff}}^2} = \frac{2}{\epsilon\epsilon_0 e N_{\text{D}}}(V + V_{\text{bi}})$$

This gives a way for the doping profiling.

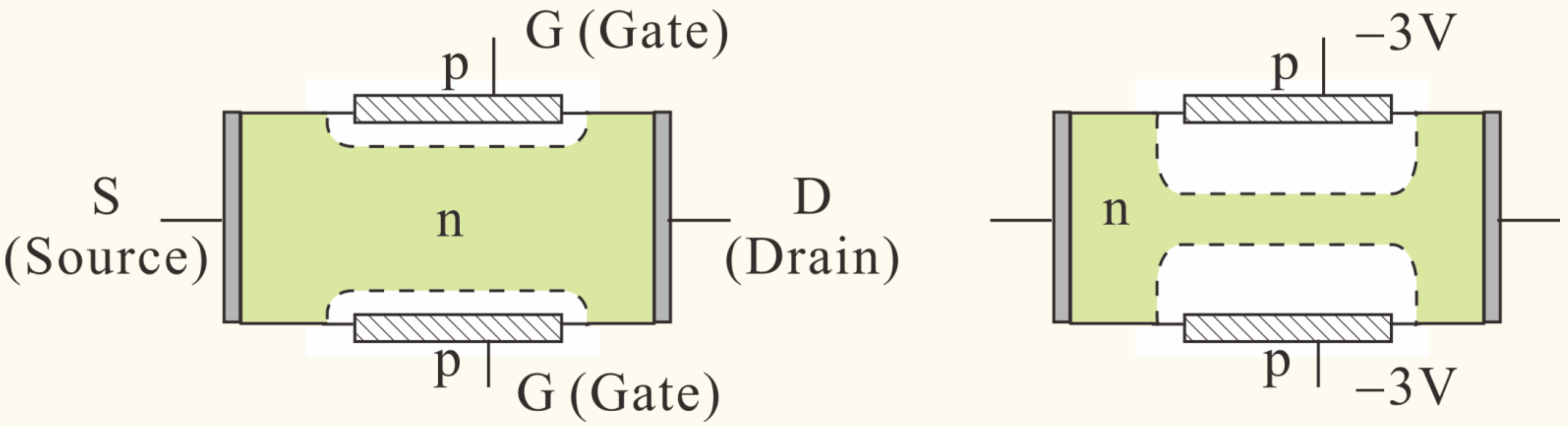
Varicap diode circuit example



KB505

Frequency modulation
Phase lock loop

pn junction field effect transistor (JFET)

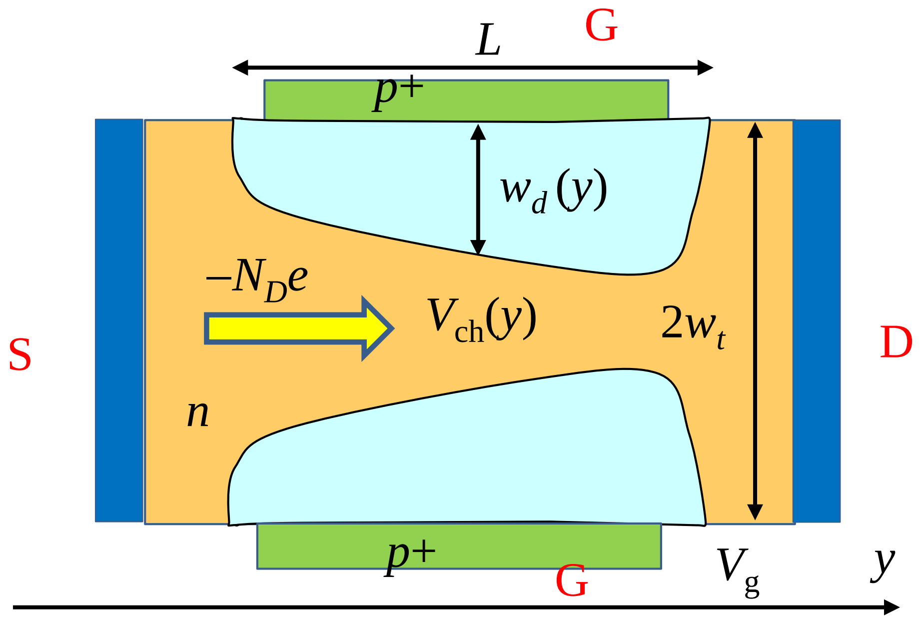


Circuit symbols

n-channel

p-channel

pn junction FET



$$V(y) = V_g + V_{bi} - V_{ch}(y)$$

$$w_d(y) = \sqrt{\frac{2\epsilon\epsilon_0 V(y)}{eN_D}}$$

$$J_{ch} = eN_D\mu_n \frac{dV_{ch}}{dy} \cdot 2[w_t - w_d(y)]W$$

conductivity — electric field — channel width

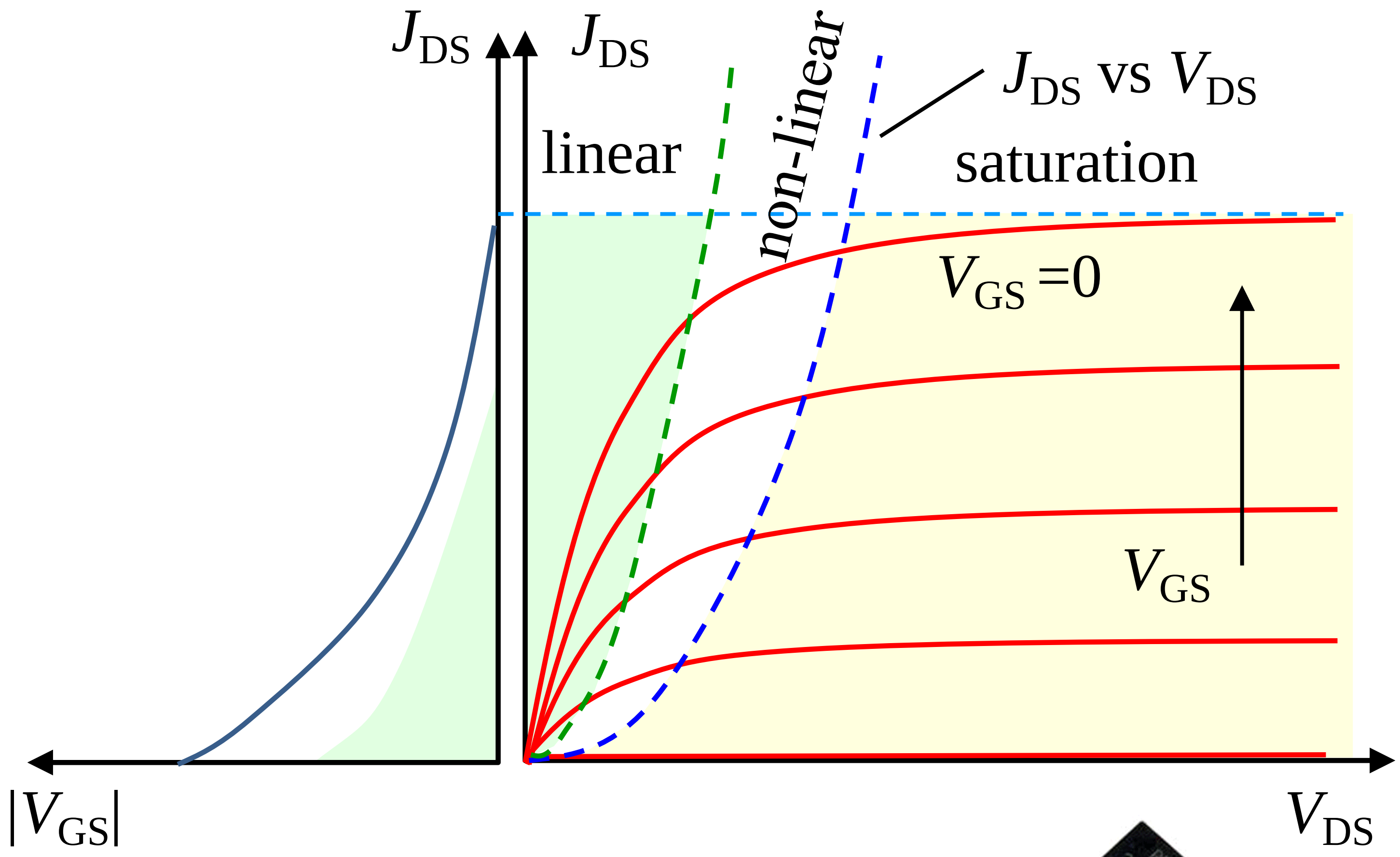
$$J_{ch}L = \int_0^L J_{ch}dy = 2eN_D\mu_n W \int_0^L (w_t - w_d)\frac{dV}{dy}dy = 2w_t eN_D\mu_n W \int_{V_0}^{V_L}\left(1 - \frac{w_d}{w_t}\right)dV$$

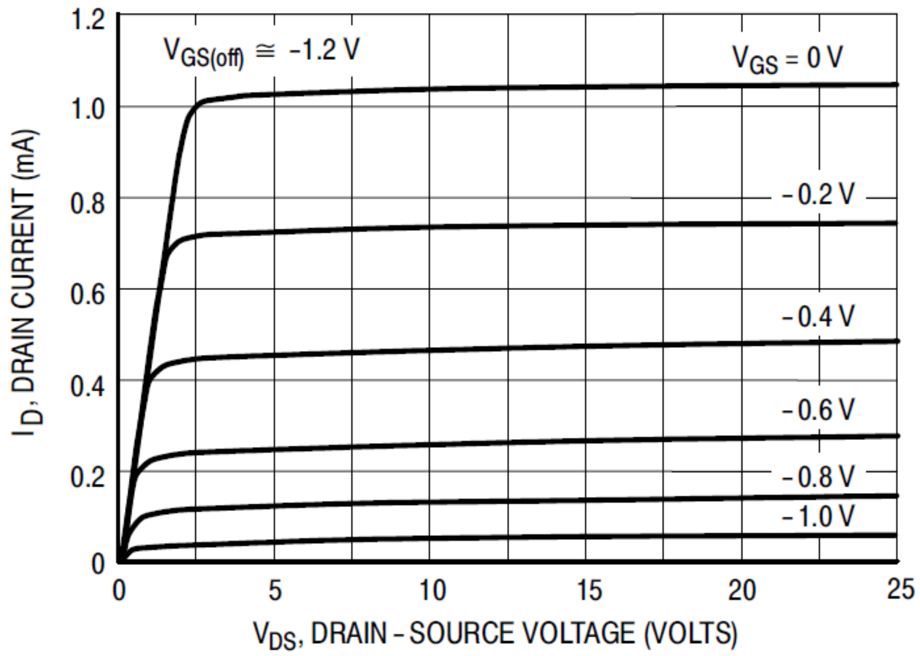
pinch off (internal) voltage: $w_d(V_c) = w_t \quad V_c = \frac{eN_D w_t^2}{2\epsilon\epsilon_0}$

$$J_{ch} = \frac{2N_D e\mu_n W w_t}{L}\left[V_L - V_0 + \frac{2}{3\sqrt{V_c}}(V(V_0)^{3/2} - V(V_L)^{3/2})\right]$$

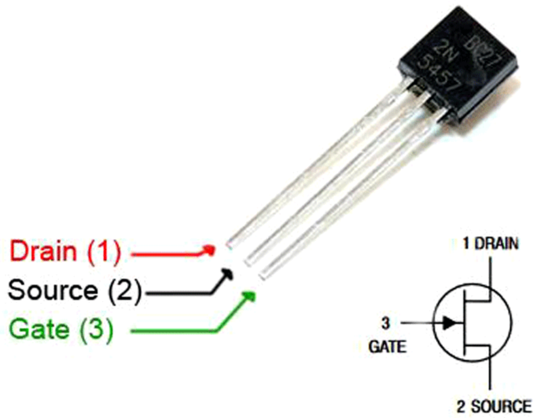
Only valid for $w_d < w_t/2$.

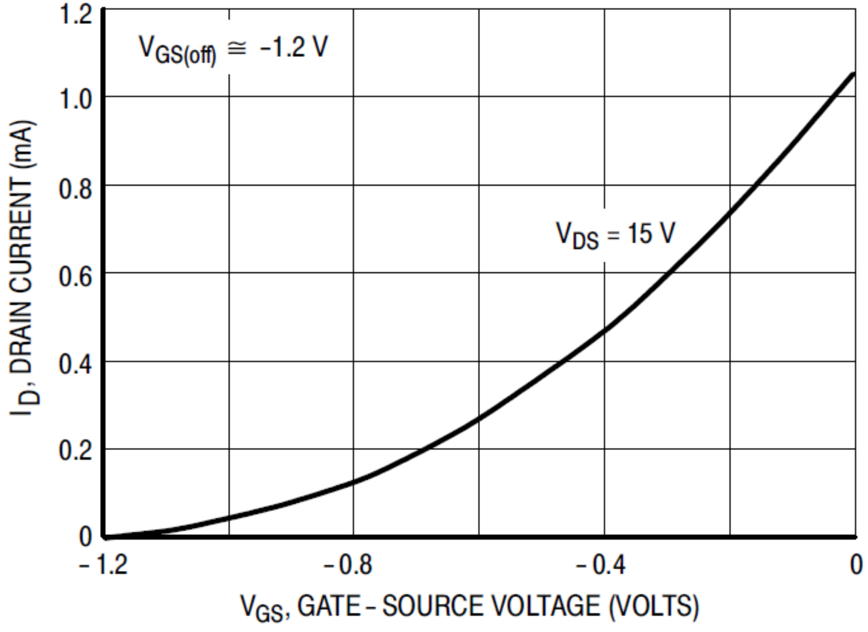
I-V characteristics of JFET





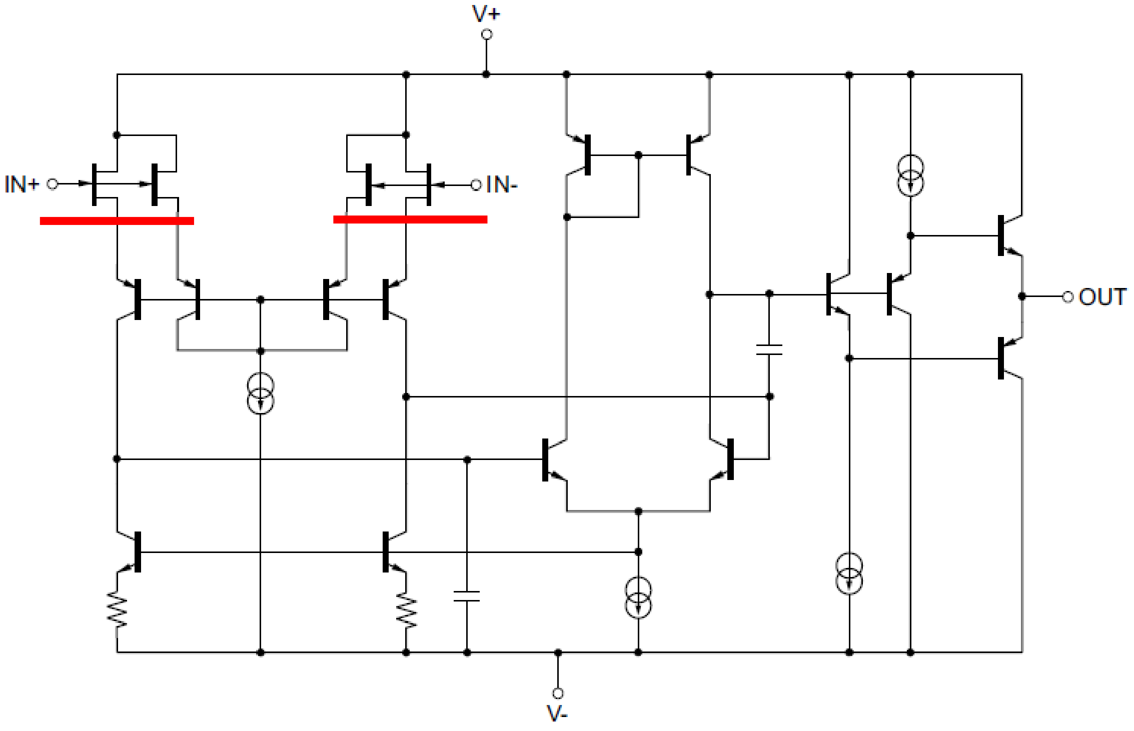
Example: 2N5457
n-channel
depletion-type



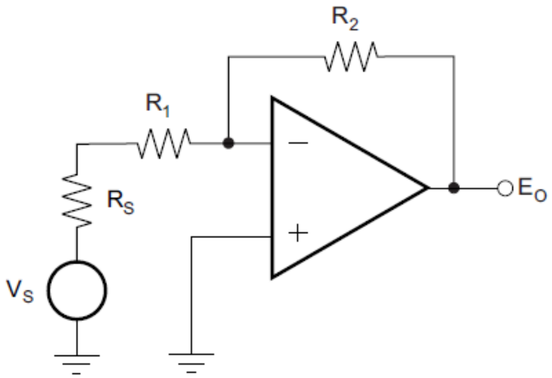


Low linearity → linearization with feedback with high gain
High input impedance, low bias current (operation at the reverse bias region)
: fit the input stage of operational amplifier

Example: OPA827



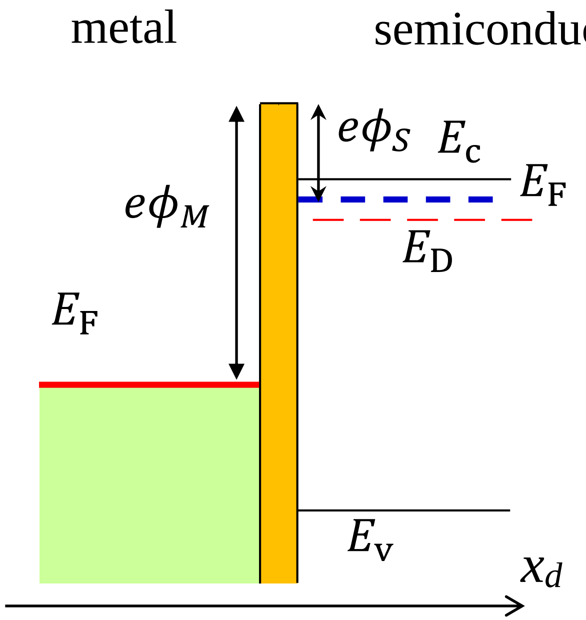
- Input voltage noise: 4 nV/$\sqrt{\text{Hz}}$ at 1 kHz
- Input bias current 10 pA max
- Input impedance 10^{13} Ω



Inverting amplifier

Schottky barrier (metal-semiconductor junction)

Walter Schottky
1886-1976



Q: space charge

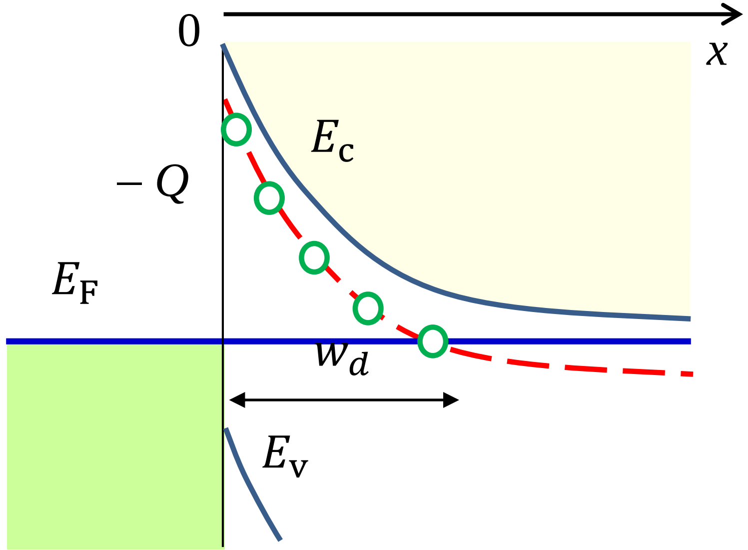
electrostatic potential

$$\phi(x_d) = \int_0^{x_d} (eN_D x - Q)/\epsilon\epsilon_0 dx = \frac{1}{\epsilon\epsilon_0}\left(\frac{eN_D}{2}x_d^2 - Qx_d\right)$$

Charge balance: $w_d = \dfrac{Q}{eN_\mathrm{D}}$ $\qquad \phi_M - \phi_S - \phi(w_d) = 0$

$$Q = \sqrt{2\epsilon\epsilon_0 N_D e(\phi_M - \phi_S)} \qquad \therefore w_d = \sqrt{\frac{2\epsilon\epsilon_0(\phi_M - \phi_S)}{eN_D}} \equiv \sqrt{\frac{2\epsilon\epsilon_0 V_s}{eN_D}}$$

Voltage V --> barrier height $e(V_s - V)$

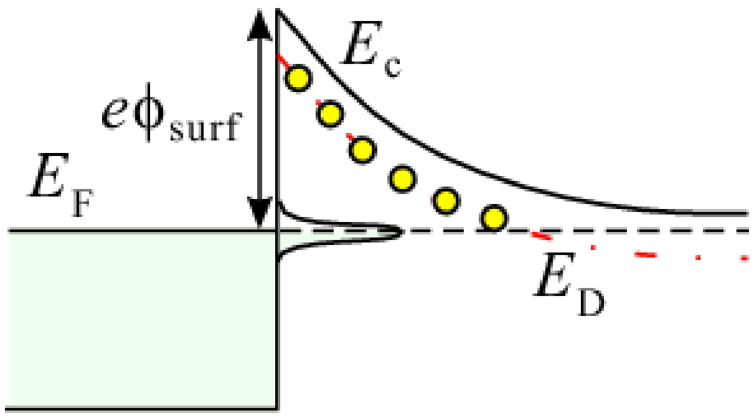


$$J = AT^2\left[\exp\left(\frac{e(V - V_s)}{k_\mathrm{B}T}\right) - \exp\left(\frac{-eV_s}{k_\mathrm{B}T}\right)\right]$$
$$= eAT^2\exp\left(\frac{-eV_s}{k_\mathrm{B}T}\right)\left[\exp\left(\frac{eV}{k_\mathrm{B}T}\right) - 1\right]$$

barrier overcoming current

No minority carrier injection

MES-FET



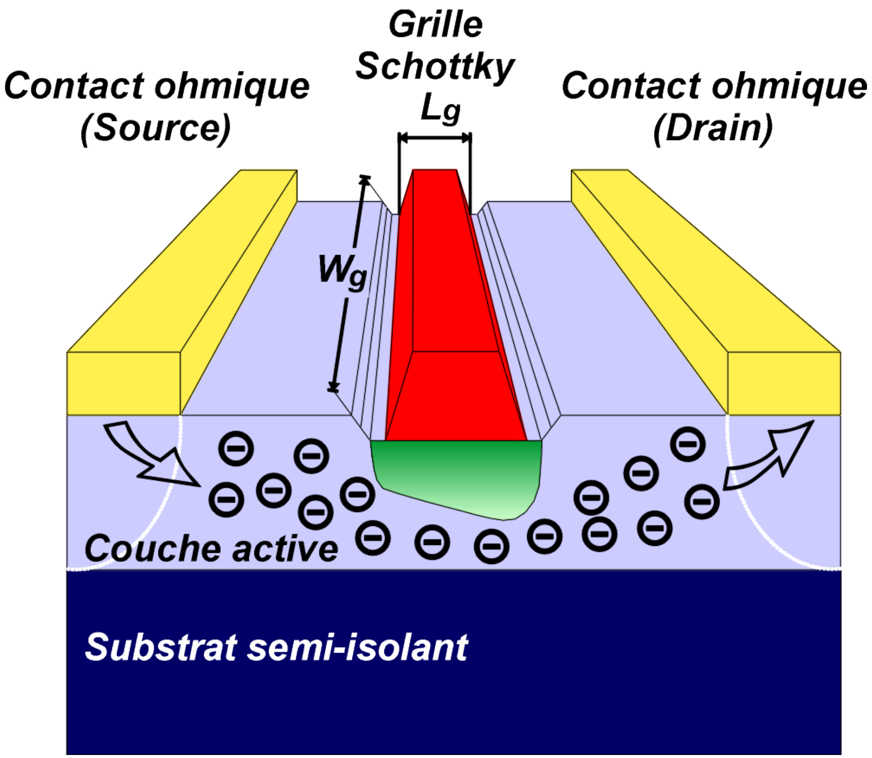
In most cases, the surface barrier is dominated by the pinning of Fermi level with the high density surface states.

MES (metal-semiconductor) FET: depletion layer device.

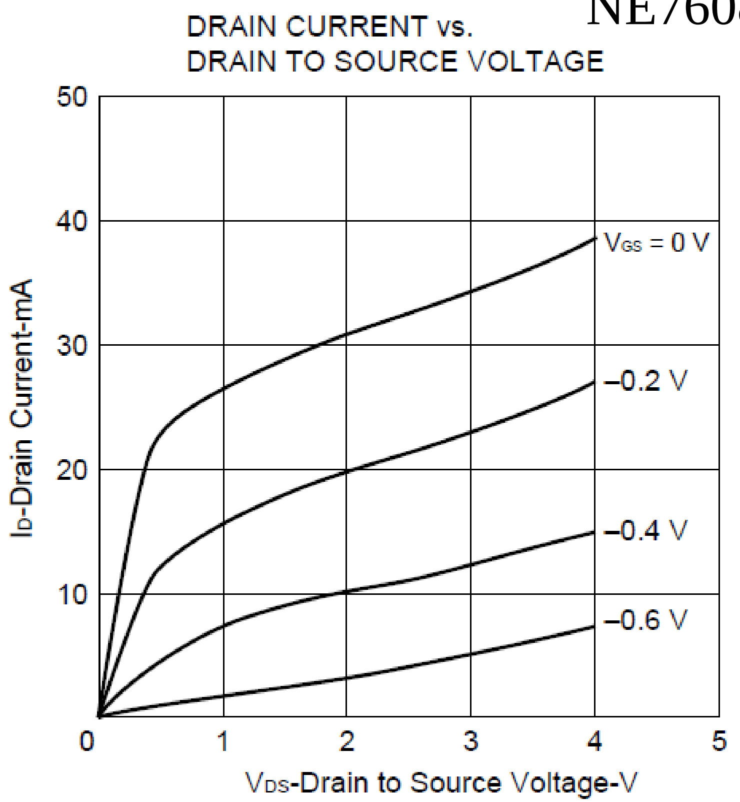
Complementary circuit is difficult.

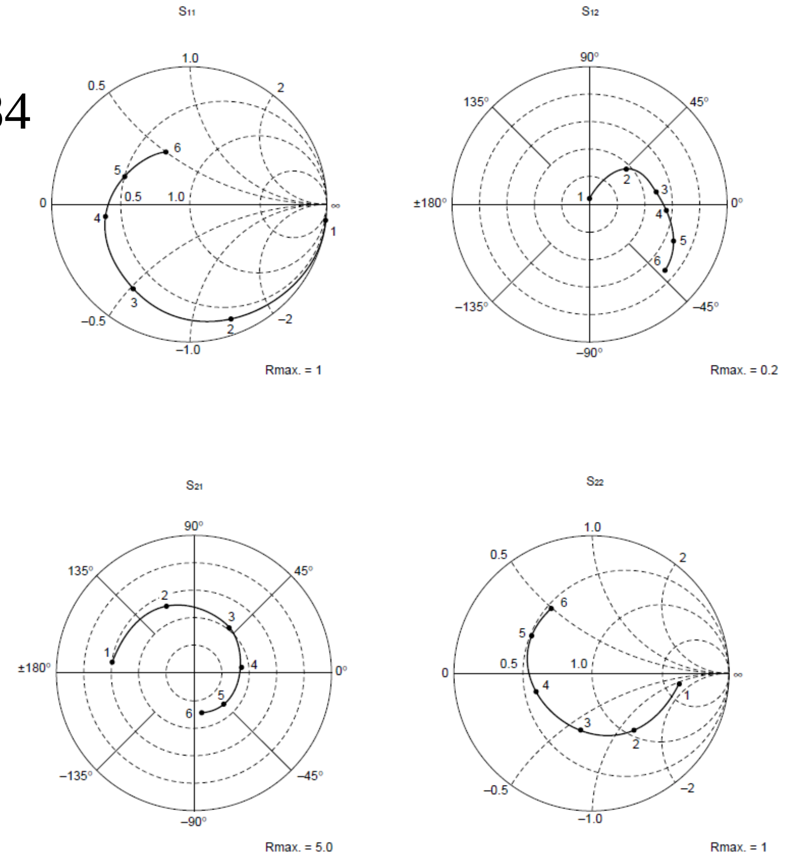
Saturation effect is a bit weak.

Data are given in S-parameters.

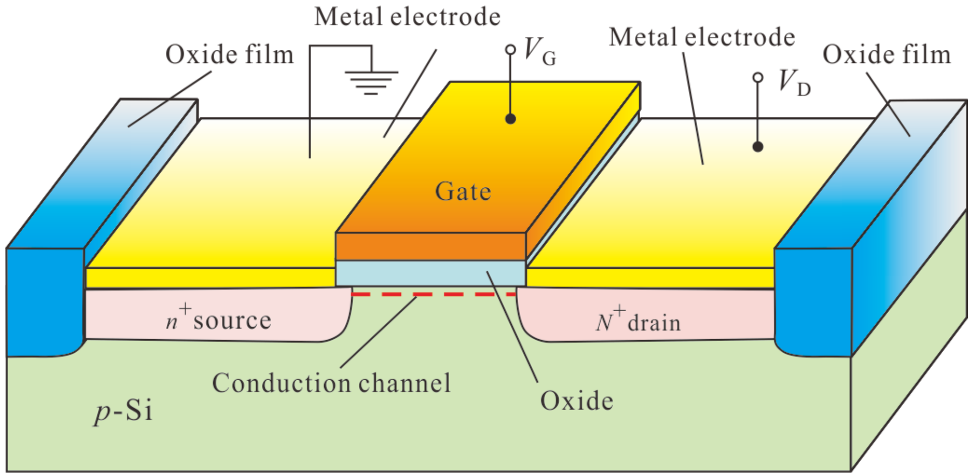


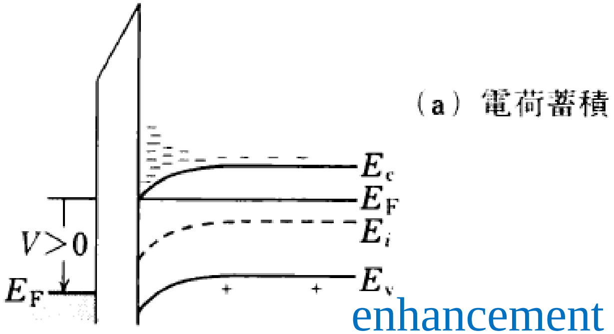
NE76084



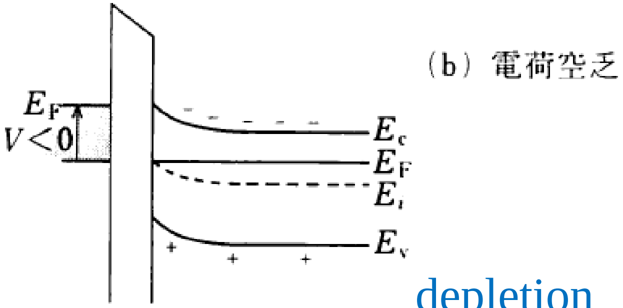


MOS FET

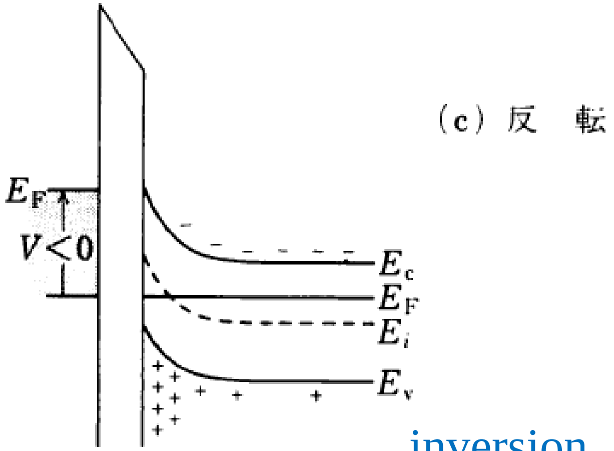




enhancement

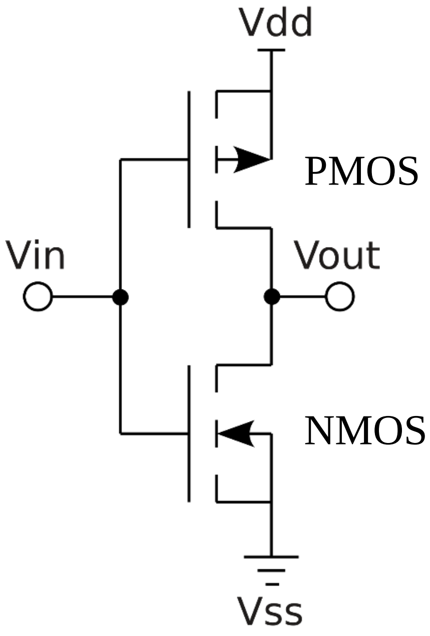


depletion

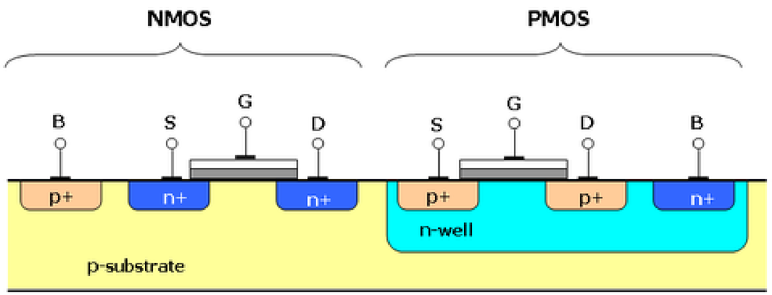


inversion

Complementary metal-oxide-semiconductor (CMOS) circuit



Simplified CMOS inverter circuit



Low leakage current

Single gate input both on/off switch

FinFET

Improvement of MOS FET

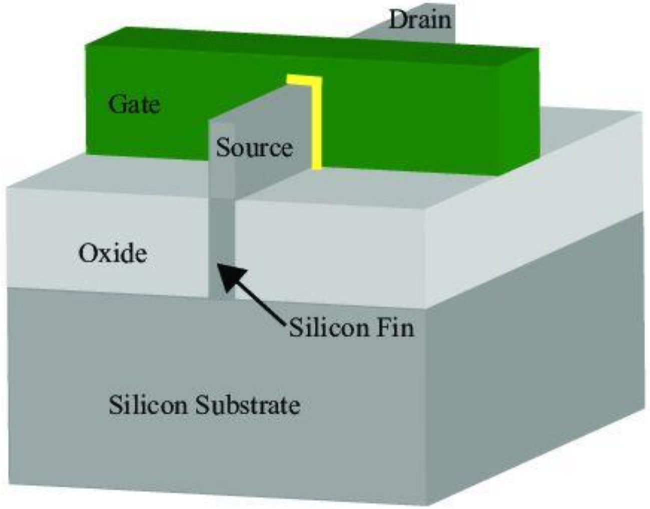
High -κ materials for dielectrics other than

	κ
SiO_2	3.9
HfO_4Si	11
Si_3N_4	7
Al_2O_3	9
ZrO_2	25
HfO_2	25

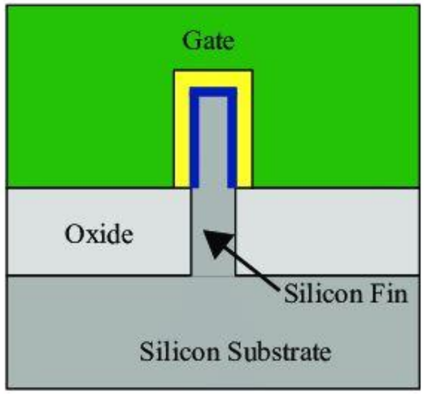
Low voltage action requirement:

Multi-gate structure to wrap up the conduction channel

FinFET structure



(a) 3D Structure



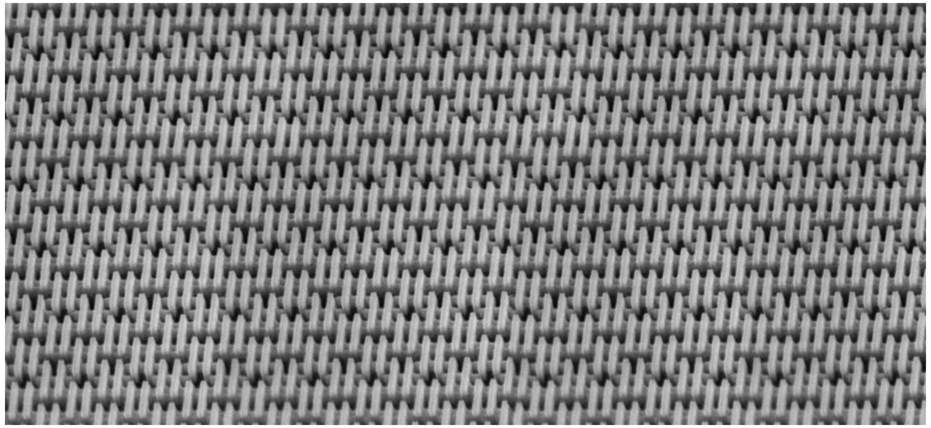
(b) Cross-sectional View

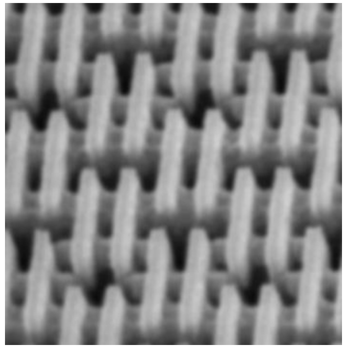
Pinch-off the channel with wrapping gate

Less than 1 ps

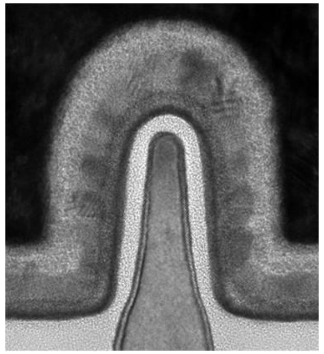
Less than 1 V

Inversion conductive mode





TSMC 7 nm transistors



TSMC 30 nm gate (2012)

Heterojunction and envelope function

Effective mass approximation

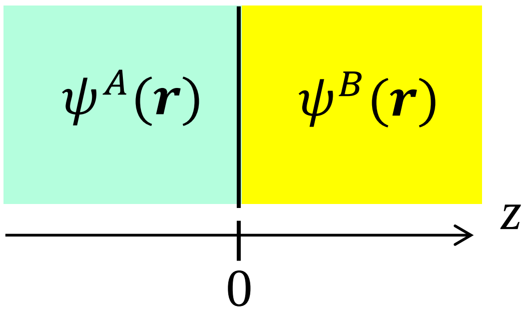
$$\left[-\frac{\hbar^2\nabla^2}{2m^*}+U(\boldsymbol{r})\right]f(\boldsymbol{r})=Ef(\boldsymbol{r})$$

$f(\boldsymbol{r})$: envelope function

This holds for spatially slow perturbation $U(\boldsymbol{r})$.

Then how about heterointerface?

$$\psi^{(\mathrm{A})}(\boldsymbol{r})=\sum_l f_l^{(\mathrm{A})}(\boldsymbol{r})u_{l\boldsymbol{k}}^{(\mathrm{A})}(\boldsymbol{r}),\quad \psi^{(\mathrm{B})}(\boldsymbol{r})=\sum_l f_l^{(\mathrm{B})}(\boldsymbol{r})u_{l\boldsymbol{k}}^{(\mathrm{B})}(\boldsymbol{r})$$



1. For simplicity we assume $u_{l\boldsymbol{k}}^{(\mathrm{A})}(\boldsymbol{r})=u_{l\boldsymbol{k}}^{(\mathrm{B})}(\boldsymbol{r}),\quad \partial\epsilon_l^{(\mathrm{A})}/\partial\boldsymbol{k}=\partial\epsilon_l^{(\mathrm{B})}/\partial\boldsymbol{k}$

Then continuity condition at z =0 becomes $f_l^{(\mathrm{A})}(\boldsymbol{r}_{xy},0)=f_l^{(\mathrm{B})}(\boldsymbol{r}_{xy},0)$

In xy-plane, the Bloch theorem tells $f_l^{(\mathrm{A,B})}=\dfrac{1}{\sqrt{S}}\exp(i\boldsymbol{k}_{xy}\cdot\boldsymbol{x})\chi_l^{(\mathrm{A,B})}(z)$

envelope function for z

For z-freedom, we apply $k\cdot p$ perturbation.

$$\mathscr{D}^{(0)}\left(z,-i\hbar\frac{\partial}{\partial z}\right)\boldsymbol{\chi}=\epsilon\boldsymbol{\chi}$$

Heterojunction and envelope function (2)

The elements of $\mathscr{D}^{(0)}$ are

$$\mathscr{D}^{(0)}_{lm}\left(z,\frac{\partial}{\partial z}\right)=\left[\epsilon_l(z)+\frac{\hbar^2k_{xy}^2}{2m_0}-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial z^2}\right]\delta_{lm}+\frac{\hbar\boldsymbol{k}_{xy}}{m_0}\cdot\langle l|\boldsymbol{p}_{xy}|m\rangle-\frac{i\hbar}{m_0}\langle l|p_z|m\rangle\frac{\partial}{\partial z}$$

with $\epsilon_l(z)=\epsilon_l^{(\mathrm{A})}\quad(z<0),\quad \epsilon_l^{(\mathrm{B})}\quad(z\geq 0)$

$$V_l(z)\equiv\begin{cases}0 & z<0\quad(z\in\mathrm{A})\\ \epsilon_l^{(\mathrm{B})}-\epsilon_l^{(\mathrm{A})} & z\geq 0\quad(z\in\mathrm{B}).\end{cases}$$

$$\sum_{m=1}^{N}\left\{\left[\epsilon_{m0}^{(\mathrm{A})}+V_m(z)+\frac{\hbar^2k_{xy}^2}{2m_0}-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial z^2}\right]\delta_{lm}-\frac{i\hbar}{m_0}\langle l|\hat{p}_z|m\rangle\frac{\partial}{\partial z}+\frac{\hbar\boldsymbol{k}_{xy}}{m_0}\cdot\langle l|\hat{\boldsymbol{p}}_{xy}|m\rangle\right\}\chi_m=\epsilon\chi_l$$

Continuity condition:

$$\mathscr{A}^{(\mathrm{A})}\chi^{(\mathrm{A})}(z_0=0)=\mathscr{A}^{(\mathrm{B})}\chi^{(\mathrm{B})}(0)$$

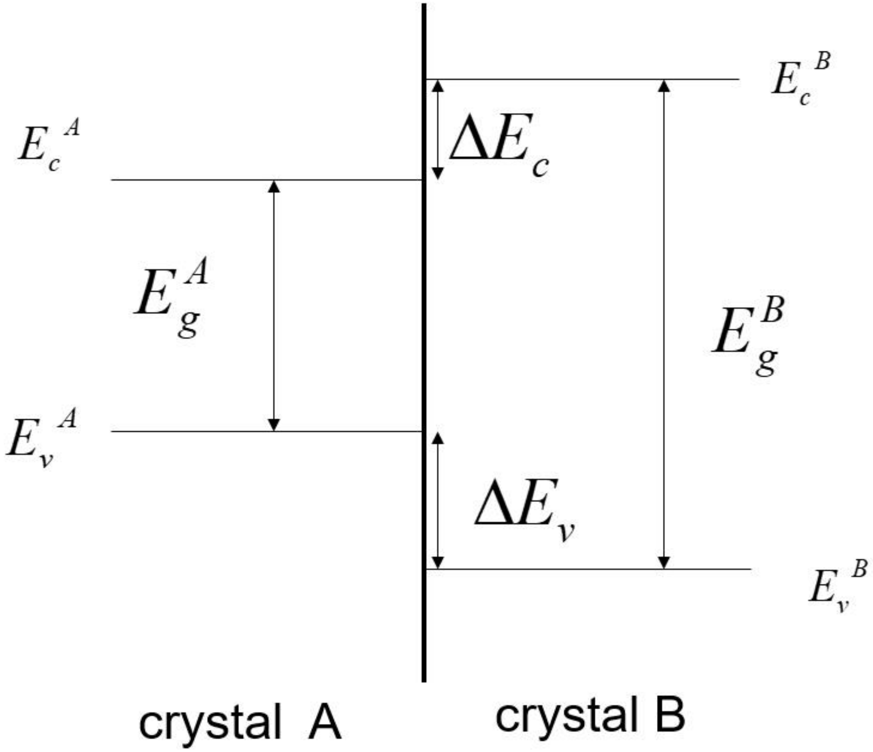
$$\mathscr{A}_{lm}=-\frac{\hbar^2}{2m_0}\left[\delta_{lm}\frac{\partial}{\partial z}+\frac{2i}{\hbar}\langle l|p_z|m\rangle\right]$$

continuity in derivative ($\frac{\partial}{\partial z}$) — discontinuity ($\langle l|p_z|m\rangle$)

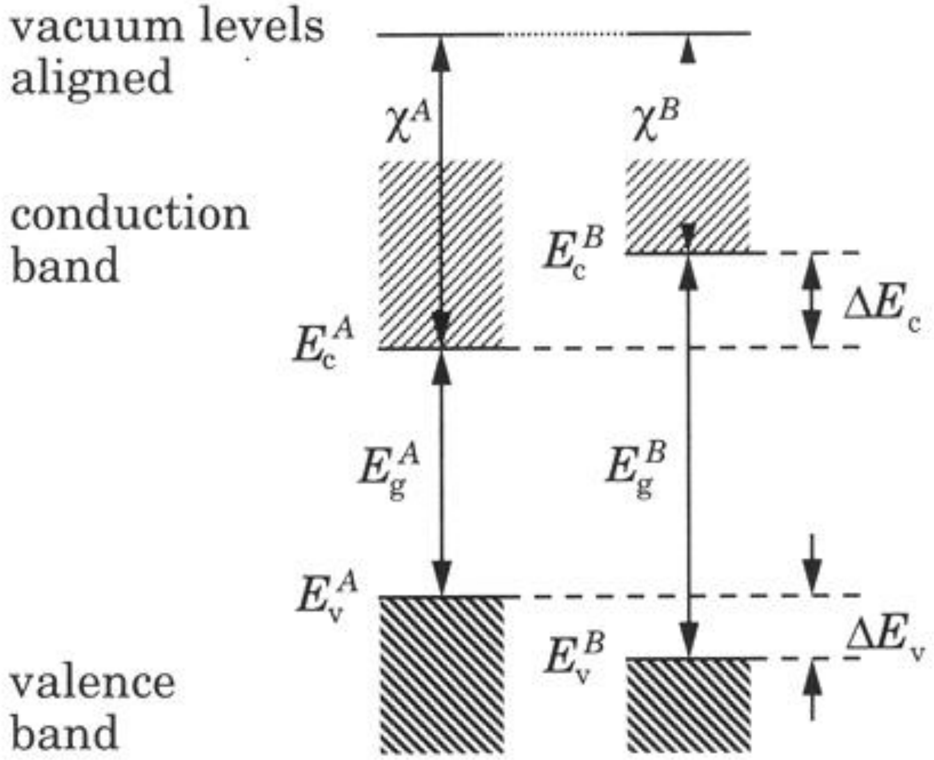
When the band mixing effect is ignorable, we can also apply the effective mass approximation for the heterojunctions.

Band discontinuity

Band discontinuity parameters

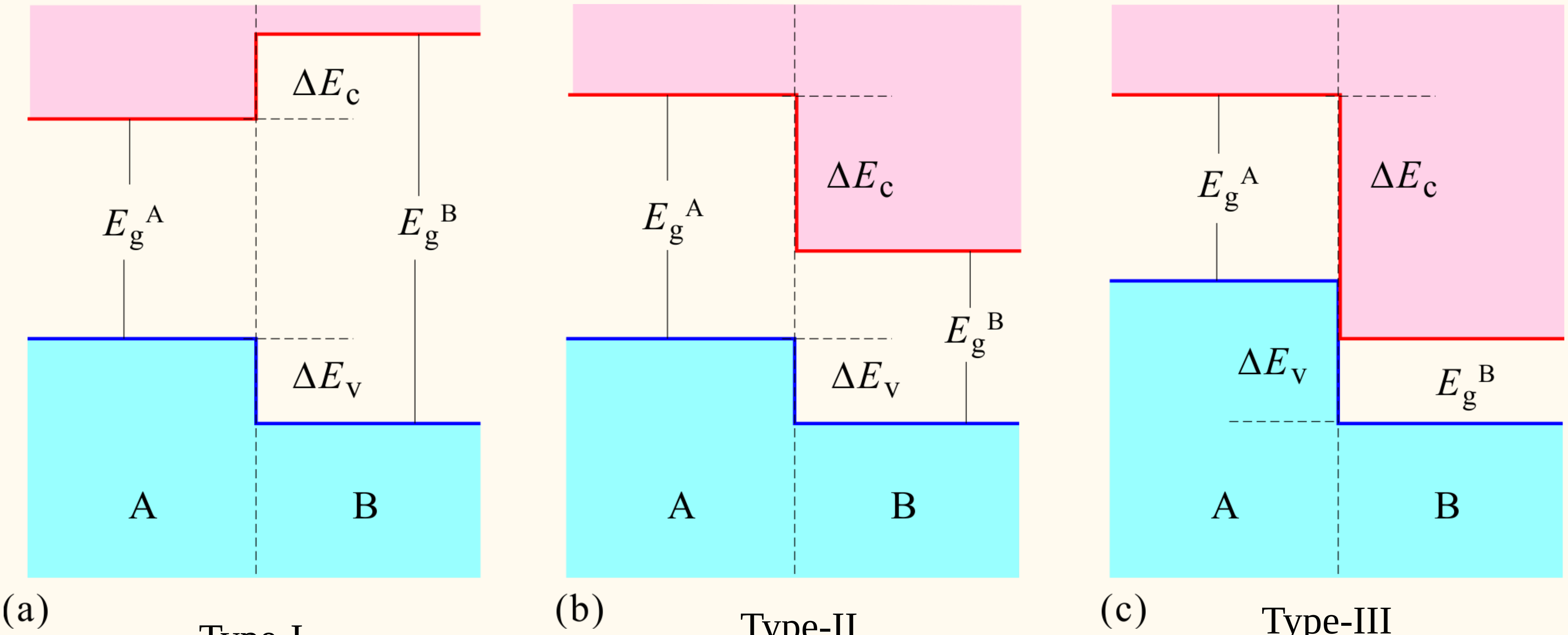


Anderson’s rule: affinity from the vacuum level determines the alignment



R. L. Anderson, IBM J. Res. Dev. **4**, 283 (1960).

Heterojunction types



Type-I

Type-II

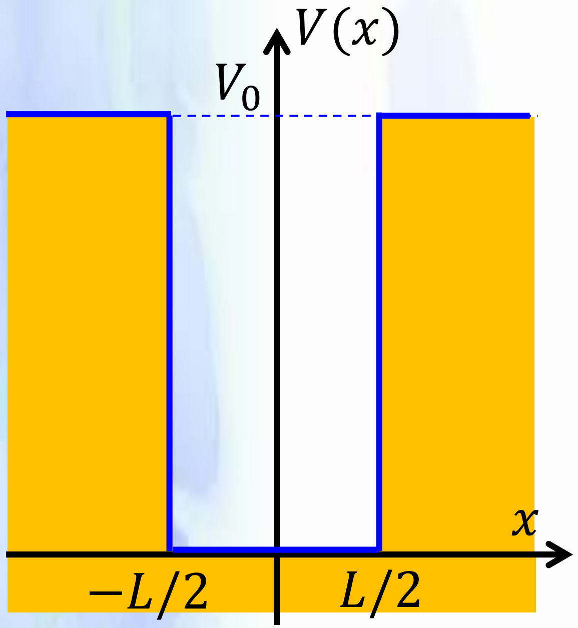
Type-III
(Type-II staggered)

Chapter 7 Quantum Structure (Quantum wells, wires, dots)

Zhores I. Alferov | Herbert Kroemer | Jack S. Kilby

The Nobel Prize in Physics 2000 was awarded *"for basic work on information and communication technology"* with one half jointly to Zhores I. Alferov and Herbert Kroemer *"for developing semiconductor heterostructures used in high-speed- and opto-electronics"* and the other half to Jack S. Kilby *"for his part in the invention of the integrated circuit"*.

Quantum well (elementary quantum mechanics)



Outside the well: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\right]\psi = E\psi, \quad x \le -\frac{L}{2}, \ \frac{L}{2} \le x, \quad \kappa \equiv \frac{\sqrt{2m|E-V_0|}}{\hbar}$

$$\psi(x) = \begin{cases} C_1\exp(i\kappa x) + C_2\exp(-i\kappa x) & E \ge V_0, \\ D_1\exp(\kappa x) + D_2\exp(-\kappa x) & E < V_0. \end{cases}$$

States localized inside the well: $E < V_0$ $\quad \frac{L}{2} < x \rightarrow D_1^+ = 0, \quad x < -\frac{L}{2} \rightarrow D_2^- = 0$

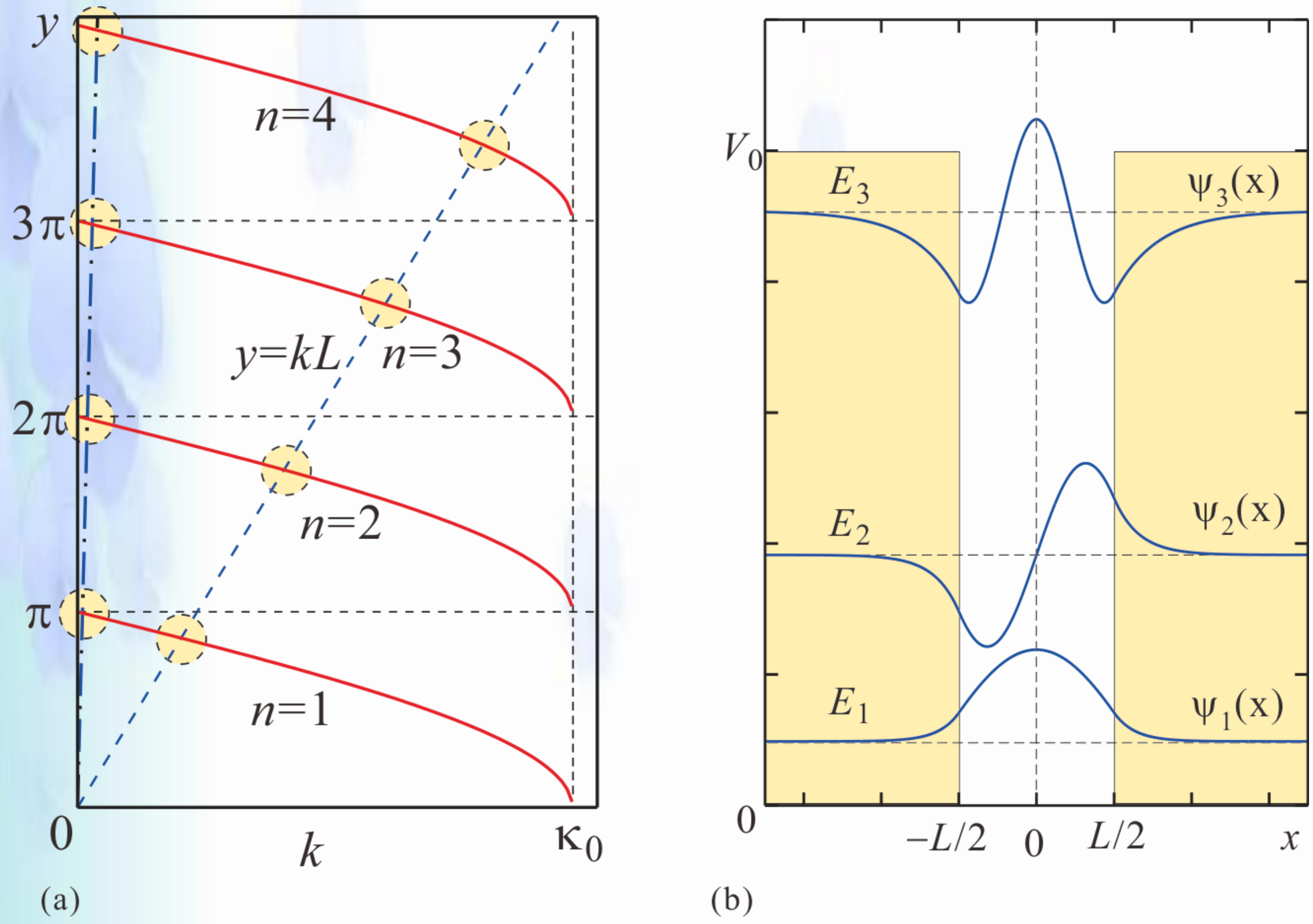
Inside the well: $\psi(x) = C_1\exp(ikx) + C_2\exp(-ikx), \ k \equiv \frac{\sqrt{2mE}}{\hbar}, \ x \in \left[-\frac{L}{2}, \frac{L}{2}\right]$

Envelope function connection

Continuity
$$\begin{cases} C_1\exp(ikL/2) + C_2\exp(-ikL/2) = D_2^+\exp(-\kappa L/2), \\ C_1\exp(-ikL/2) + C_2\exp(ikL/2) = D_1^-\exp(-\kappa L/2), \end{cases}$$

Differentiability
$$\begin{cases} ikC_1\exp(ikL/2) - ikC_2\exp(-ikL/2) = -\kappa D_2^+\exp(-\kappa L/2), \\ ikC_1\exp(-ikL/2) - ikC_2\exp(ikL/2) = \kappa D_1^-\exp(-\kappa L/2), \end{cases}$$

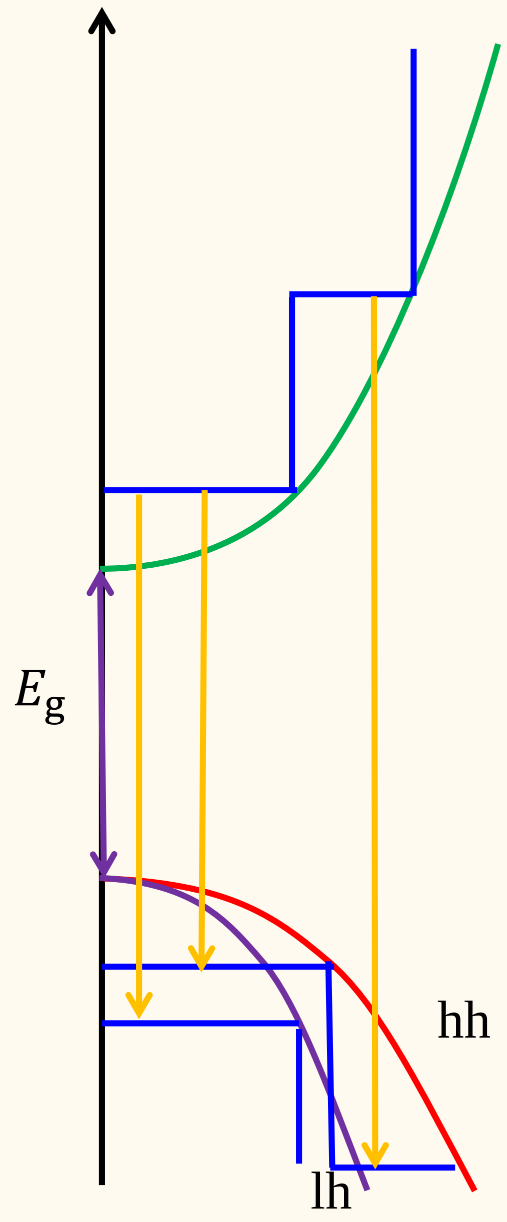
Quantum well



$$kL = -2\arctan\frac{k}{\sqrt{\kappa_0^2 - k^2}} + n\pi$$

$$\kappa_0^2 \equiv \frac{2mV_0}{\hbar^2}, \quad n = 1, 2, \cdots$$

Optical absorption of quantum wells



$$\left.\begin{aligned}\psi_e(\boldsymbol{r}) &= \phi_e(z)\exp(i\boldsymbol{k}_{xy}\cdot\boldsymbol{r}_{xy})u_c(\boldsymbol{r}),\\ \psi_h(\boldsymbol{r}) &= \phi_h(z)\exp(i\boldsymbol{k}_{xy}\cdot\boldsymbol{r}_{xy})u_v(\boldsymbol{r}).\end{aligned}\right\}$$

Envelope functions

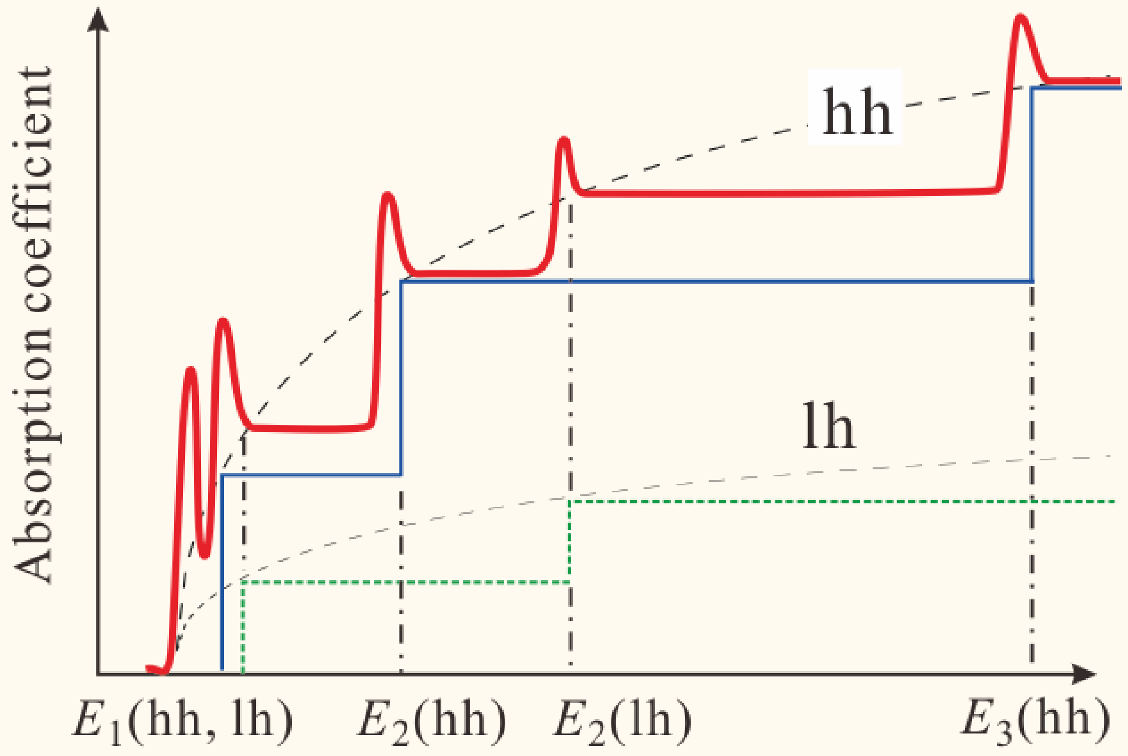
Lattice periodic functions

Direct transition rate: $P_{cv} \propto \langle u_c(\boldsymbol{r})|\boldsymbol{\nabla}|u_v(\boldsymbol{r})\rangle \int_{-\infty}^{\infty} dz\phi_e(z)^*\phi_h(z)$

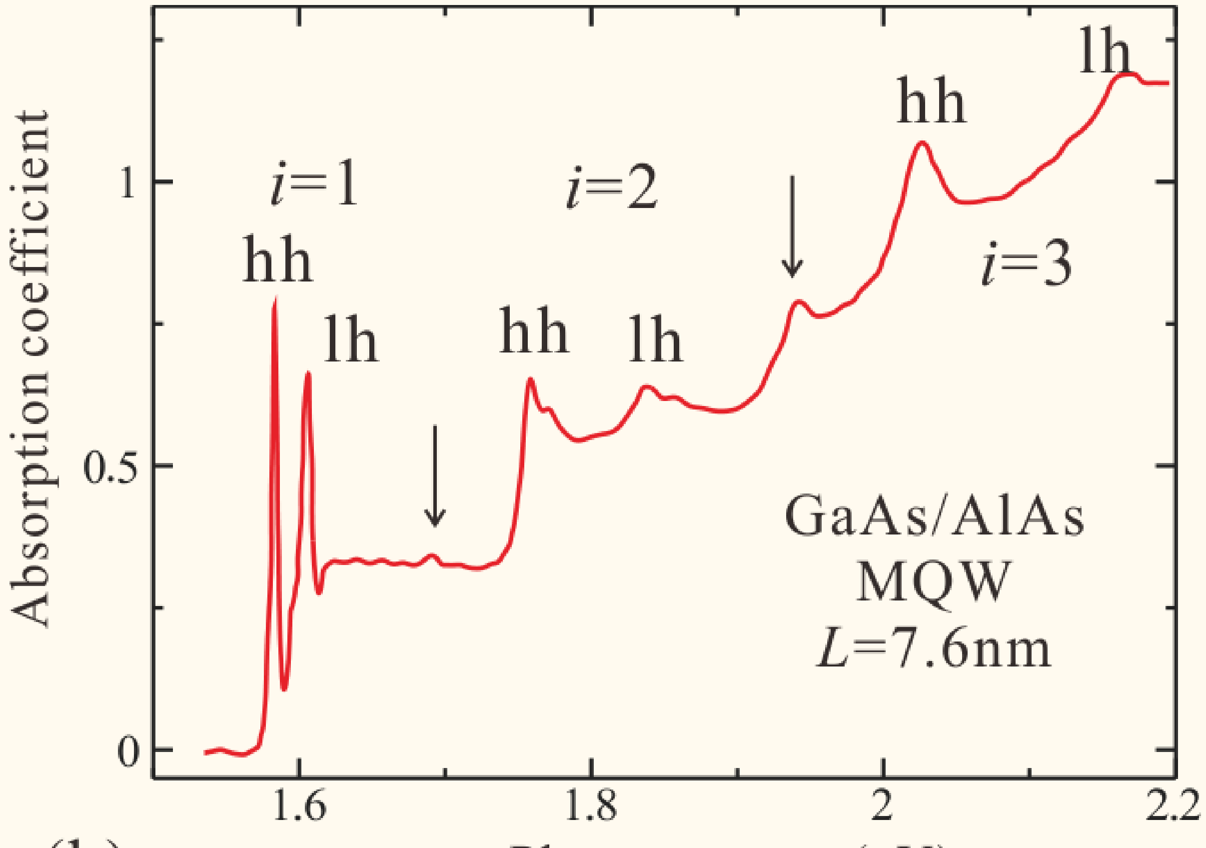
Transition energy: $E = E_{\rm g} + \Delta E_n^{(eh)} + \dfrac{\hbar^2}{2\mu}k_{xy}^2$

Two dimensional density of states: $\dfrac{dn}{dE} = \dfrac{m^*}{2\pi\hbar^2}H(E) \quad (H(x)$: Heaviside function$)$

Optical absorption of quantum wells



(a)



(b)

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.6.09 Lecture 09

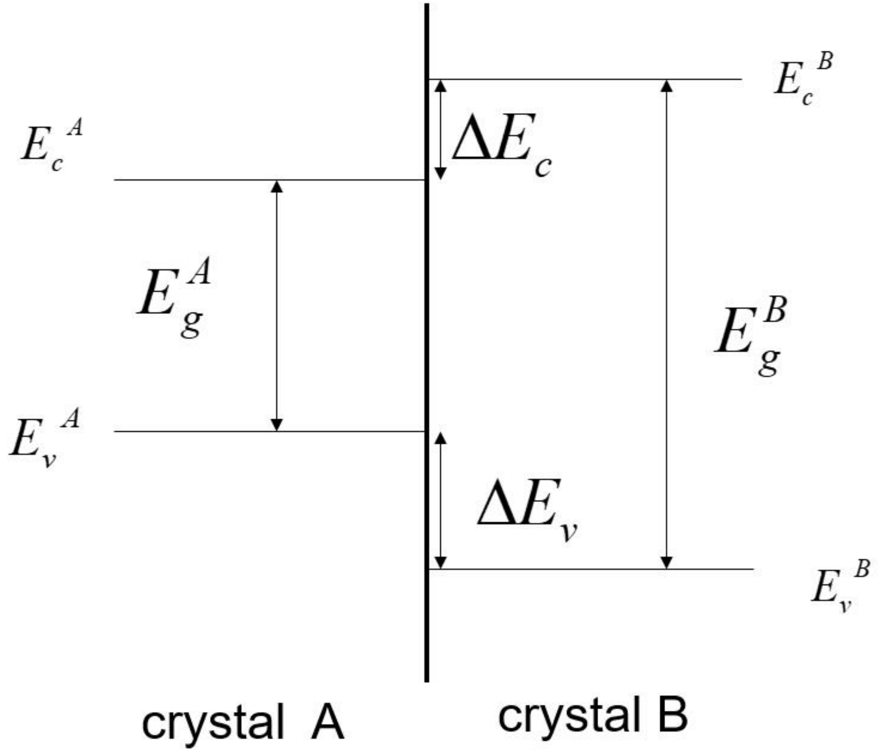
10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Band discontinuity

Band discontinuity parameters



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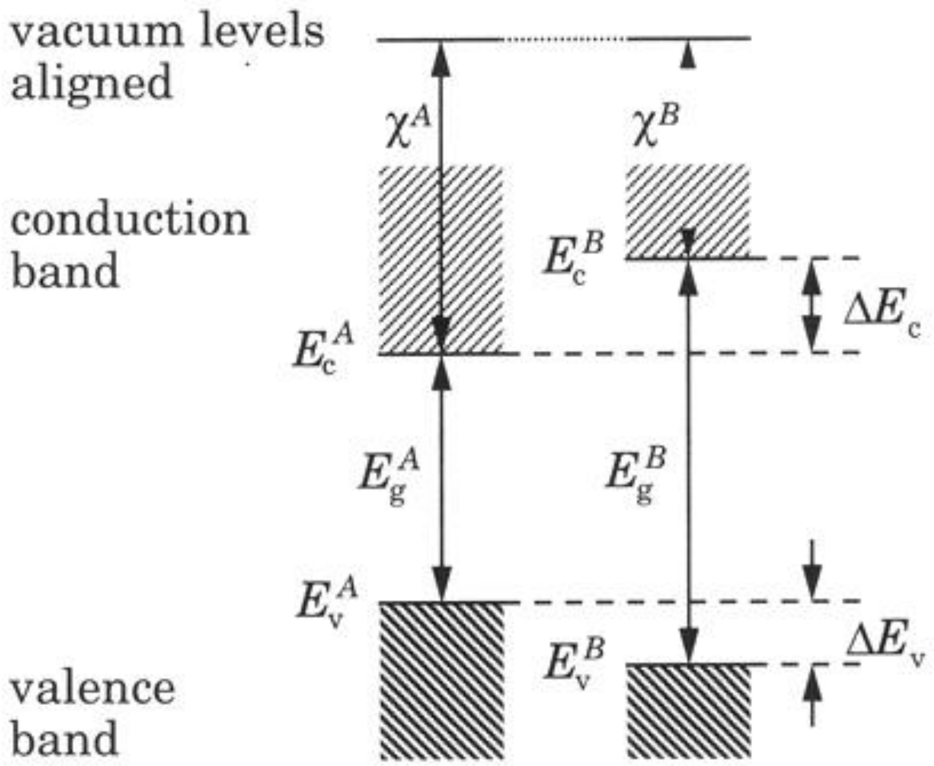

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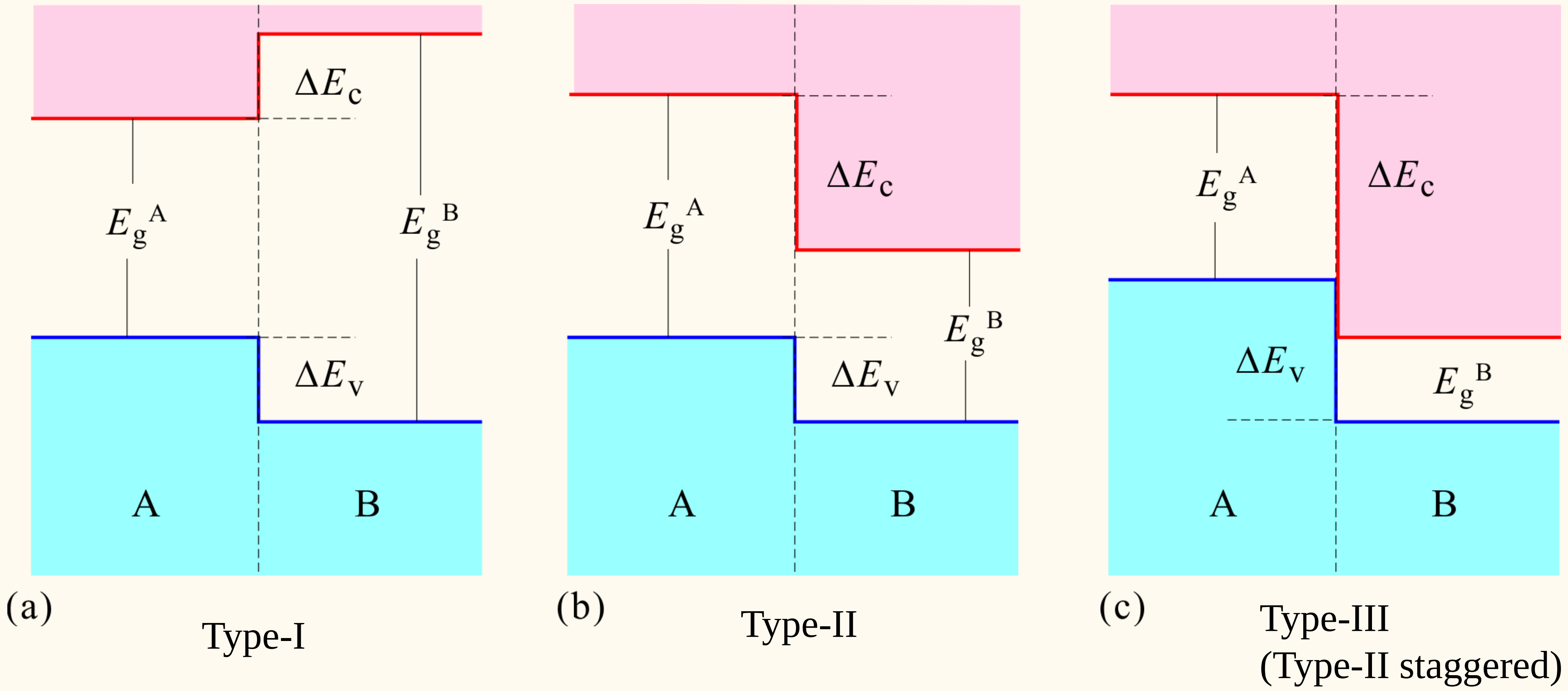
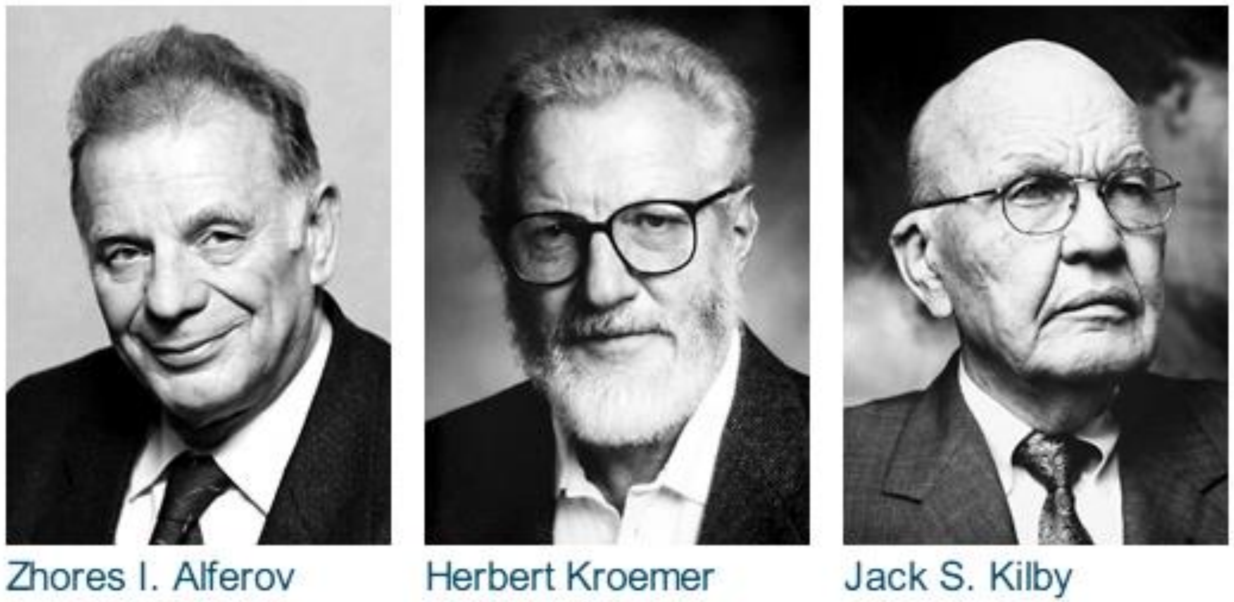
Heterojunction types



Chapter 7 Quantum Structure (Quantum wells, wires, dots)



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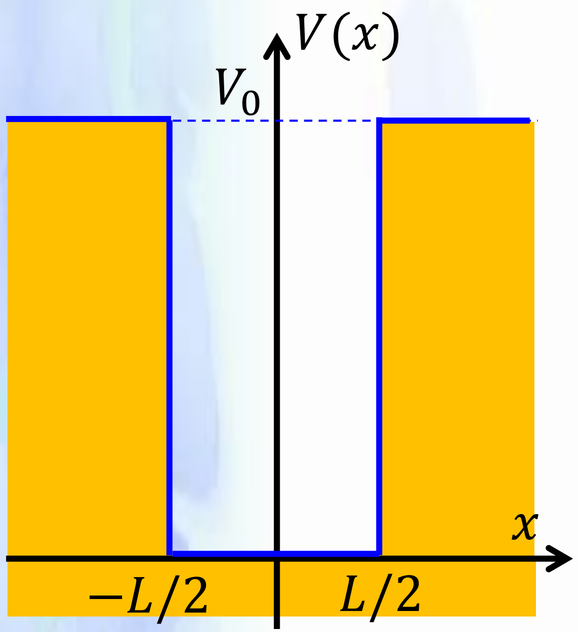

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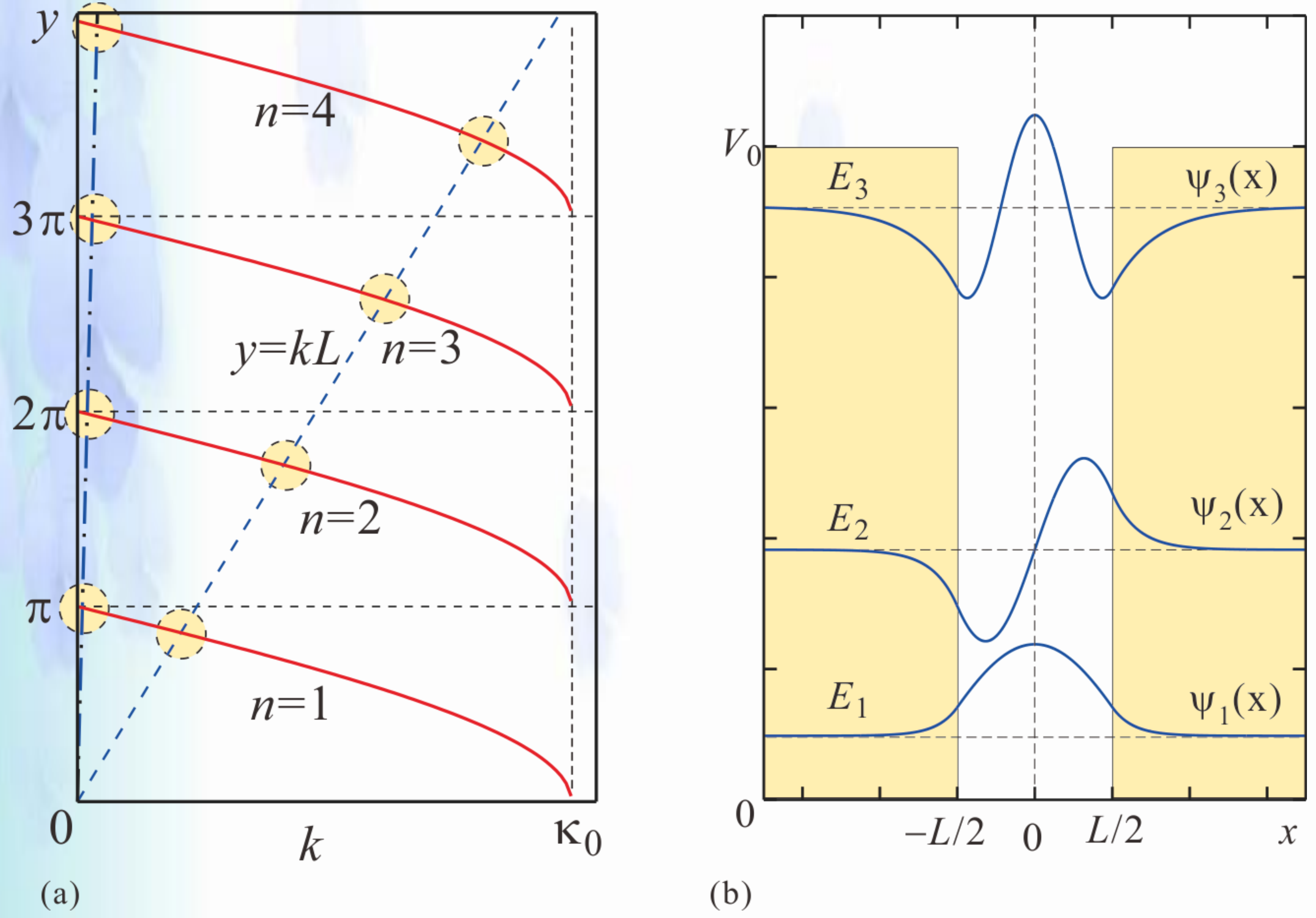
Quantum well



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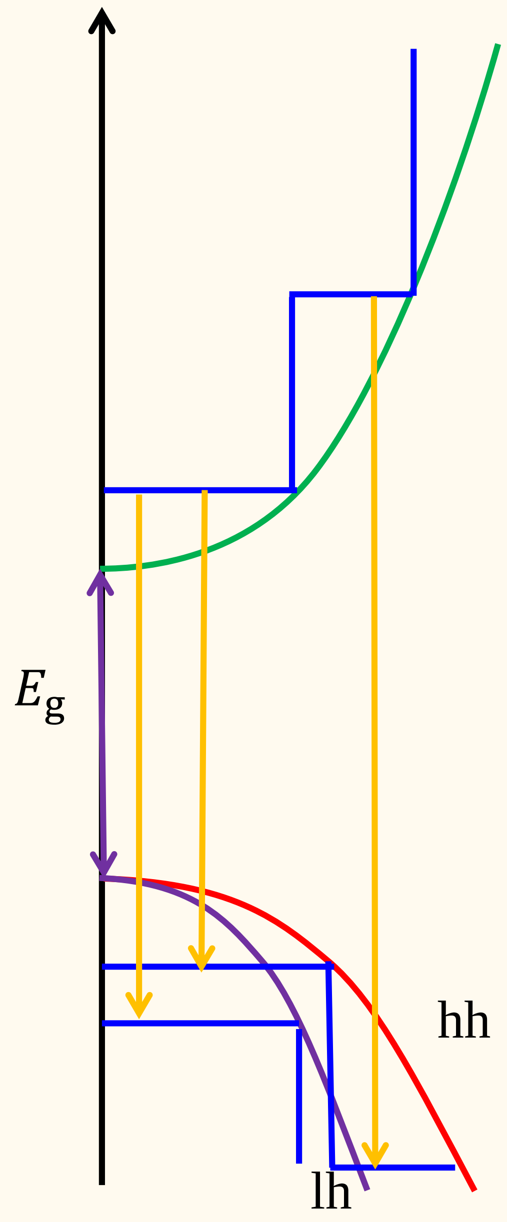
Optical absorption of quantum wells



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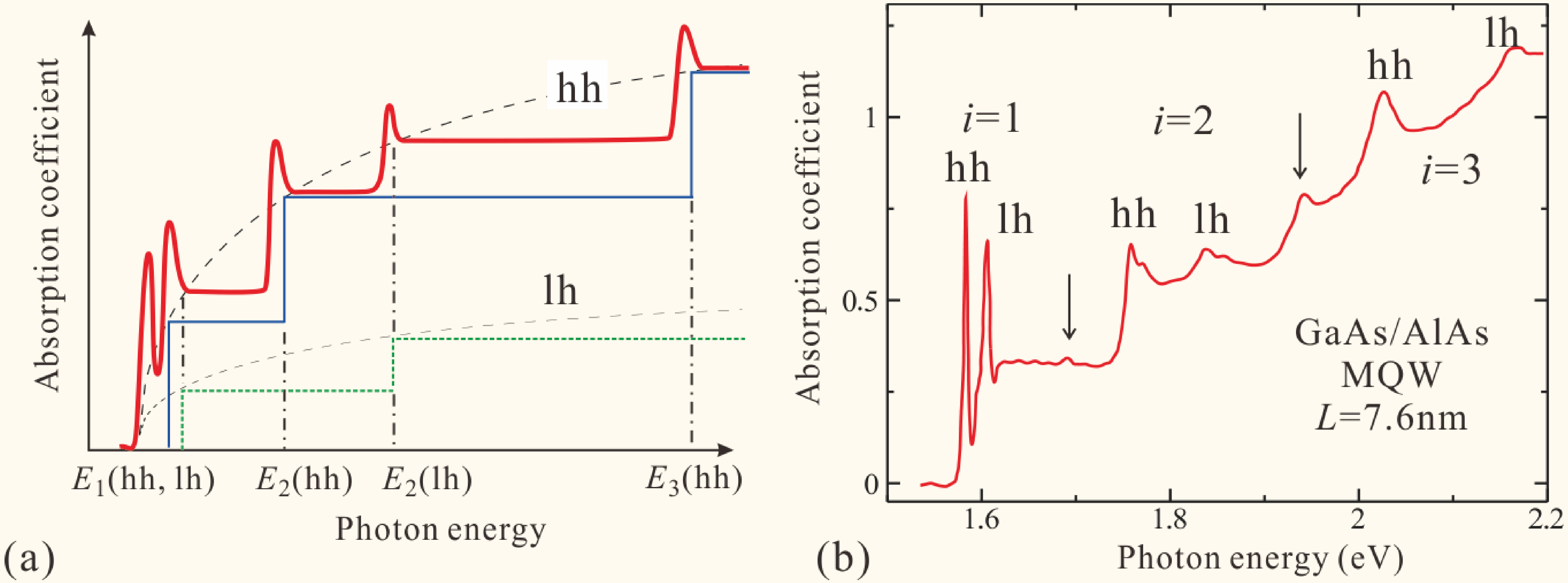
Lattice periodic functions

Direct transition rate: $P_{cv} \propto \langle u_c(\boldsymbol{r})|\boldsymbol{\nabla}|u_v(\boldsymbol{r})\rangle \int_{-\infty}^{\infty} dz\phi_e(z)^*\phi_h(z)$

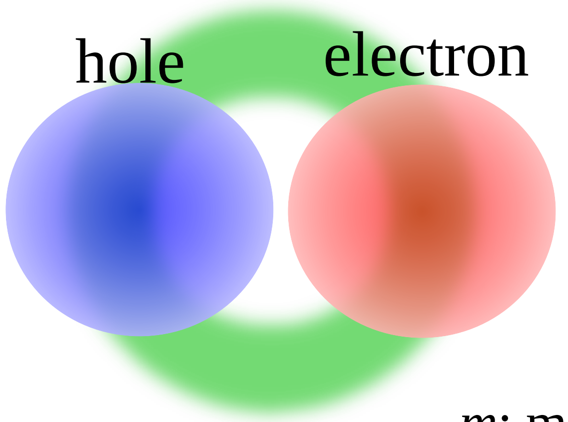
Transition energy: $E = E_{\rm g} + \Delta E_n^{(eh)} + \dfrac{\hbar^2}{2\mu}k_{xy}^2$

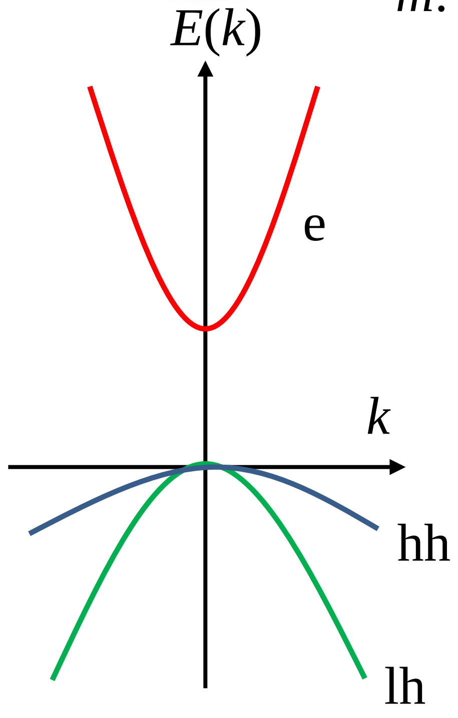
Two dimensional density of states: $\dfrac{dn}{dE} = \dfrac{m^*}{2\pi\hbar^2}H(E)$ $\quad (H(x)$: Heaviside function)

Optical absorption of quantum wells



Excitons in quantum well





Schrödinger equation

$$\left(-\frac{\hbar^2}{2m_\mathrm{r}^*}\nabla^2 - \frac{e^2}{4\pi\epsilon\epsilon_0|\boldsymbol{r}|}\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

Variable separation

$$\psi^{2\mathrm{d}} = \rho^{|m|}e^{-\rho/2}R(\rho)e^{im\varphi} \qquad \rho = \frac{\sqrt{-8m_\mathrm{r}^*E}}{\hbar}r$$

Radial wavefunction

m: magnetic quantum number

$$\left[\rho\frac{\partial^2}{\partial\rho^2} + (2|m| + 1 - \rho)\frac{\partial}{\partial\rho} + \lambda - |m| + \frac{1}{2}\right]R(\rho) = 0$$

$$\lambda \equiv \frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{-\frac{m_\mathrm{r}^*}{2E}}$$

Power series expansion

$$R(\rho) = \sum_\nu \beta_\nu\rho^\nu, \qquad \beta_{\nu+1} = \beta_\nu\frac{\nu - \lambda + |m| + 1/2}{(\nu+1)(\nu+p+1)}$$

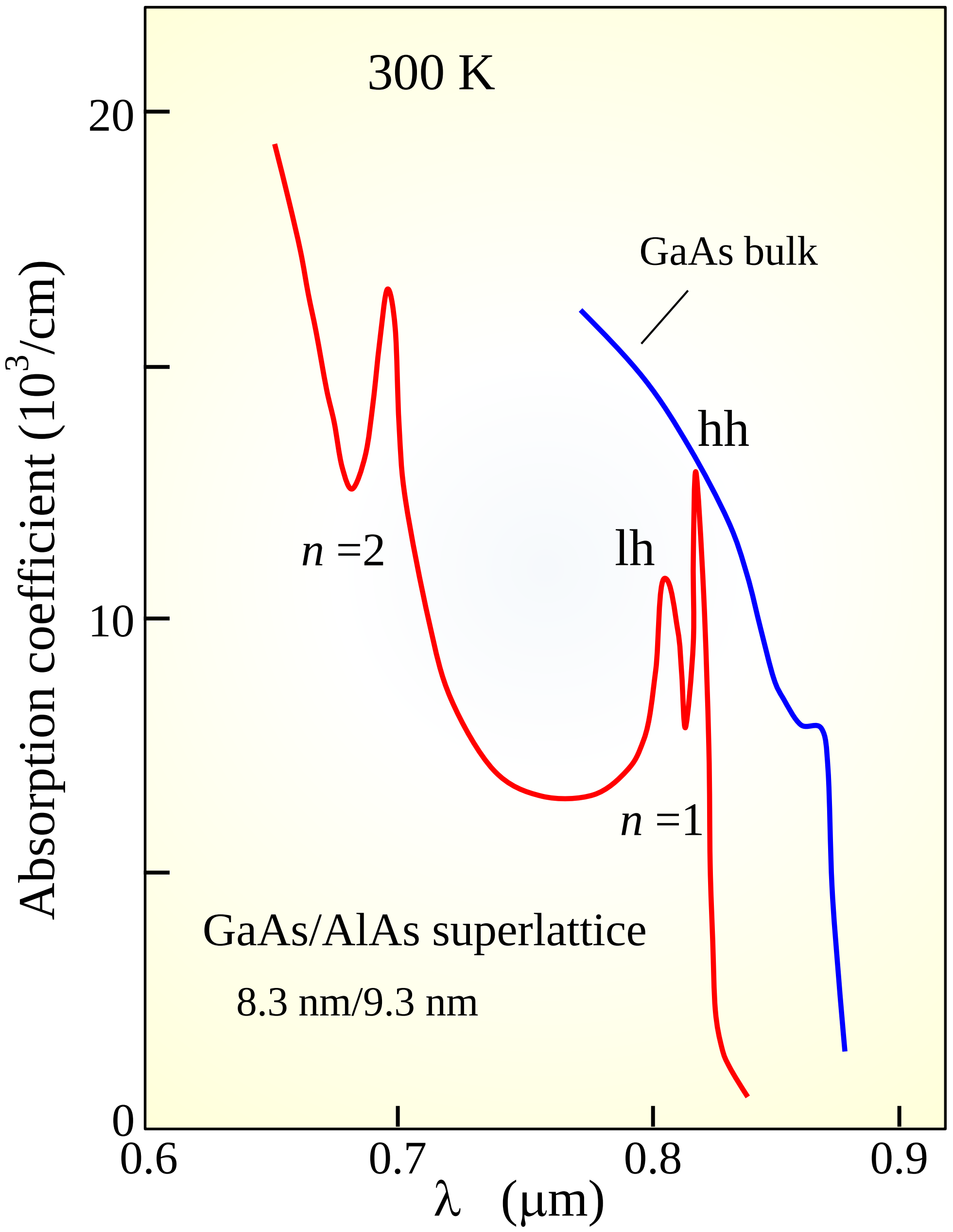
The series to be stopped at a finite length

$$E_{\mathrm{b}n}^{2\mathrm{d}} = -\frac{E_0}{(n+1/2)^2} \qquad n = 0, 1, \cdots$$

$$E_0 = \frac{e^2}{8\pi\epsilon\epsilon_0 a_0^*}, \qquad a_0^* = \frac{4\pi\epsilon\epsilon_0\hbar^2}{m_\mathrm{r}^* e^2}$$

$$E_\mathrm{ground}^{2\mathrm{d}} = 4E_0, \qquad a_0^{2\mathrm{d}} = a_0^*/2$$

Excitons in quantum well



$$\left(-\frac{\hbar^2}{2m_{\rm r}^*}\nabla^2 - \frac{e^2}{4\pi\epsilon\epsilon_0|\boldsymbol{r}|}\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

$$\psi^{2{\rm d}} = \rho^{|m|}e^{-\rho/2}R(\rho)e^{im\varphi} \qquad \rho = \frac{\sqrt{-8m_{\rm r}^*E}}{\hbar}r$$

$$\left[\rho\frac{\partial^2}{\partial\rho^2} + (2|m|+1-\rho)\frac{\partial}{\partial\rho} + \lambda - |m| + \frac{1}{2}\right]R(\rho) = 0$$

$$\lambda \equiv \frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{-\frac{m_{\rm r}^*}{2E}}$$

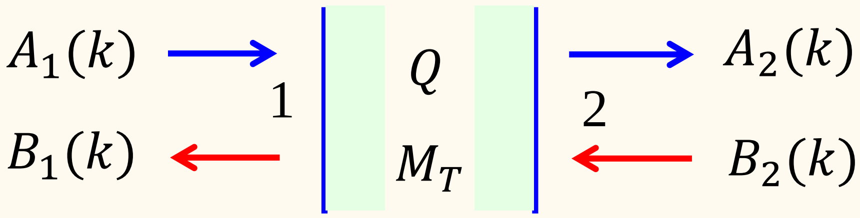
$$R(\rho) = \sum_\nu \beta_\nu\rho^\nu, \qquad \beta_{\nu+1} = \beta_\nu\frac{\nu-q}{(\nu+1)(\nu+p+1)}$$

$$E_{{\rm b}n}^{2{\rm d}} = -\frac{E_0}{(n+1/2)^2} \qquad n = 0, 1, \cdots$$

$$E_0 = \frac{e^2}{8\pi\epsilon\epsilon_0 a_0^*}, \quad a_0^* = \frac{4\pi\epsilon\epsilon_0\hbar^2}{m_{\rm r}^*e^2}$$

$$E_{\rm ground}^{2{\rm d}} = 4E_0, \quad a_0^{2{\rm d}} = a_0^*/2$$

Quantum barrier



momentum conservation

→ relation between wavefunctions

Simpler way to consider tunneling through energy barriers

Generally $\sqrt{v_g}\psi$

- Transfer matrix: T-matrix
- Scattering matrix: S-matrix

Transfer matrix: M_T $\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \equiv M_T \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$

M_T for a barrier width L height V_0 $\quad \kappa \equiv \sqrt{2m(V_0 - E(k))}/\hbar$

Inside the barrier $\quad V_2 = V_1 e^{-\kappa L}, \quad W_2 = W_1 e^{\kappa L}$

Boundary condition: value $\quad A_1 + B_1 = V_1 + W_1, \qquad A_2 + B_2 = e^{-\kappa L} V_1 + e^{\kappa L} W_1,$

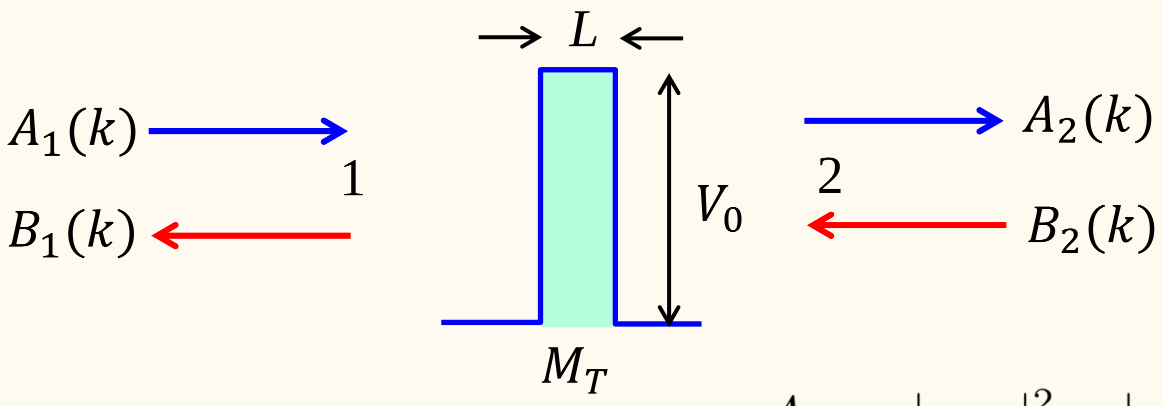
derivative $\quad ik(A_1 - B_1) = \kappa(-V_1 - W_1), \qquad ik(A_2 - B_2) = \kappa(-e^{-\kappa L} V_1 + e^{\kappa L} W_1)$

Then $M_T = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$

is obtained as

$$\begin{cases} m_{11} = \left[\cosh(\kappa L) + i\dfrac{k^2 - \kappa^2}{2k\kappa}\sinh(\kappa L)\right], \\ m_{12} = -i\dfrac{k^2 + \kappa^2}{2k\kappa}\sinh(\kappa L), \\ m_{21} = m_{12}^*, \qquad m_{22} = m_{11}^*, \end{cases}$$

Transfer matrix for rectangular barrier



$$\begin{cases} m_{11} = \left[\cosh(\kappa L) + i\frac{k^2-\kappa^2}{2k\kappa}\sinh(\kappa L)\right], \\ m_{12} = -i\frac{k^2+\kappa^2}{2k\kappa}\sinh(\kappa L), \\ m_{21} = m_{12}^*, \qquad m_{22} = m_{11}^*, \end{cases}$$

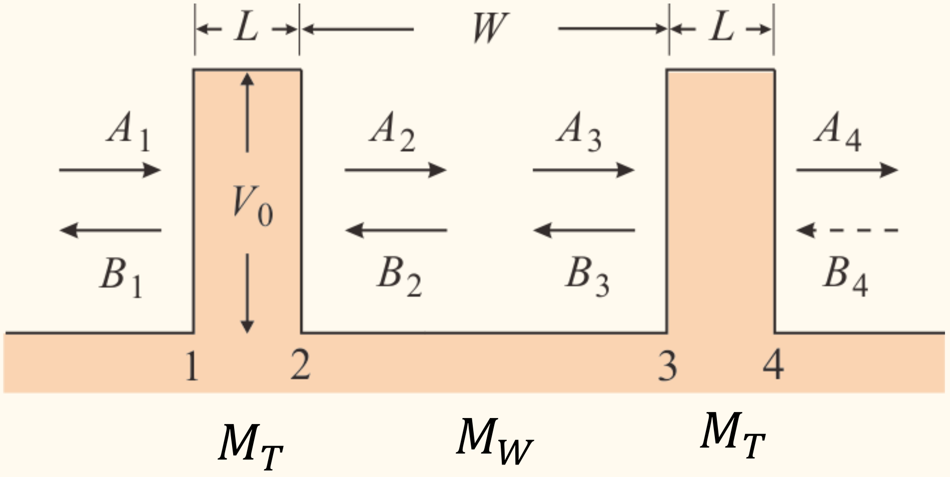
$$\begin{cases} t \equiv \frac{A_2}{A_1} = \frac{|m_{11}|^2 - |m_{12}|^2}{m_{11}^*} = \frac{1}{m_{11}^*} \\ \quad = \frac{2ik\kappa}{(k^2-\kappa^2)\sinh(\kappa L) + 2ik\kappa\cosh(\kappa L)} \\ r \equiv \frac{B_1}{A_1} = -\frac{m_{21}}{m_{22}} = \frac{(k^2+\kappa^2)\sinh(\kappa L)}{(k^2-\kappa^2)\sinh(\kappa L) - 2ik\kappa\cosh(\kappa L)} \end{cases}$$

t, r : complex transmission and reflection coefficients

Transmission coefficient $T = |t|^2$, reflection coefficient $R = |r|^2$

Then the transfer matrix is expressed as $M_T = \begin{pmatrix} 1/t^* & -r^*/t^* \\ -r/t & 1/t \end{pmatrix}$

Application of transfer matrix: double barrier transmission



T-matrix for well $M_W = \begin{pmatrix} \exp(ikW) & 0 \\ 0 & \exp(-ikW) \end{pmatrix}$

$$M_{DB} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} e^{ikW} & 0 \\ 0 & e^{-ikW} \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$
$$\equiv \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}$$

Calculation of transmission coefficient

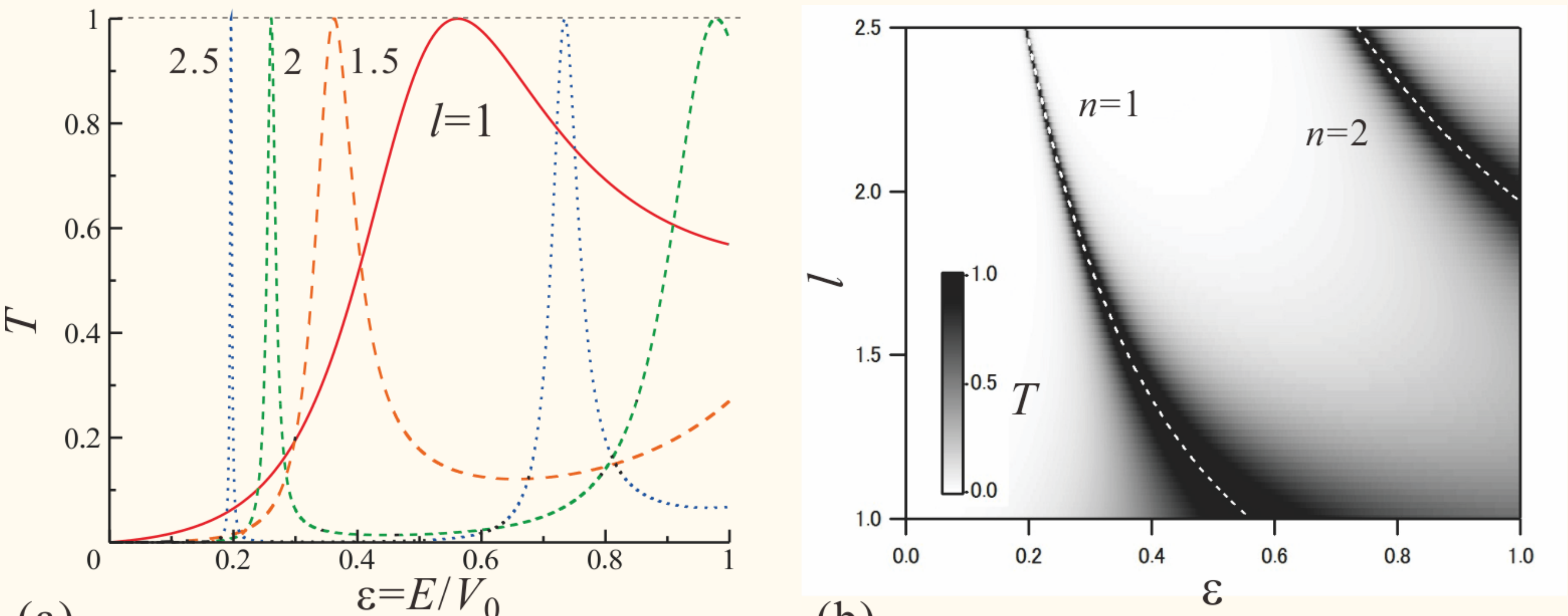
$$\begin{cases} m_{11} = \left[\cosh(\kappa L) + i\frac{k^2 - \kappa^2}{2k\kappa}\sinh(\kappa L)\right], \\ m_{12} = -i\frac{k^2 + \kappa^2}{2k\kappa}\sinh(\kappa L), \\ m_{21} = m_{12}^*, \quad m_{22} = m_{11}^*, \end{cases}$$

$$T_{11} = m_{11}^2 \exp(ikW) + |m_{12}|^2 \exp(-ikW) \quad (\because m_{12} = m_{21}^*)$$

$$T_{11}T_{11}^* = ((|m_{11}|^2 e^{2i\varphi} e^{ikW} + |m_{12}|^2 e^{-ikW})(|m_{11}|^2 e^{-2i\varphi} e^{-ikW} + |m_{12}|^2 e^{ikW})$$
$$= (|m_{11}^2 - |m_{12}|^2)^2 + 2|m_{11}|^2|m_{12}|^2 (1 + \cos(2(\varphi + kW)))$$
$$= 1 + 4|m_{11}|^2|m_{12}|^2 \cos^2(\varphi + kW)$$

$$T = \frac{1}{|T_{11}|^2} = \frac{1}{1 + 4|m_{11}|^2|m_{12}|^2 \cos^2(\varphi + kW)}$$

Double barrier transmission



(a) (b)

$$T = \frac{1}{|T_{11}|^2} = \frac{1}{1 + 4|m_{11}|^2|m_{12}|^2 \cos^2(\varphi + kW)}$$

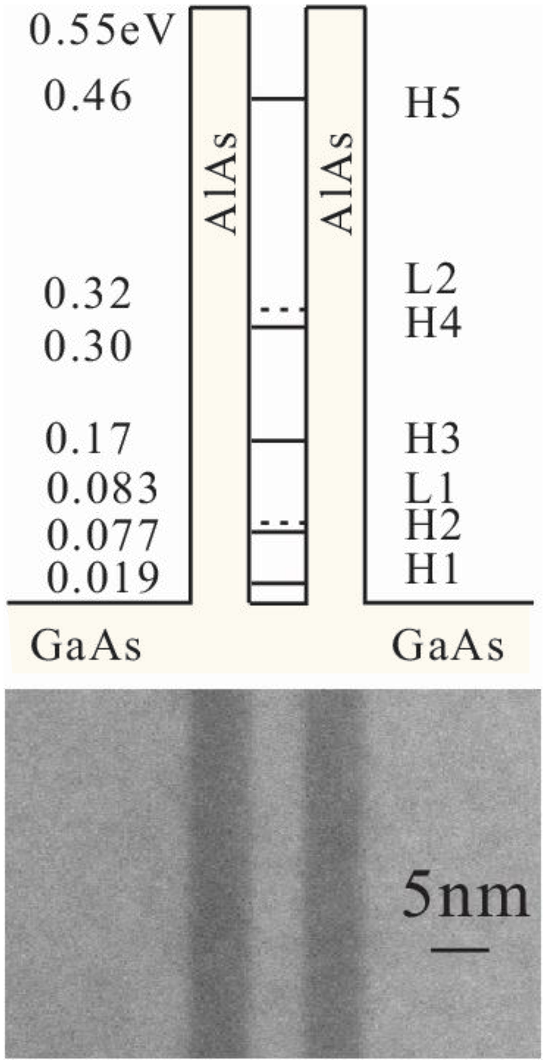
Resonant transmission condition: zero points of cosine term

$$\varphi + kW = \left(n - \frac{1}{2}\right)\pi \quad (n = 1, 2, \cdots)$$

$$\varphi = \arctan\left[\frac{k^2 - \kappa^2}{2k\kappa}\tanh(\kappa L)\right]$$

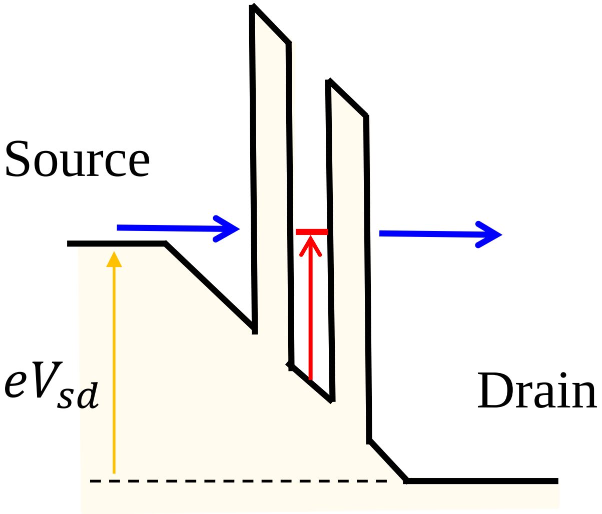
Transport experiment of double barrier conduction

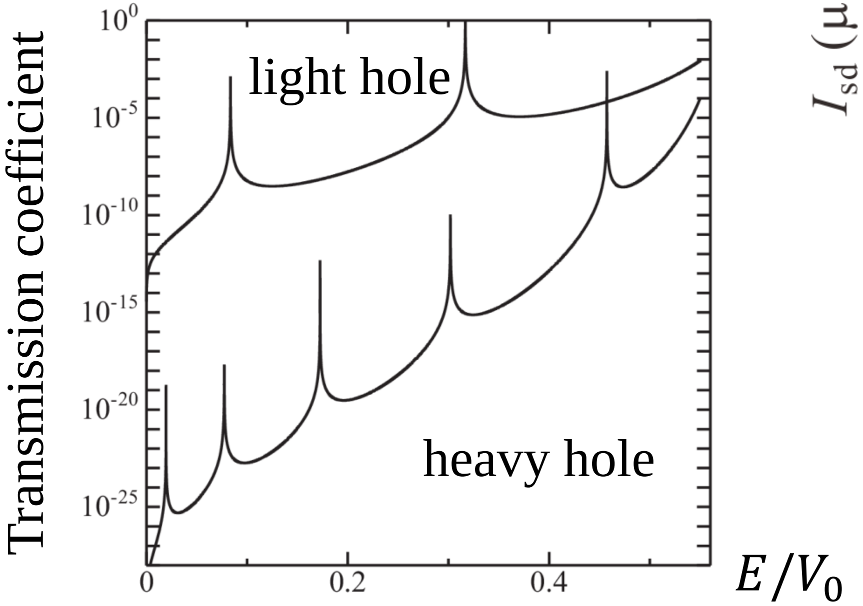
Sample structure



STEM image

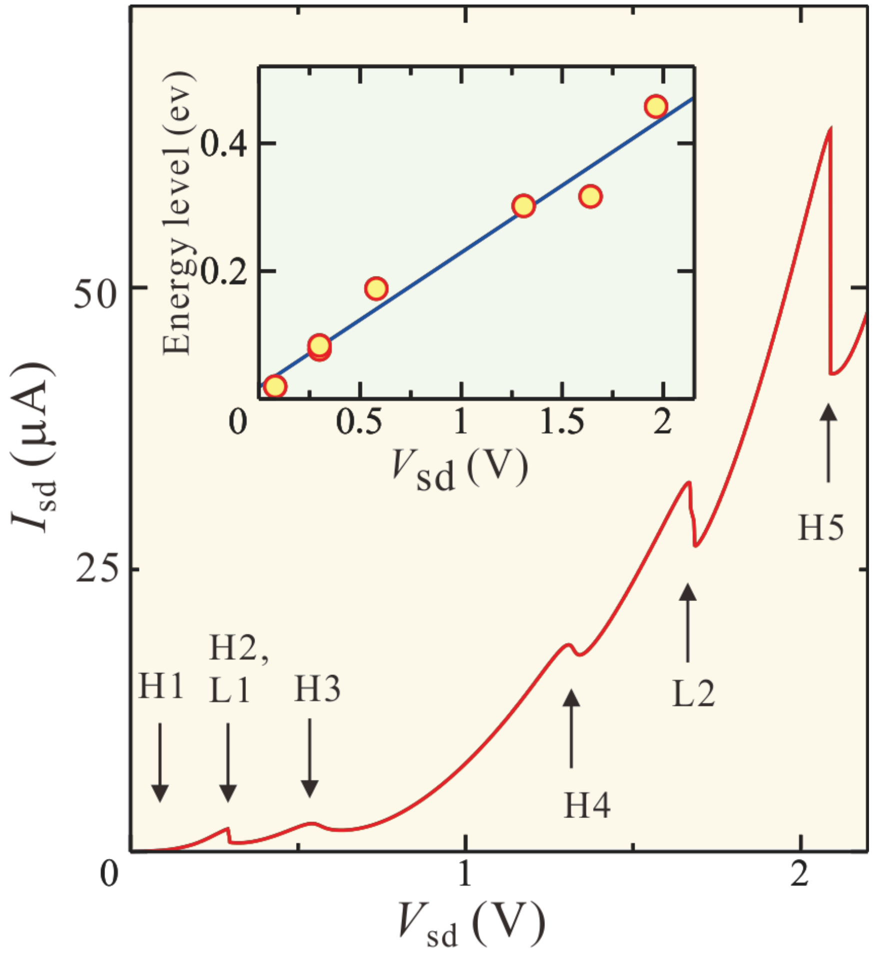
Measurement scheme



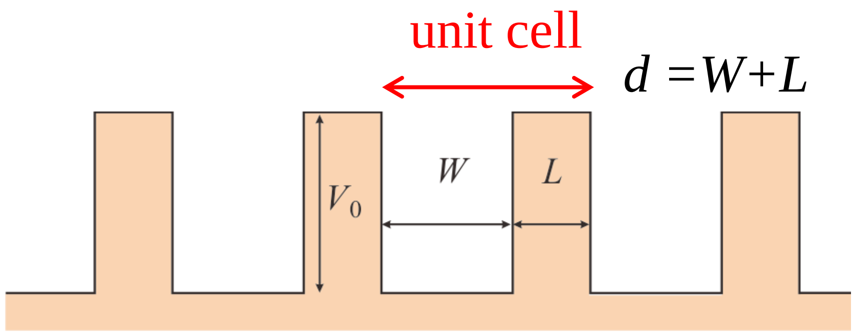


Calculated transmission coefficient

Result at 4.2 K



Application of T-matrix (2): Semiconductor superlattice



Kronig-Penny potential: $V_{KP}(x)$

Schrödinger equation

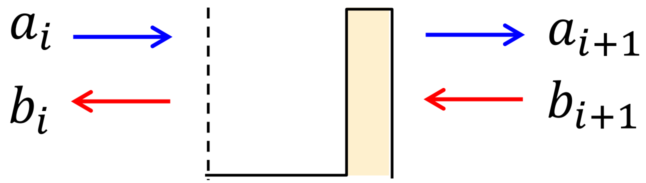
$$\left[-\frac{\hbar^2 d^2}{2m dx^2} + V_{\mathrm{KP}}(x)\right]\psi(x) = E\psi(x), \qquad V_{\mathrm{KP}}(x) = V_{\mathrm{KP}}(x+d)$$

Bloch theorem

$$\psi_K(x) = u_K(x)e^{iKx}, \quad u_K(x+d) = u_K(x), \quad K \equiv \frac{\pi s}{Nd}$$

$$s = -N+1, \cdots, N-1$$

Unit cell transfer matrix



$$M_d(k) = \begin{pmatrix} e^{ikW} & 0 \\ 0 & e^{-ikW} \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} = \begin{pmatrix} m_{11}e^{ikW} & m_{12}e^{ikW} \\ m_{21}e^{-ikW} & m_{22}e^{-ikW} \end{pmatrix}$$

$$\begin{pmatrix} a_{i+1} \\ b_{i+1} \end{pmatrix} = M_d \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \underline{e^{iKd}} \begin{pmatrix} a_i \\ b_i \end{pmatrix}$$

Eigenvalues $e^{\pm Kd}$ (M_d: unitary)

Theorem: $\mathrm{Tr}(A) = \sum(\text{eigenvalue})$ ⟶

$$e^{iKd} + e^{-iKd} = 2\cos Kd = \mathrm{Tr} M_d = 2\mathrm{Re}(e^{-ikW} m_{11}^*)$$

$$\cos\left[K(L+W)\right] = \cosh(\kappa L)\cos(kW) - \frac{k^2 - \kappa^2}{2k\kappa}\sinh(\kappa L)\sin(kW)$$

The relation between k (free electron wavenumber) and K (crystal wavenumber)

Semiconductor superlattice

$$\cos[K(L+W)] = \cosh(\kappa L)\cos(kW) - \frac{k^2-\kappa^2}{2k\kappa}\sinh(\kappa L)\sin(kW)$$

$L \to 0\ (W \to d),\ V_0 \to +\infty$ with $V_0 L = C$(constant)

δ-function series with the coefficient C.

$$\cos(Kd) = \cos(kd) + \frac{mC}{\hbar^2 k}\sin(kd)$$

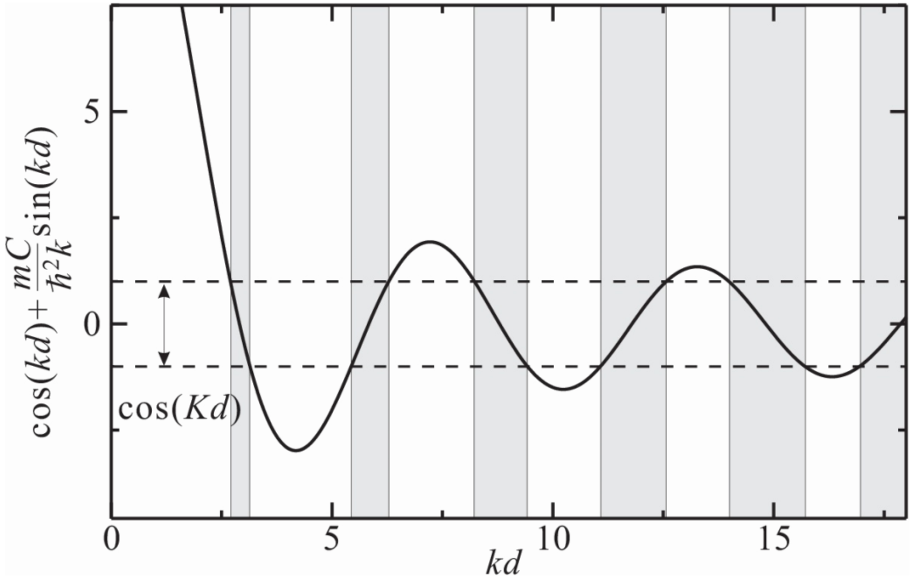
effect of superlattice potential

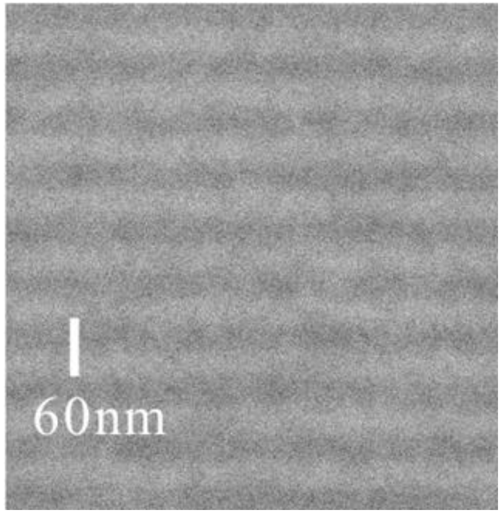
$$\left|\cos(kd) + \frac{mC}{\hbar^2 k}\sin(kd)\right| > 1$$

:no solution → band gap

Around $kd = n\pi$ $(n = 1,2,\cdots)$

Raphael Tsu and Leo Esaki, 1975

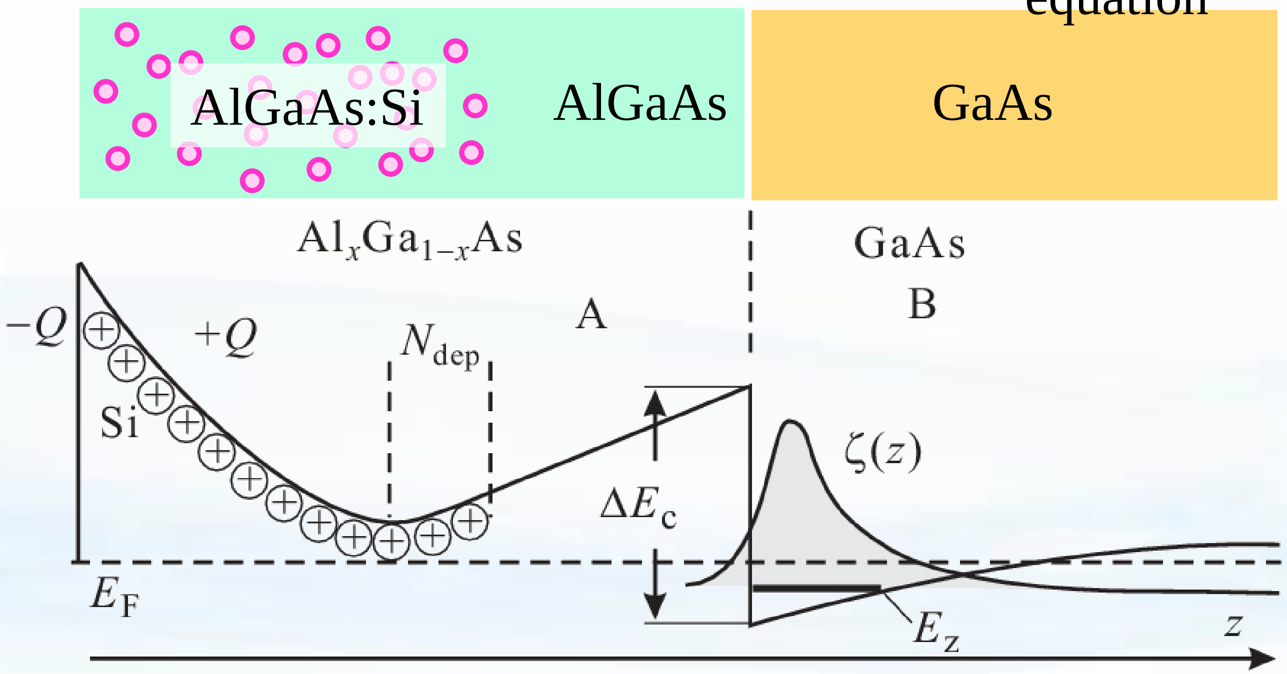




STEM image of
AlAs (30 nm)/GaAs (30nm)
superlattice

Modulation doping and 2-dimensional electrons

equation



Donor potential $V_D(z) = \frac{4\pi e^2}{\epsilon\epsilon_0} N_{\rm dep} z \quad z > 0$

$$\Psi(\boldsymbol{r}) = \psi(x, y)\zeta(z)$$

Electric field of sheet charge at z' $-\frac{4\pi e^2}{\epsilon\epsilon_0} n_{2d} |\zeta(z')|^2 |z - z'|$

$$V_{2d}(z) = -\frac{4\pi e^2}{\epsilon\epsilon_0} n_{2d}(E_z) \int_{-\xi}^{\infty} |\zeta(z')|^2 |z - z'| dz'$$

Heterointerface potential $V_h(z) = \Delta E_{\rm c}[1 - H(z)]$

Poisson-Schrödinger scheme

potential $$V(z) = V_h(z) + \frac{4\pi e^2}{\epsilon\epsilon_0}\left[N_{\rm dep} z - n_{2d}(E_z)\int_{-\xi}^{\infty} |z - z'||\zeta(z')|^2 dz'\right]$$

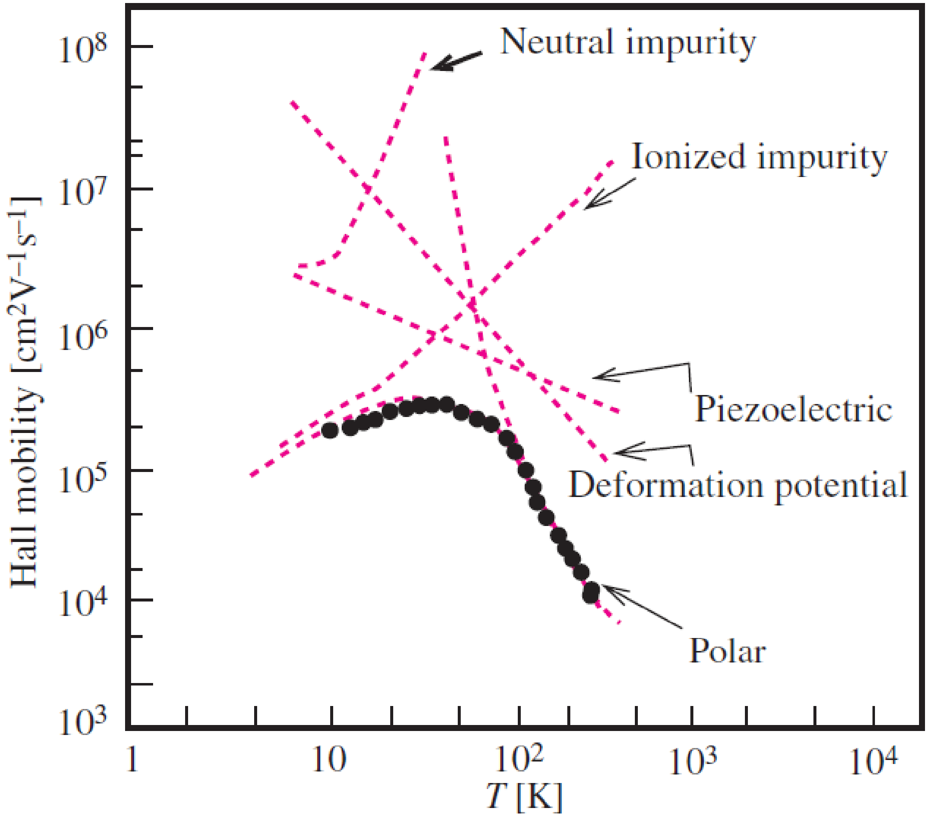
Schrödinger equation $$\left[-\frac{\hbar^2}{2m^*(z)}\frac{\partial^2}{\partial z^2} + V(z)\right]\zeta(z) = E_z\zeta(z)$$

Boundary condition $$\zeta(0)^{(\rm A)} = \zeta(0)^{(\rm B)}, \quad \frac{1}{m_{\rm A}^*}\frac{d\zeta^{(\rm A)}}{dz}\Bigg| = \frac{1}{m_{\rm B}^*}\frac{d\zeta^{(\rm B)}}{dz}\Bigg|$$

Electron mobility in MODFET

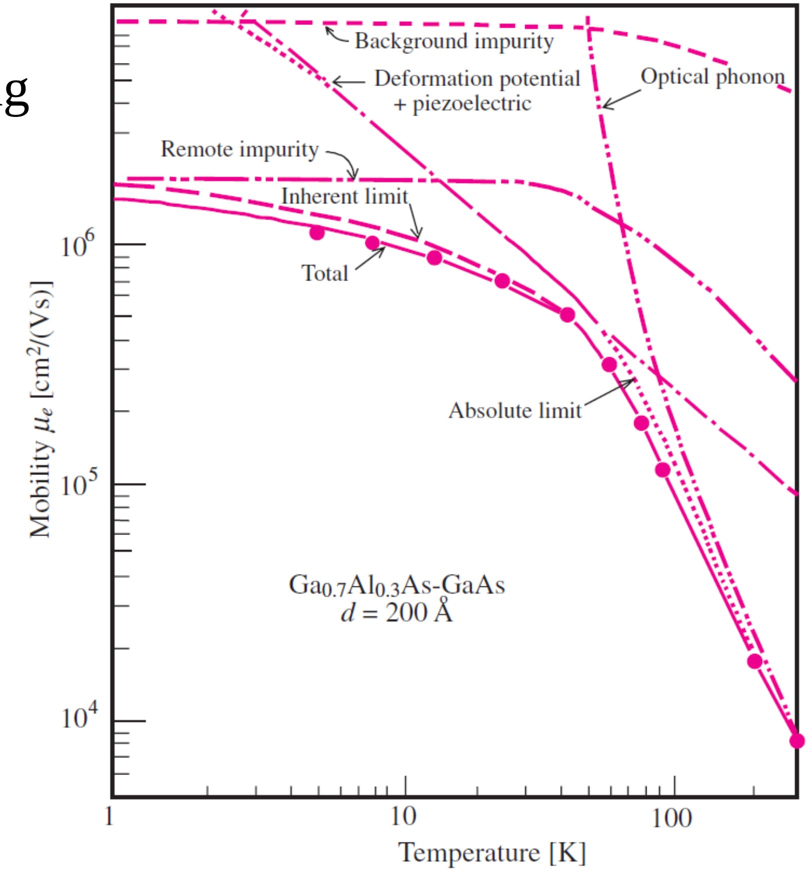
Matthiessen's rule (series connection of scattering)

$$\frac{1}{\tau_{\text{total}}} = \sum_{\beta} \frac{1}{\tau_{\beta}} = \frac{1}{\tau_{\text{defects}}} + \frac{1}{\tau_{\text{cattier}}} + \frac{1}{\tau_{\text{lattice}}} + \cdots \qquad \frac{1}{\mu_{\text{total}}} = \sum_{\beta} \frac{1}{\mu_{\beta}} = \frac{1}{\mu_{\text{defects}}} + \frac{1}{\mu_{\text{cattier}}} + \frac{1}{\mu_{\text{lattice}}} + \cdots$$



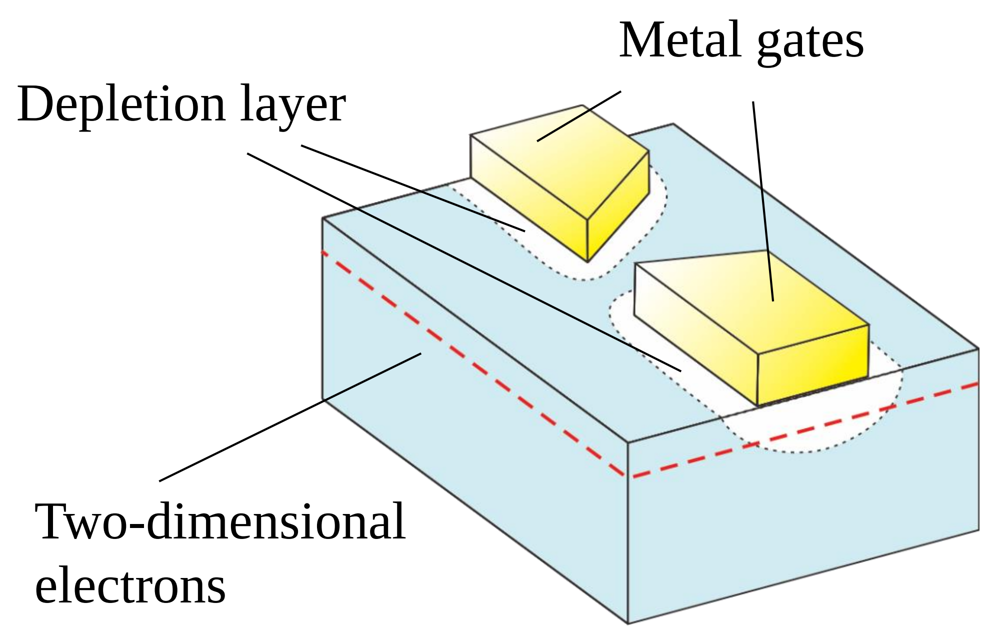
Fletcher *et al.*, J. Phys. C **5**, 212 (1972)

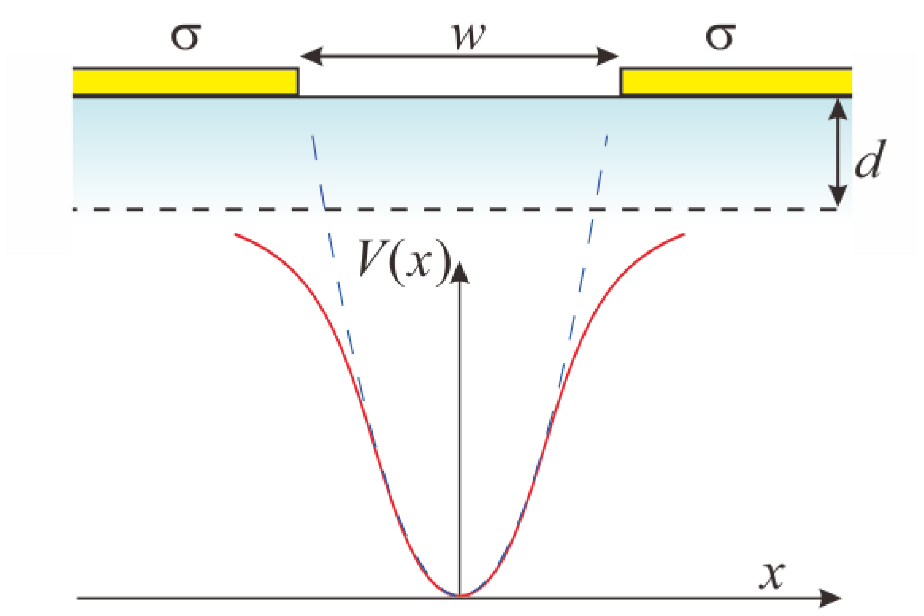
Reduction of impurity scattering by modulation doping structure



Walukiewicz *et al.* Phys. Rev. B **30**, 4571 (1984).

Formation of quantum wires: split gate



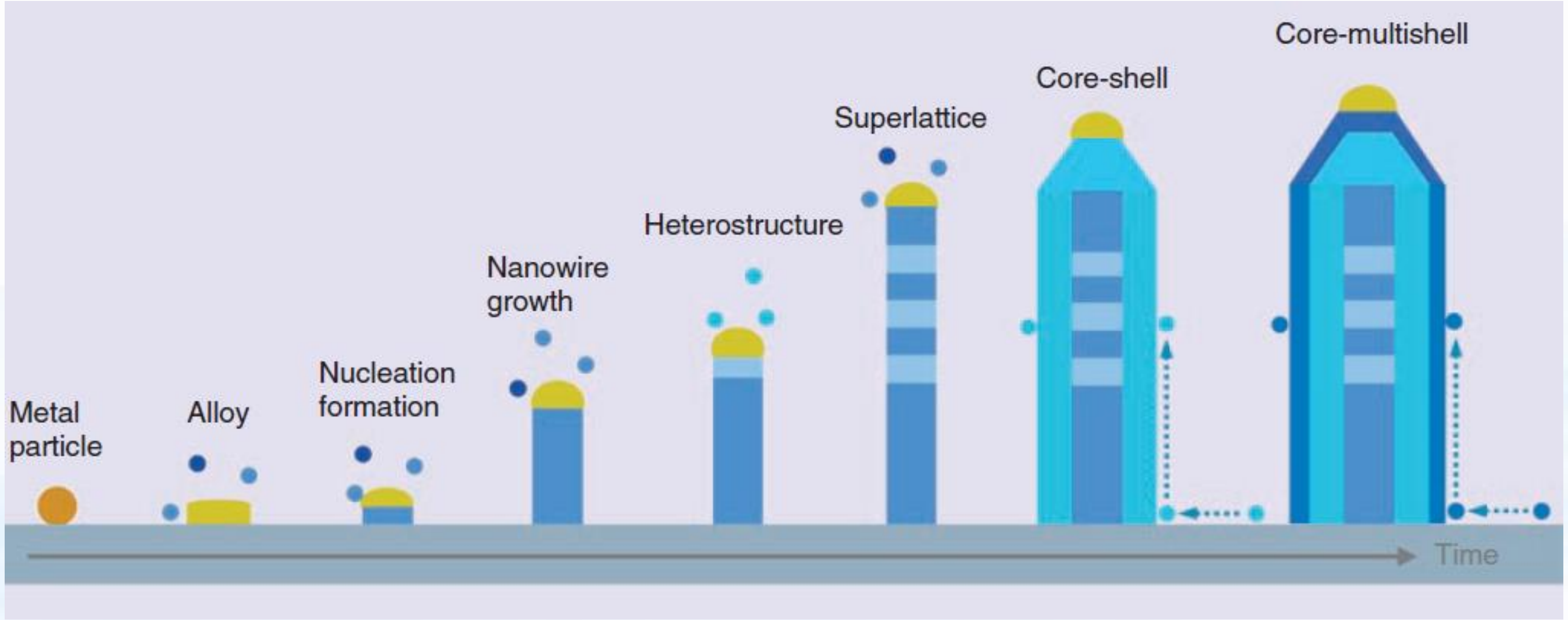


Two-dimensional electrons are pinched with depletion layers from Schottky gates to a one-dimensional system.

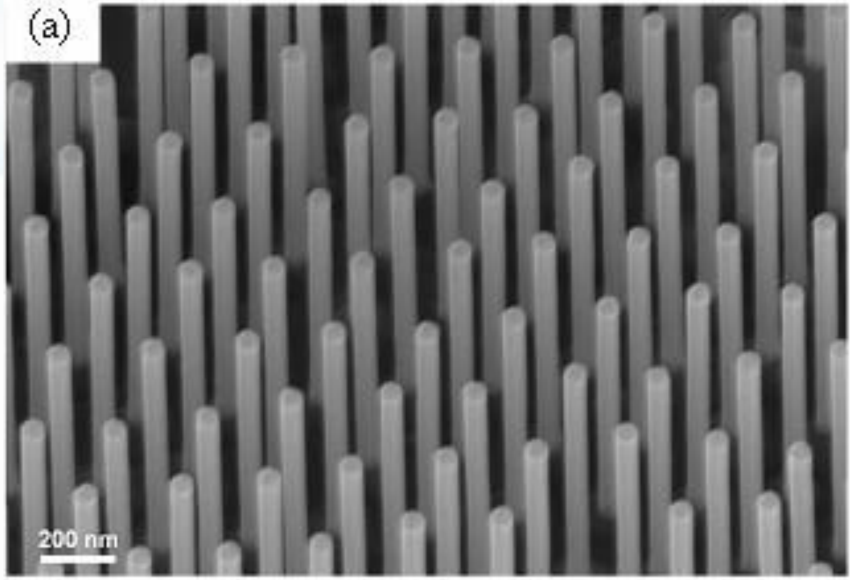
Electric field along z-axis can be approximated as $\mathcal{E}_z(d) = \frac{-\sigma}{2\pi\epsilon\epsilon_0}\left[\pi + \arctan\frac{x-w/2}{d} - \arctan\frac{x+w/2}{d}\right]$

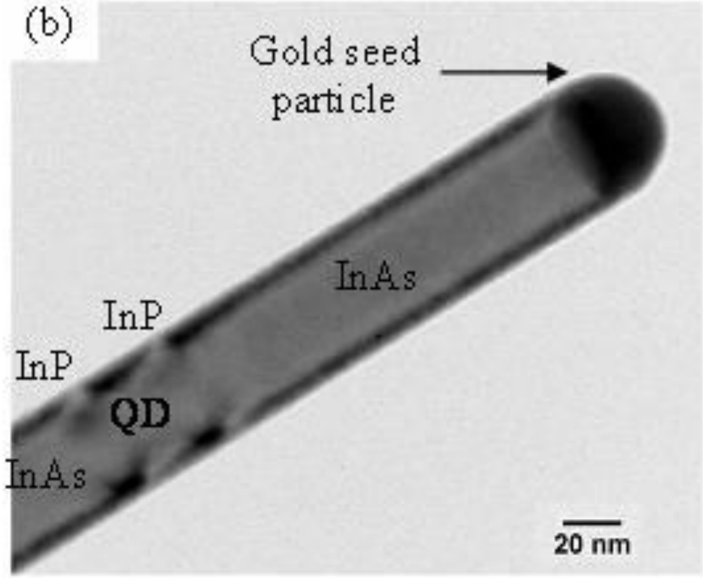
The bottom part of the confinement potential can be approximated by harmonic potential.

Self-assembled nano-wires



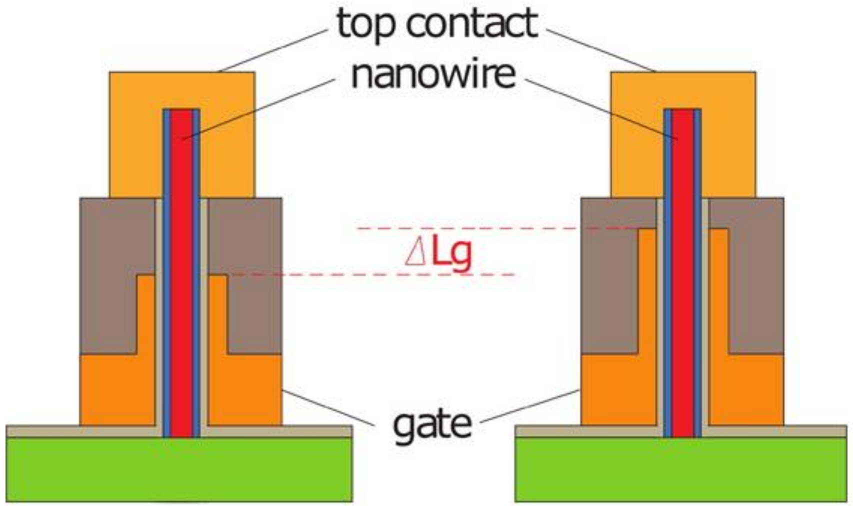
G. Zhang et al. NTT technical Review

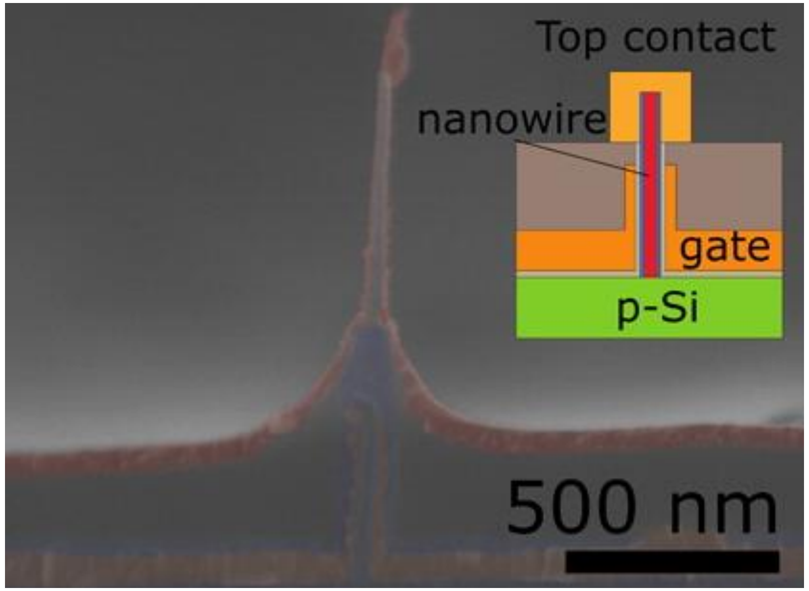


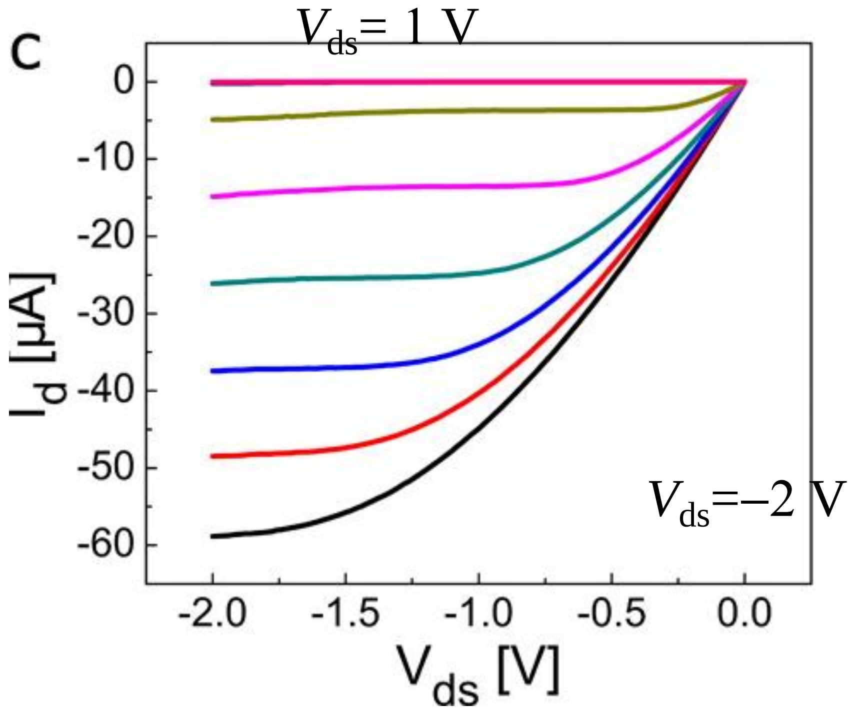


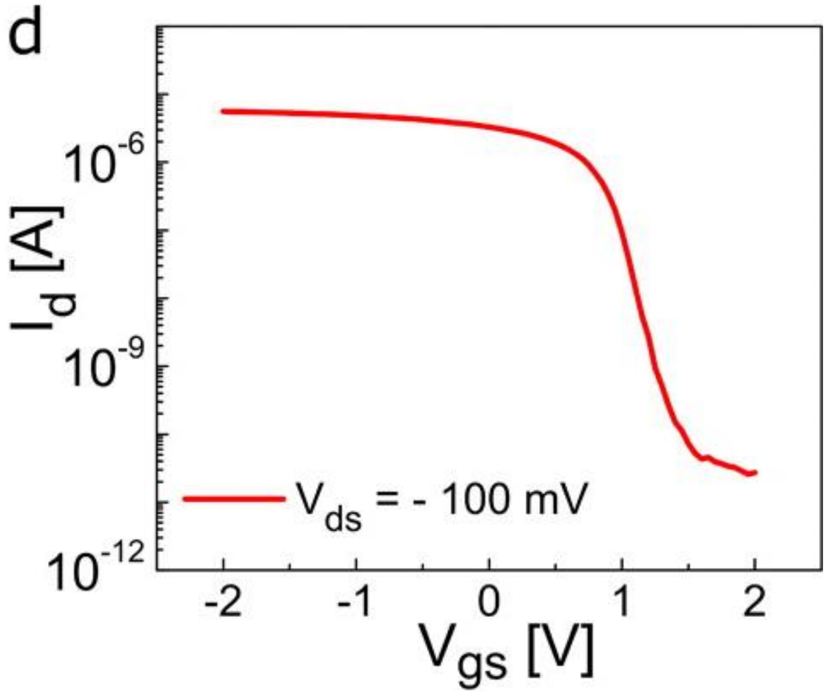
http://iemn.univ-lille1.fr/sites_perso/vignaud/english/35_nanowires.htm

Core-shell nanowire transistor



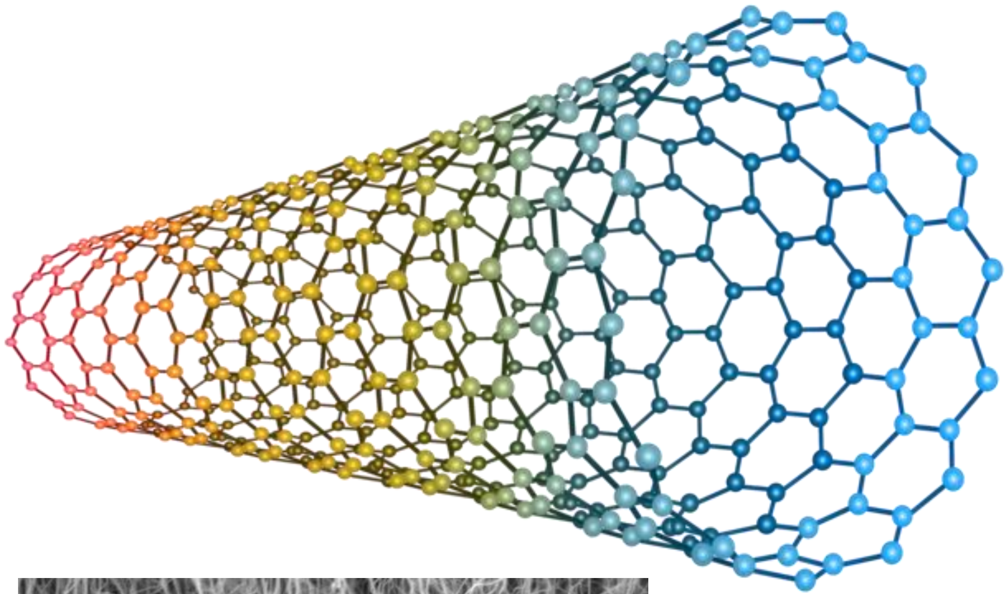


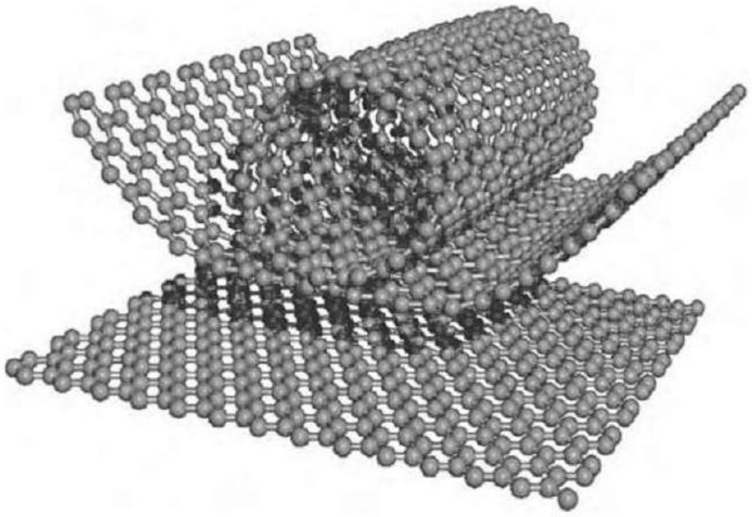


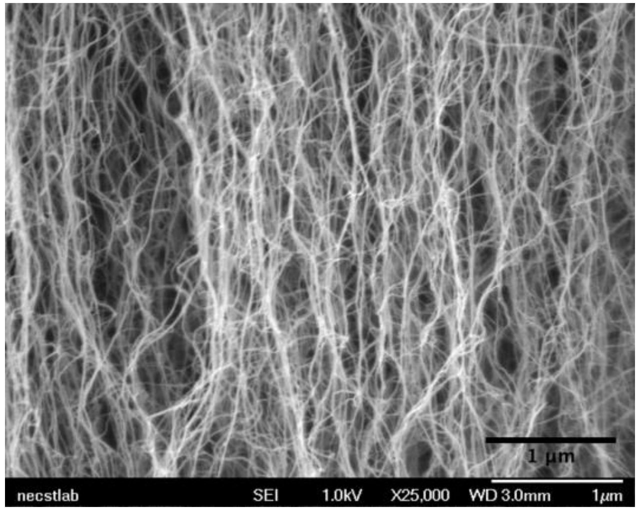


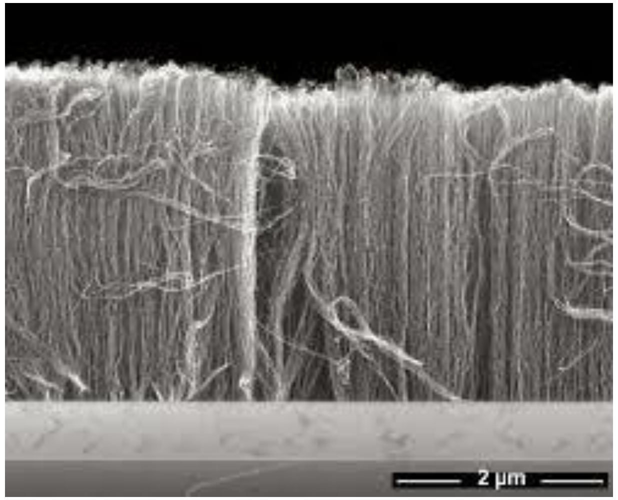
L. Chen *et al.*,
Nano Letters **16**, 420 (2016).

Carbon nanotube



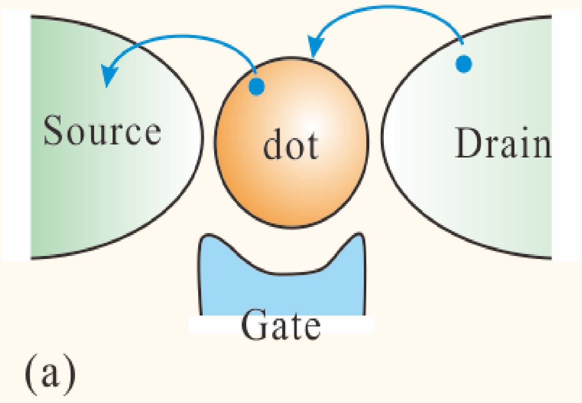


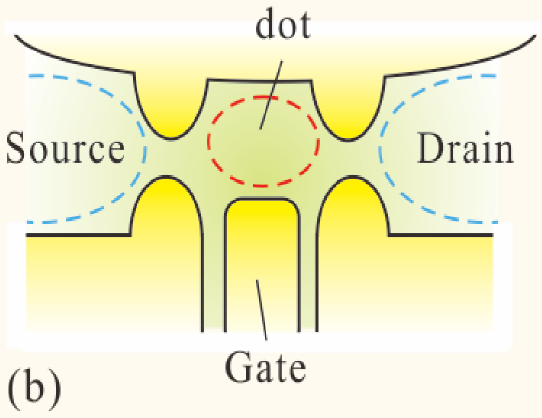


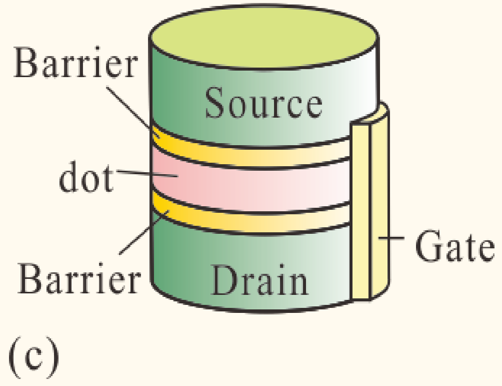


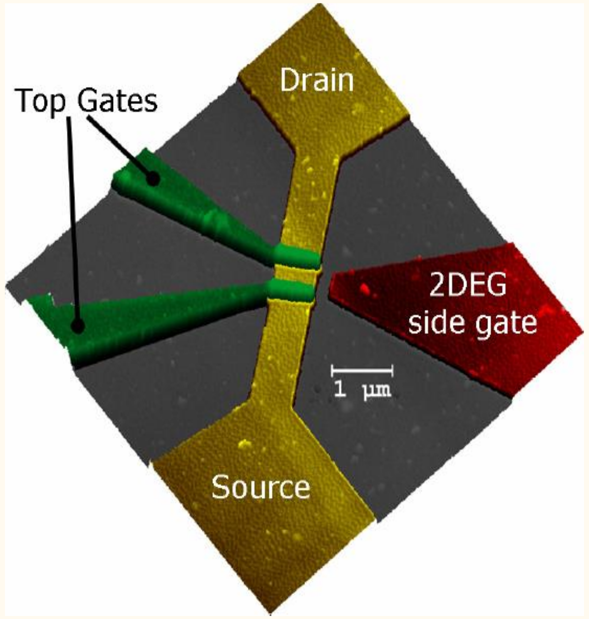
Quantum dots: zero-dimensional system

Quantum dots with nano-fabrication techniques

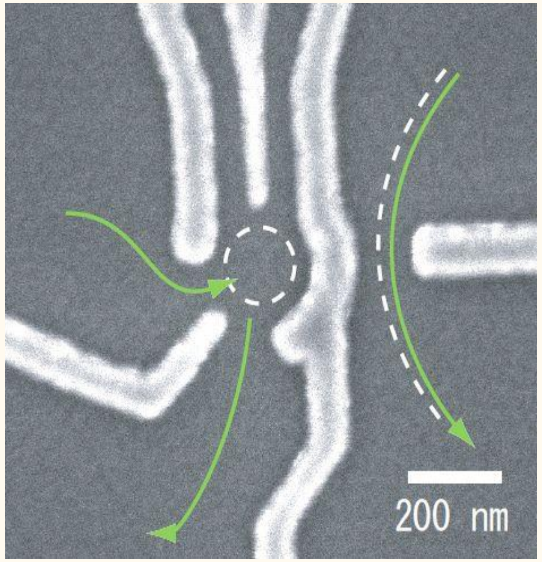






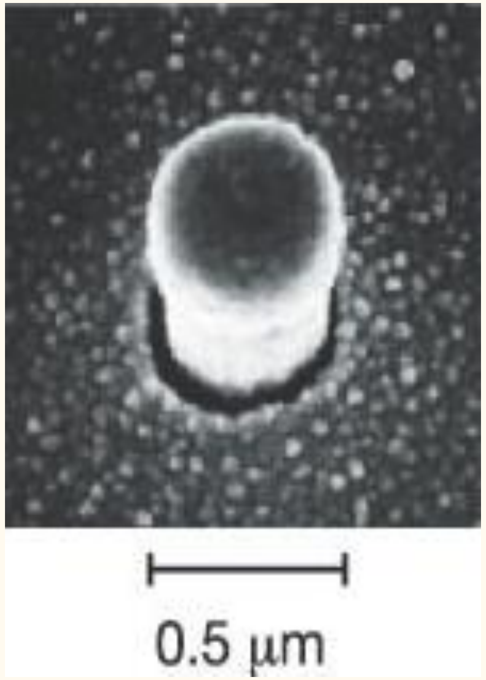


wrap gate



split gate

with charge detector

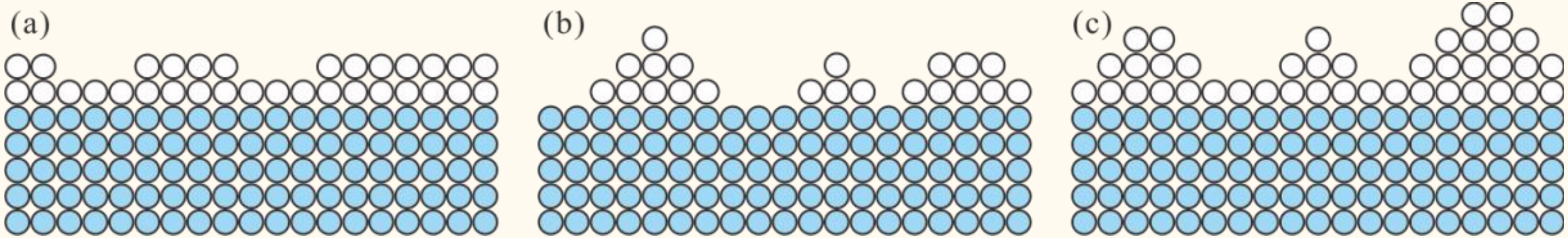


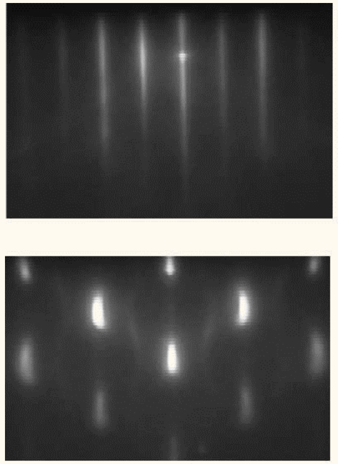
vertical type

Formation of quantum dots: self assemble

MBE growth modes

Frank-van der Merve Volmer-Weber Stranski-Krastanow





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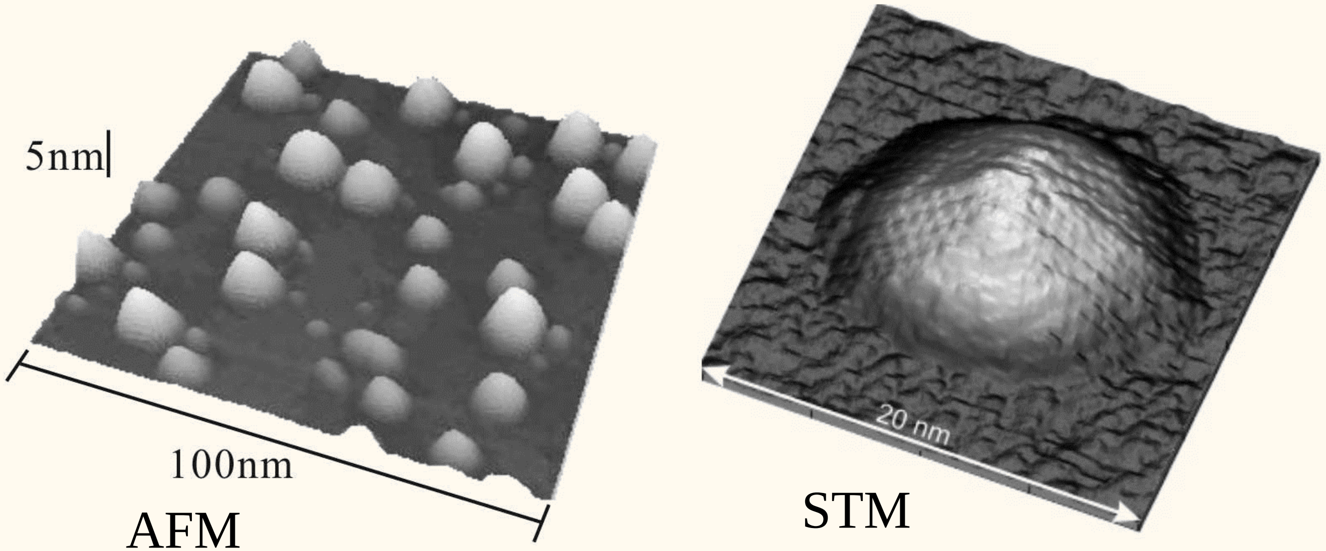
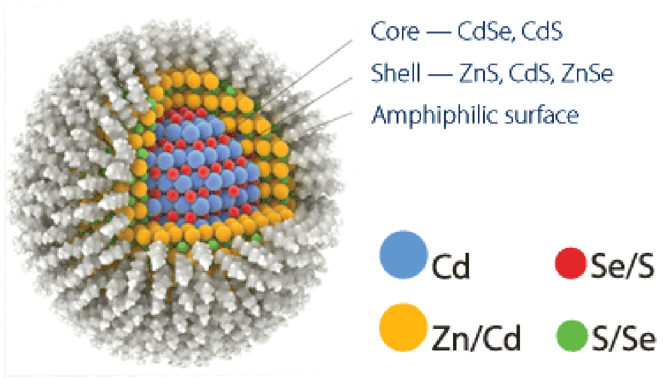
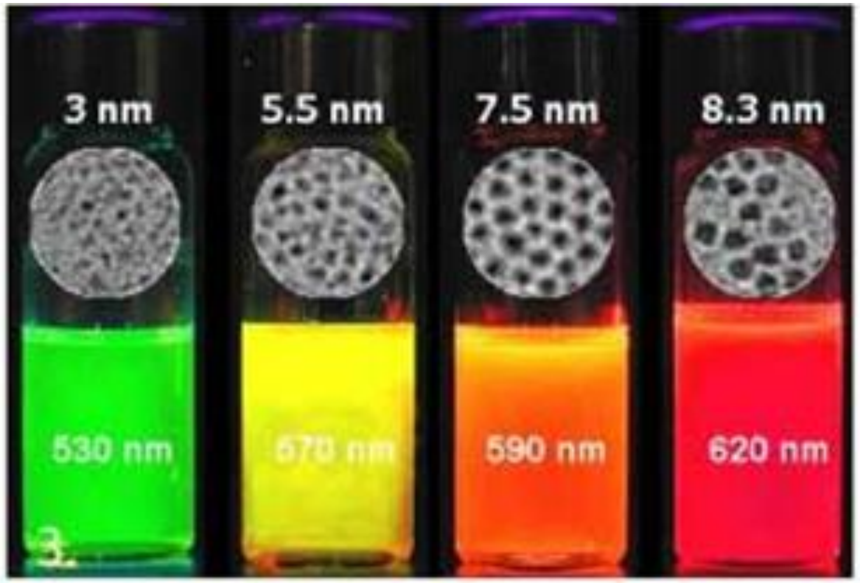


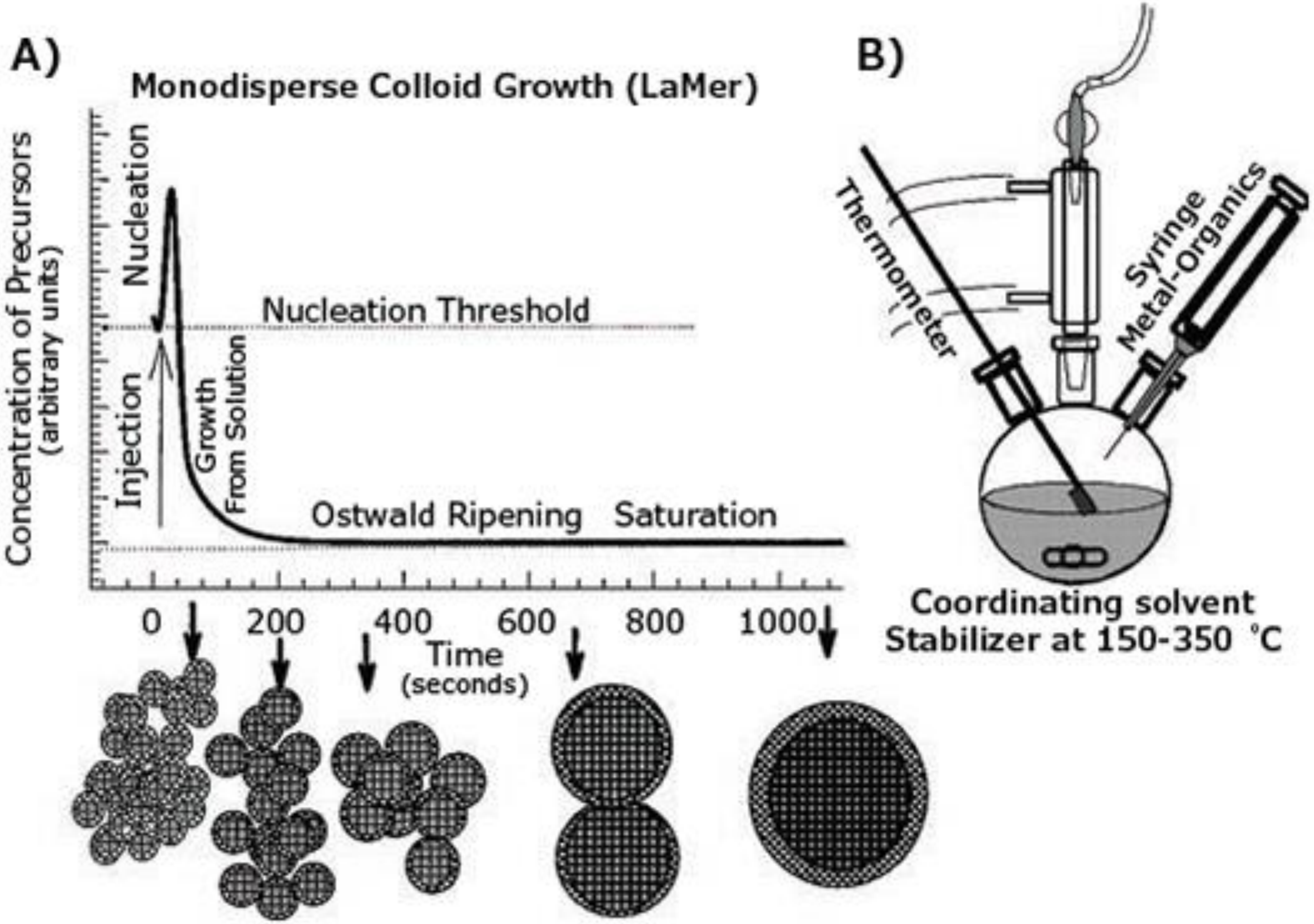
AFM

STM

Formation of quantum dots: Colloidal nano-crystals







Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.6.16 Lecture 10

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

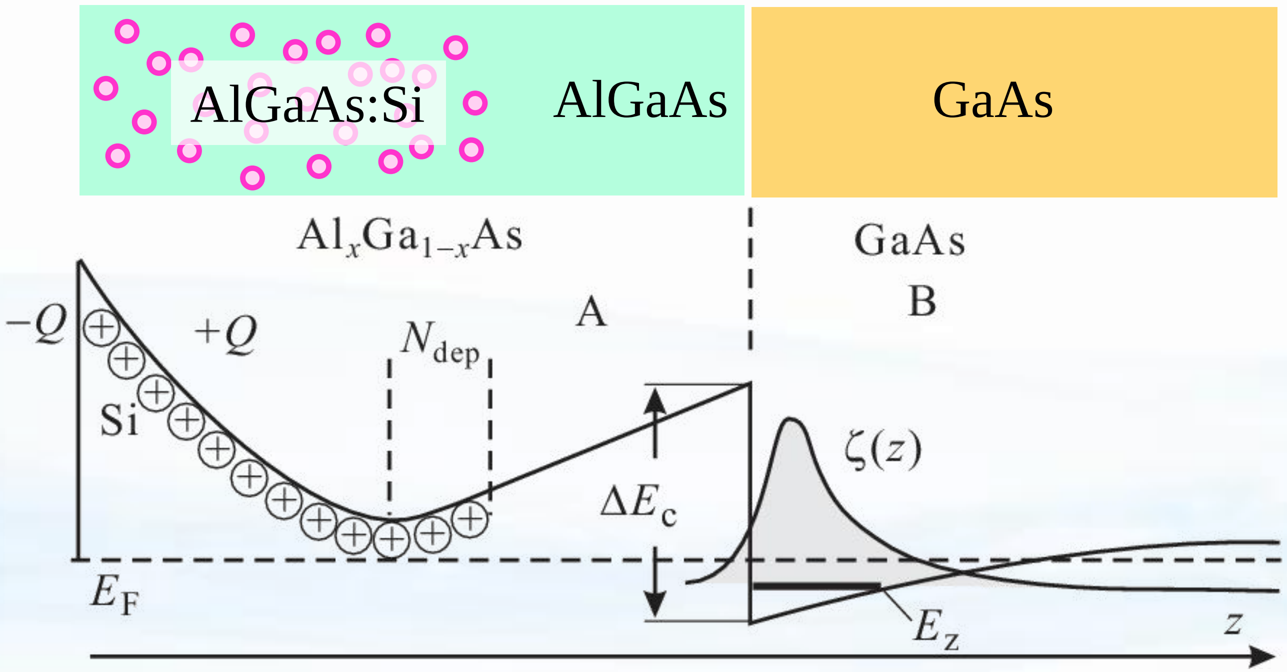
Review of last week

- Band discontinuity at heterojunction

Chapter 7 Quantum Structure (Quantum wells, wires, dots)

- Quantum wells
- Excitons in quantum wells
- Quantum barriers

Modulation doping and 2-dimensional electrons



Donor potential $V_D(z) = \frac{4\pi e^2}{\epsilon\epsilon_0} N_{\rm dep} z \quad z > 0$

$$\Psi(\boldsymbol{r}) = \psi(x, y)\zeta(z)$$

Electric field of sheet charge at z' $-\frac{4\pi e^2}{\epsilon\epsilon_0} n_{2d} |\zeta(z')|^2 |z - z'|$

$$V_{2d}(z) = -\frac{4\pi e^2}{\epsilon\epsilon_0} n_{2d}(E_z) \int_{-\xi}^{\infty} |\zeta(z')|^2 |z - z'| dz'$$

Heterointerface potential $V_h(z) = \Delta E_c [1 - H(z)]$

Poisson-Schrödinger scheme

potential $V(z) = V_h(z) + \frac{4\pi e^2}{\epsilon\epsilon_0} \left[N_{\rm dep} z - n_{2d}(E_z) \int_{-\xi}^{\infty} |z - z'| |\zeta(z')|^2 dz' \right]$

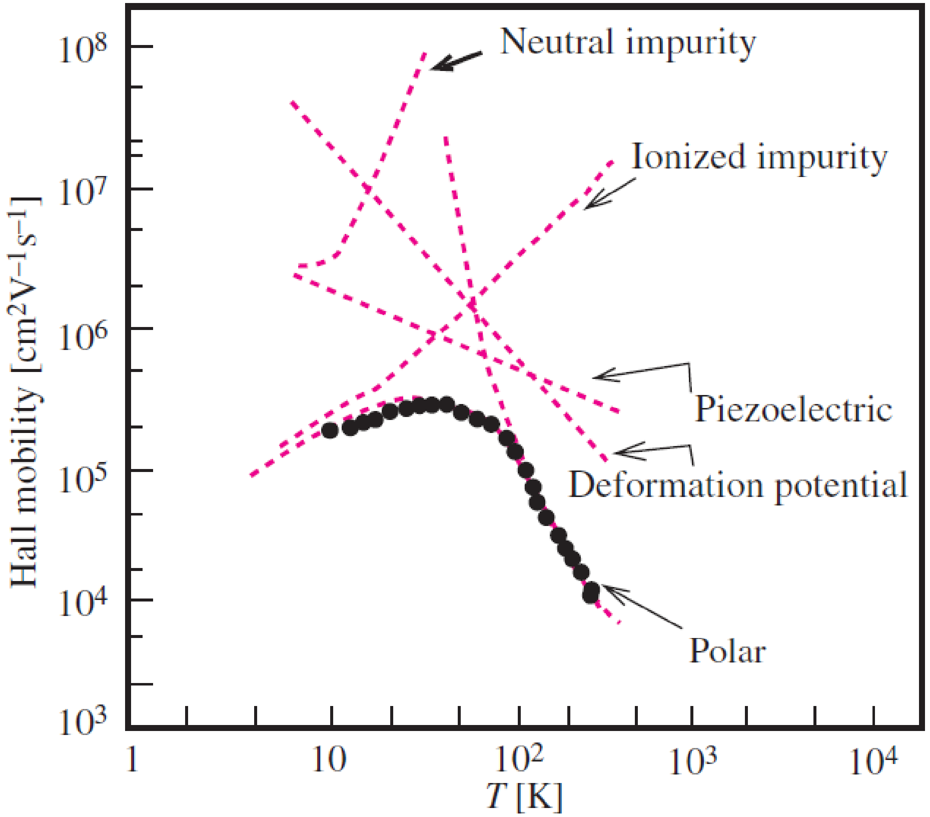
Schrödinger equation $\left[-\frac{\hbar^2}{2m^*(z)} \frac{\partial^2}{\partial z^2} + V(z) \right] \zeta(z) = E_z \zeta(z)$

Boundary condition $\zeta(0)^{(A)} = \zeta(0)^{(B)}, \quad \frac{1}{m_A^*} \frac{d\zeta^{(A)}}{dz} \Big| = \frac{1}{m_B^*} \frac{d\zeta^{(B)}}{dz} \Big|$

Electron mobility in MODFET

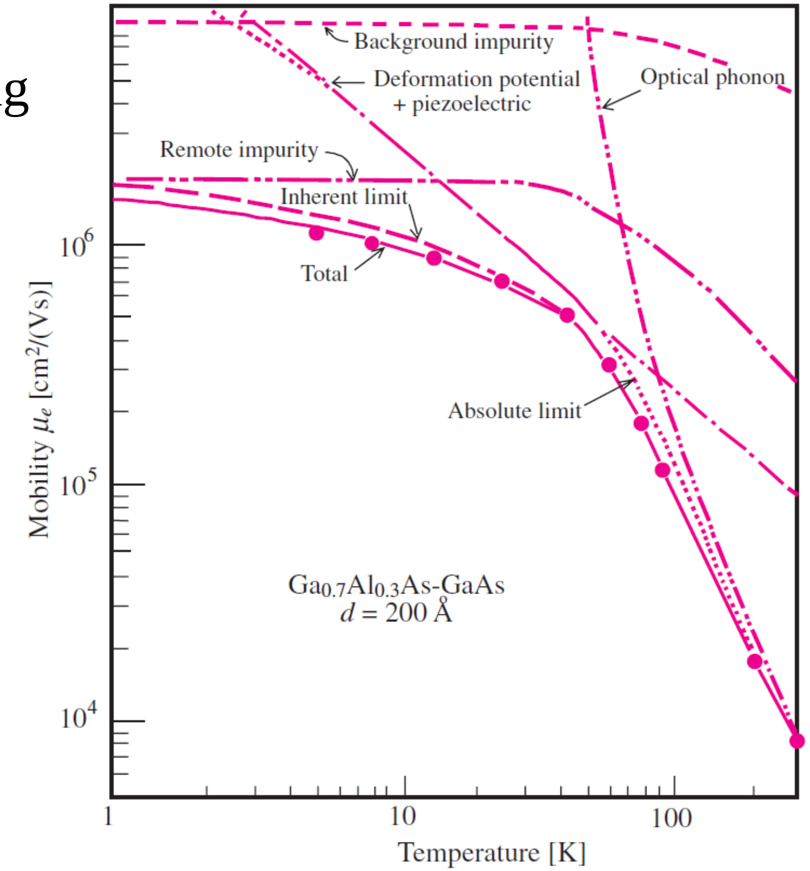
Matthiessen's rule (series connection of scattering)

$$\frac{1}{\tau_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\tau_{\beta}} = \frac{1}{\tau_{\mathrm{defects}}} + \frac{1}{\tau_{\mathrm{cattier}}} + \frac{1}{\tau_{\mathrm{lattice}}} + \cdots \qquad \frac{1}{\mu_{\mathrm{total}}} = \sum_{\beta} \frac{1}{\mu_{\beta}} = \frac{1}{\mu_{\mathrm{defects}}} + \frac{1}{\mu_{\mathrm{cattier}}} + \frac{1}{\mu_{\mathrm{lattice}}} + \cdots$$



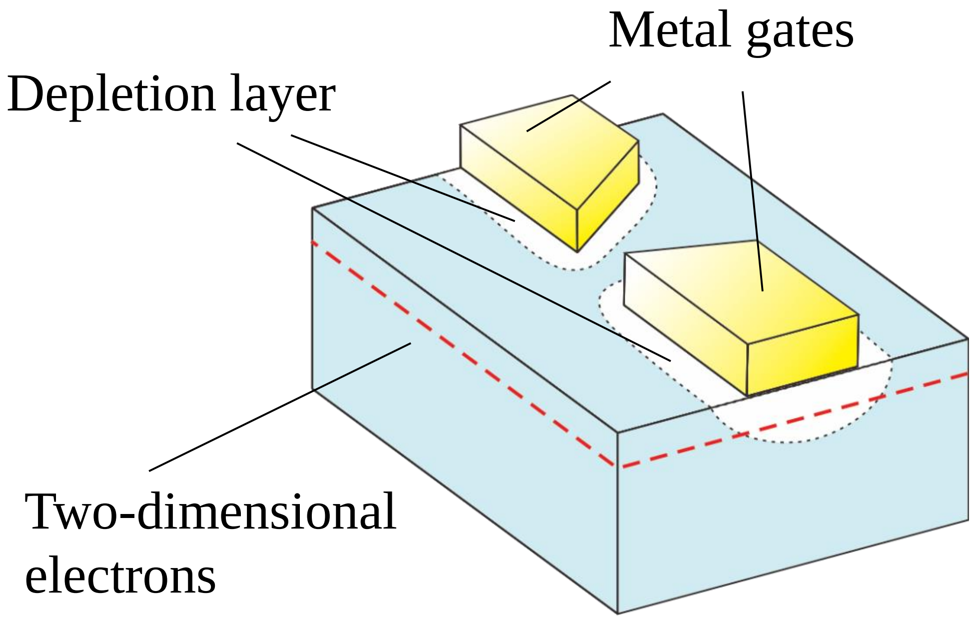
Fletcher *et al.*, J. Phys. C **5**, 212 (1972)

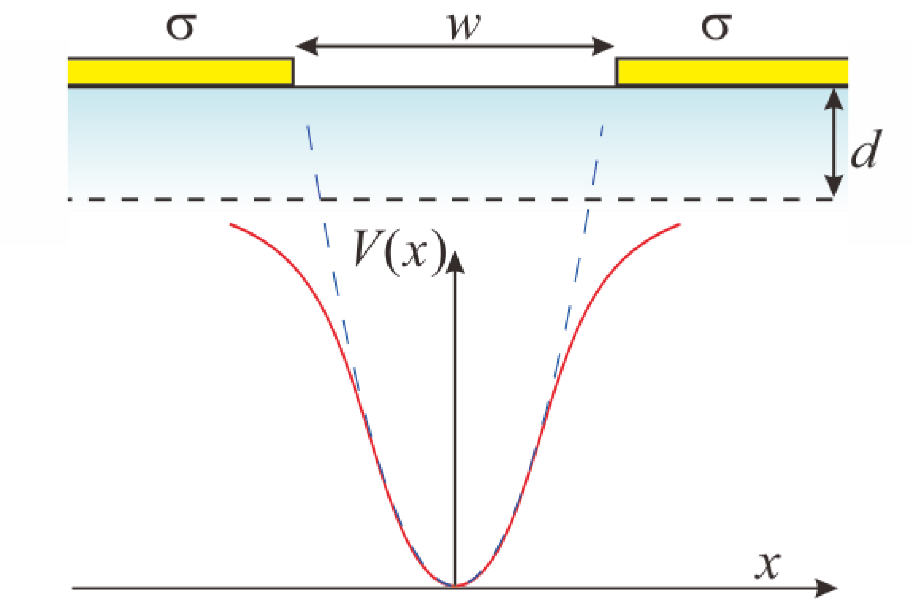
Reduction of impurity scattering by modulation doping structure



Walukiewicz *et al.* Phys. Rev. B **30**, 4571 (1984).

Formation of quantum wires: split gate



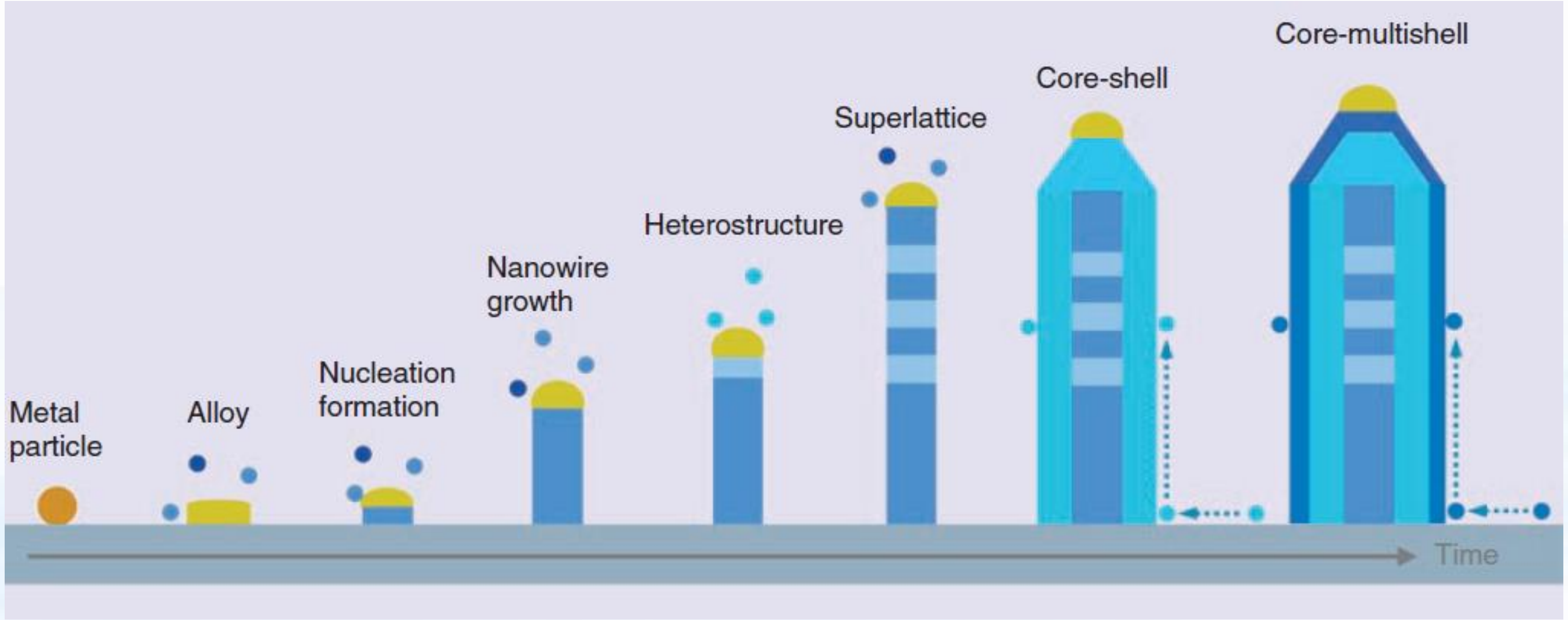


Two-dimensional electrons are pinched with depletion layers from Schottky gates to a one-dimensional system.

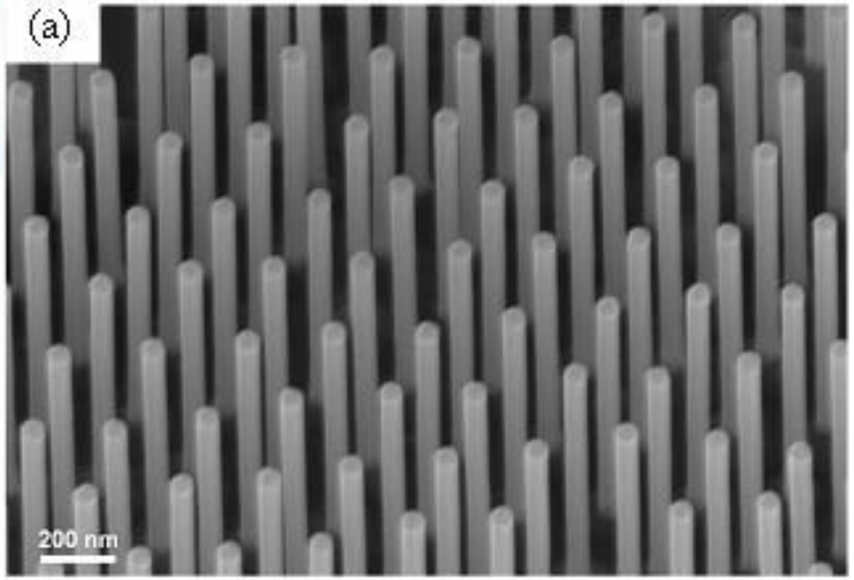
Electric field along z-axis can be approximated as $$\mathcal{E}_z(d) = \frac{-\sigma}{2\pi\epsilon\epsilon_0}\left[\pi + \arctan\frac{x - w/2}{d} - \arctan\frac{x + w/2}{d}\right]$$

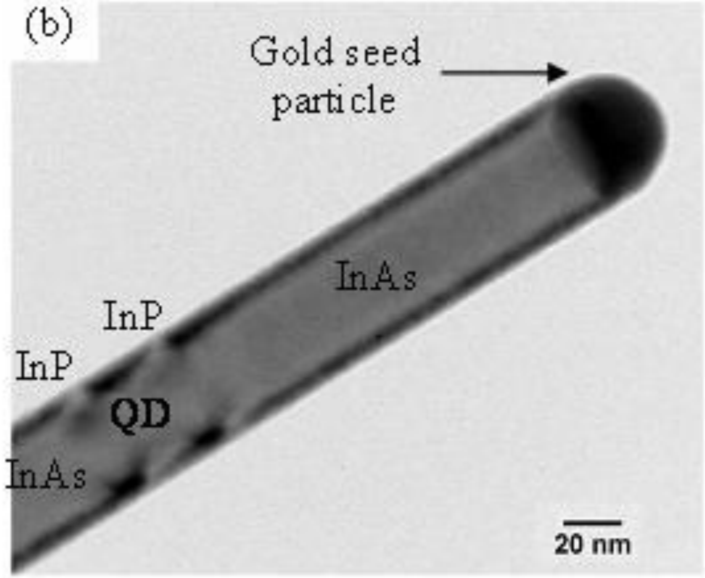
The bottom part of the confinement potential can be approximated by harmonic potential.

Self-assembled nano-wires



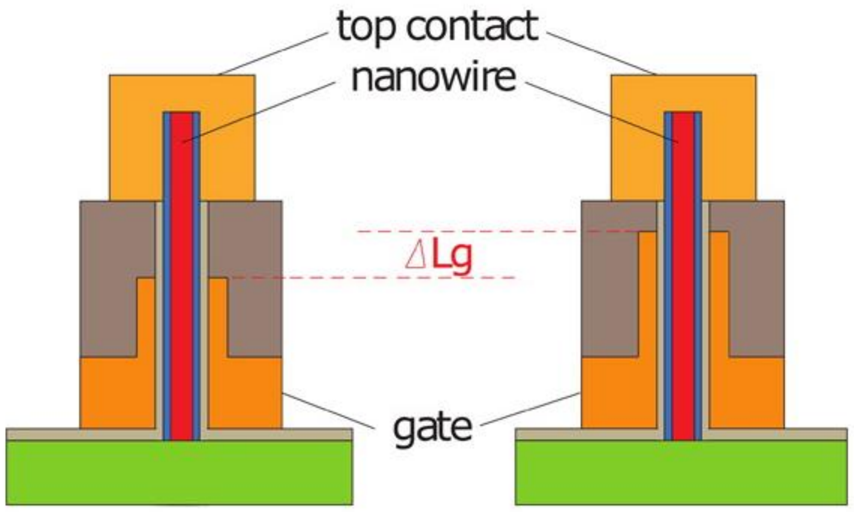
G. Zhang et al.
NTT technical
Review

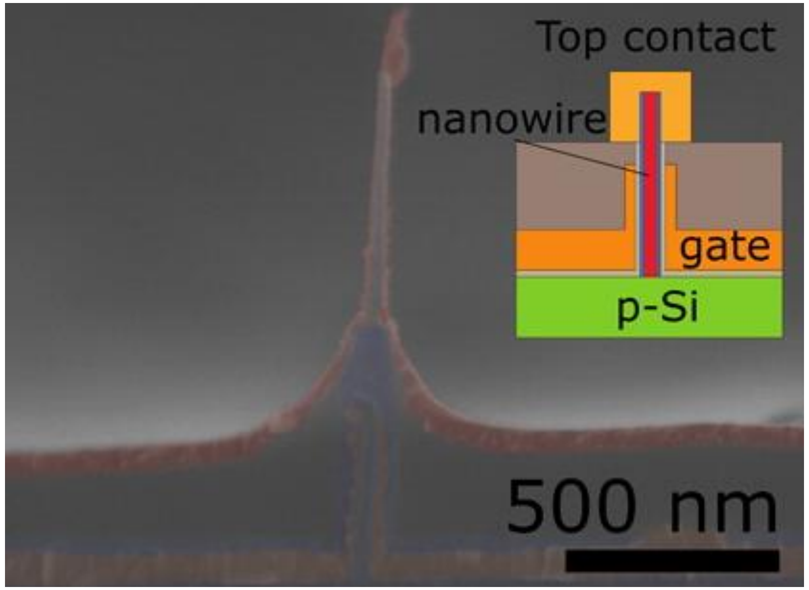


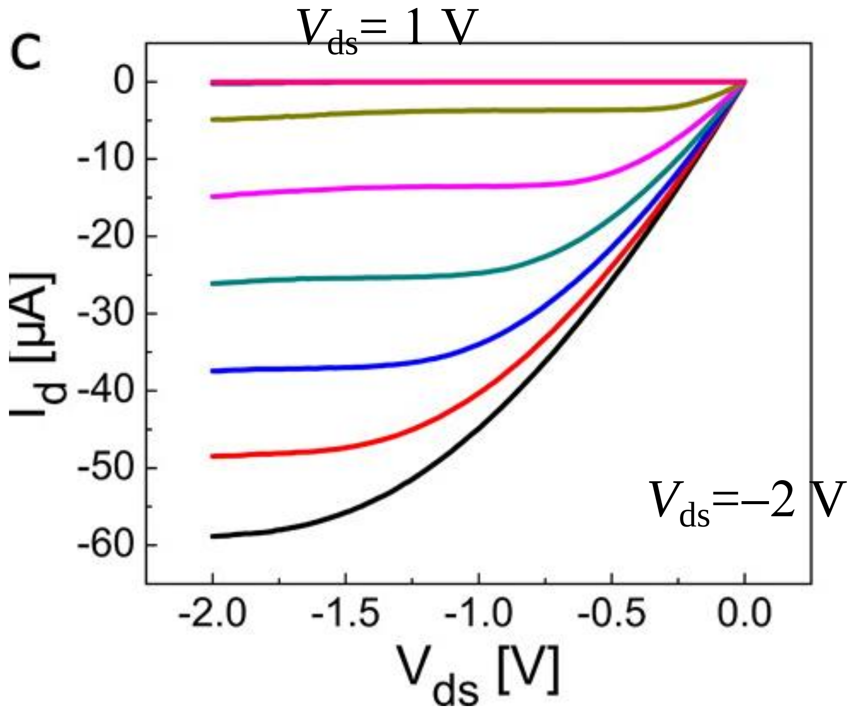


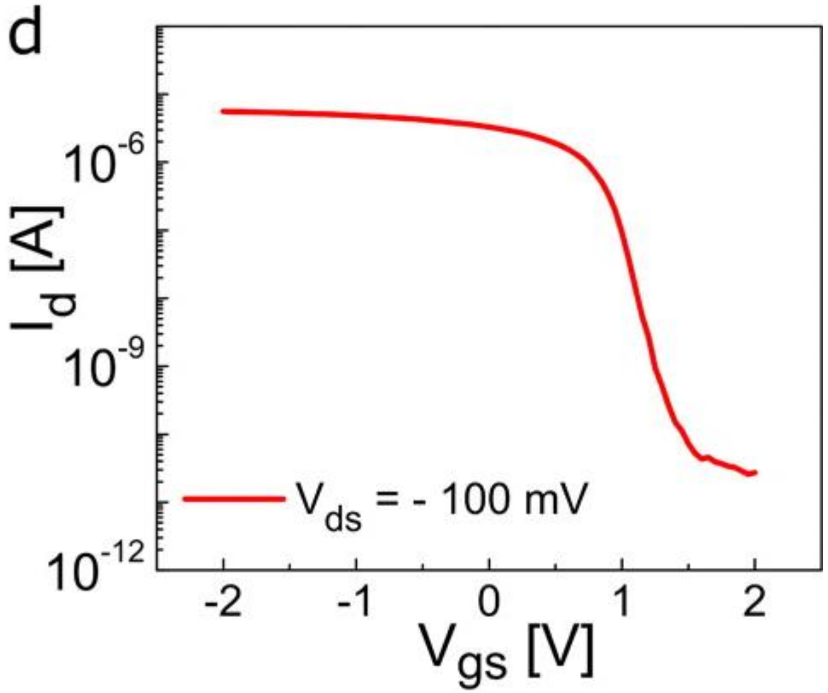
http://iemn.univ-lille1.fr/sites_perso/vignaud/english/35_nanowires.htm

Core-shell nanowire transistor



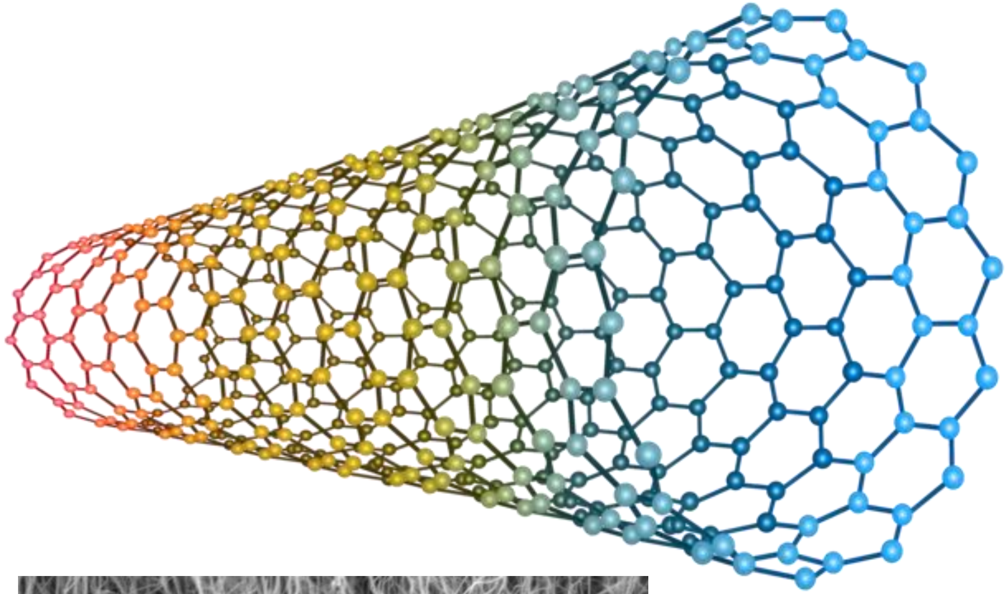


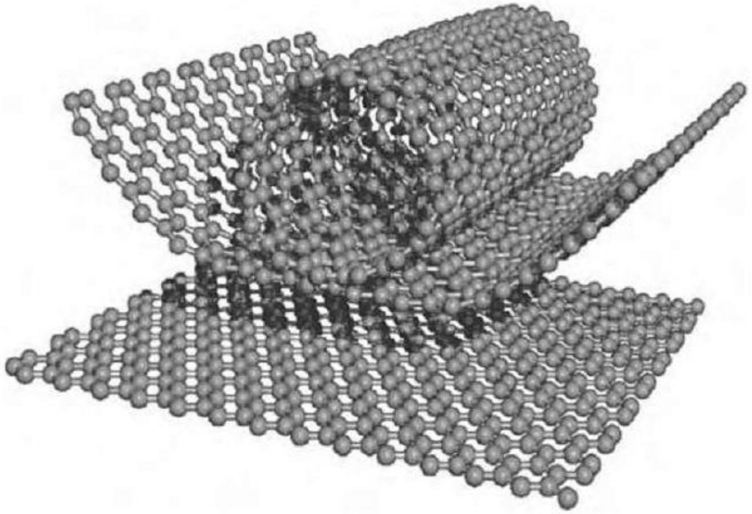


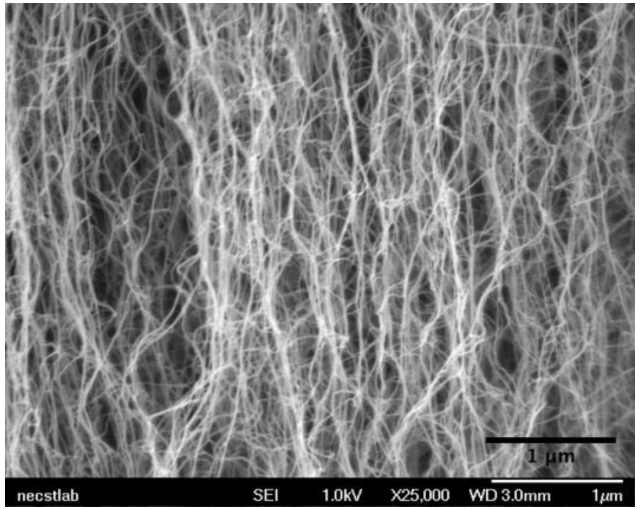


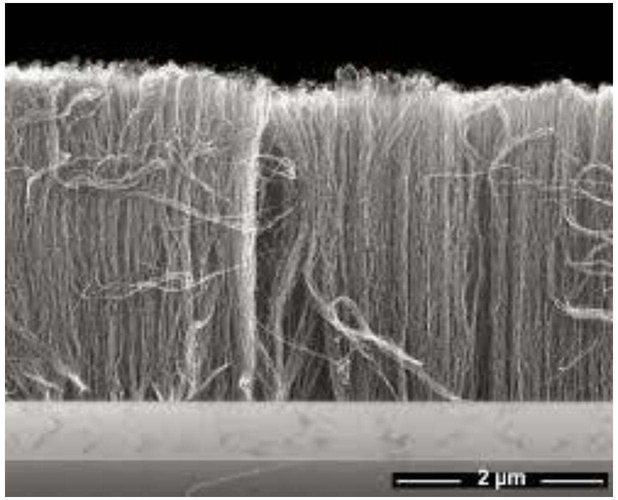
L. Chen *et al.*,
Nano Letters **16**, 420 (2016).

Carbon nanotube



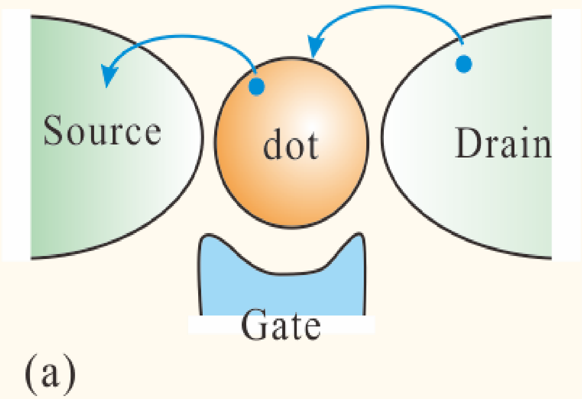


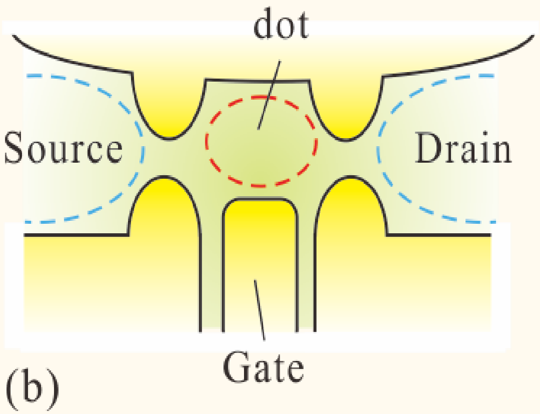


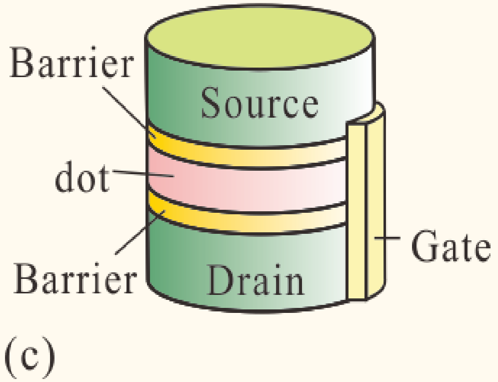


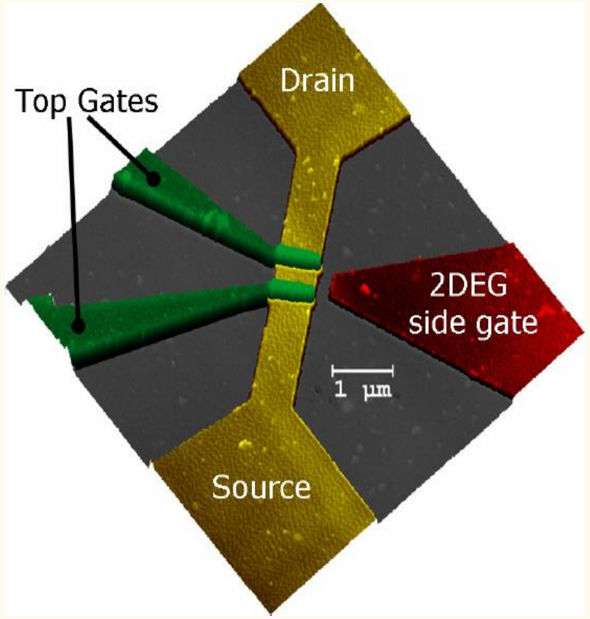
Quantum dots: zero-dimensional system

Quantum dots with nano-fabrication techniques

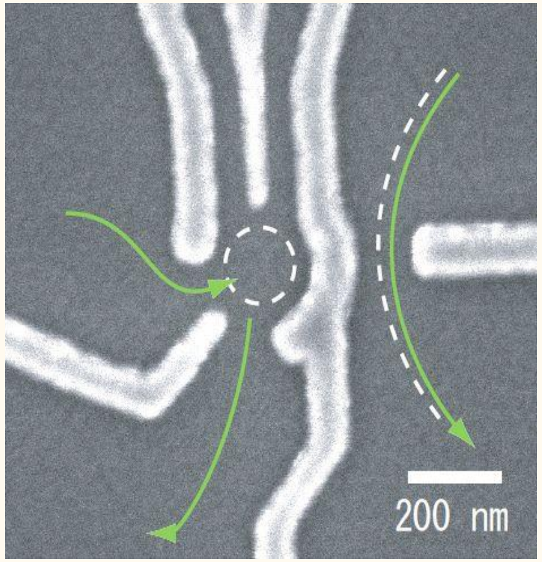






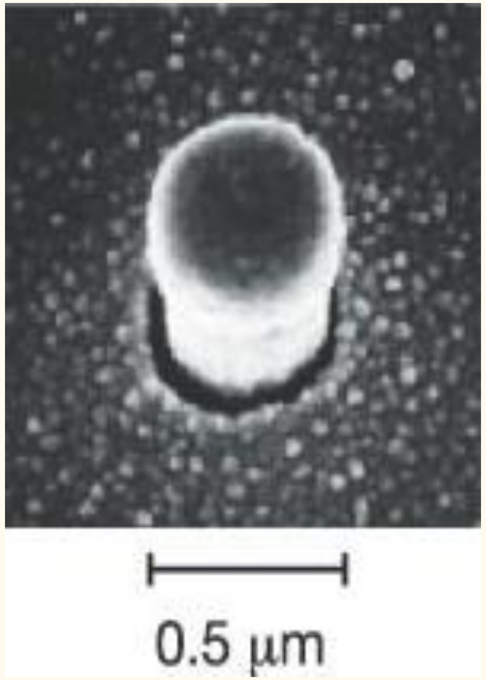


wrap gate



split gate

with charge detector

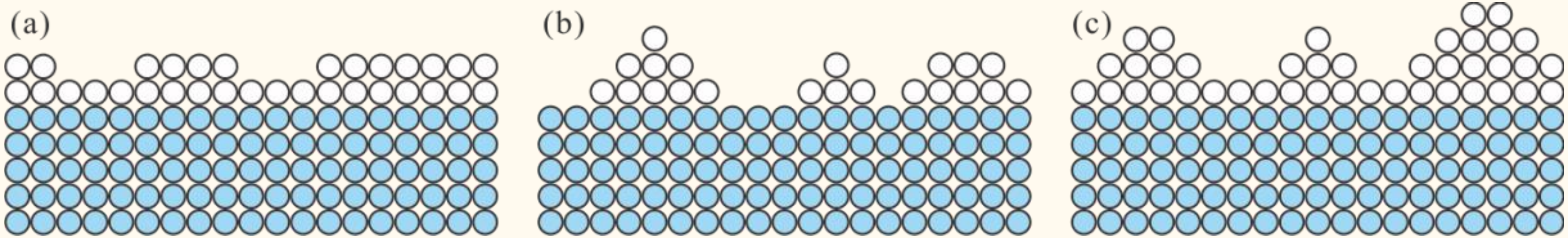


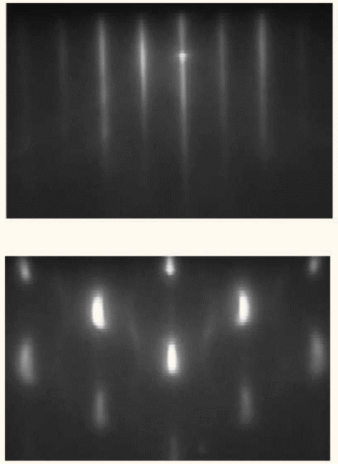
vertical type

Formation of quantum dots: self assemble

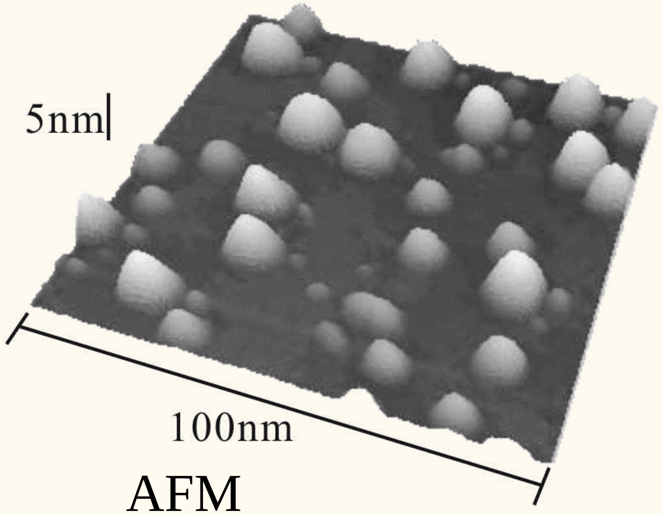
MBE growth modes

Frank-van der Merve   Volmer-Weber   Stranski-Krastanow

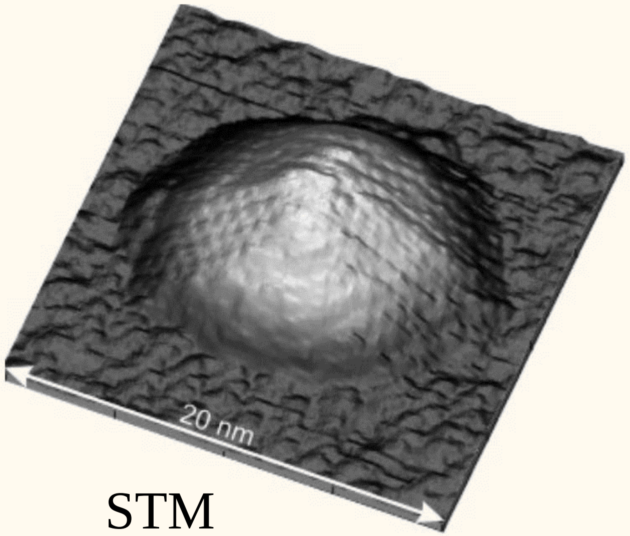




RHEED

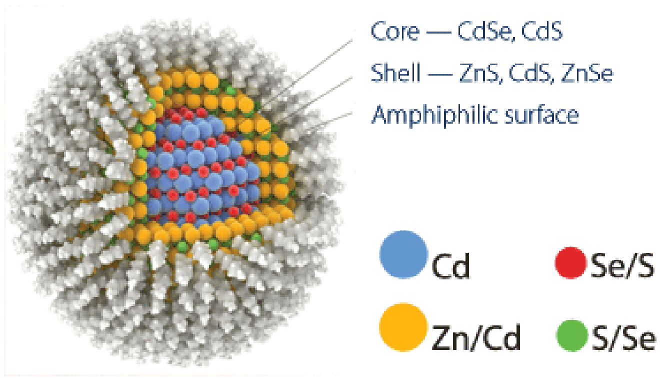


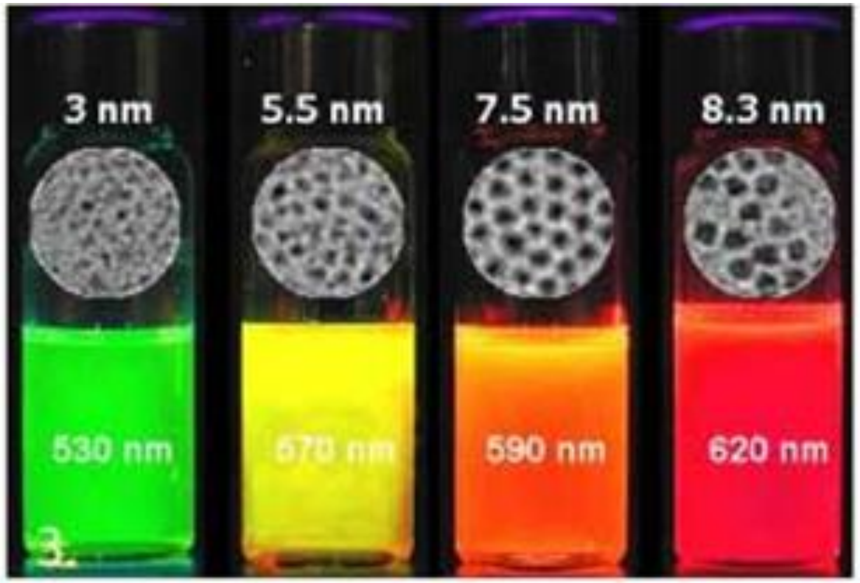
AFM

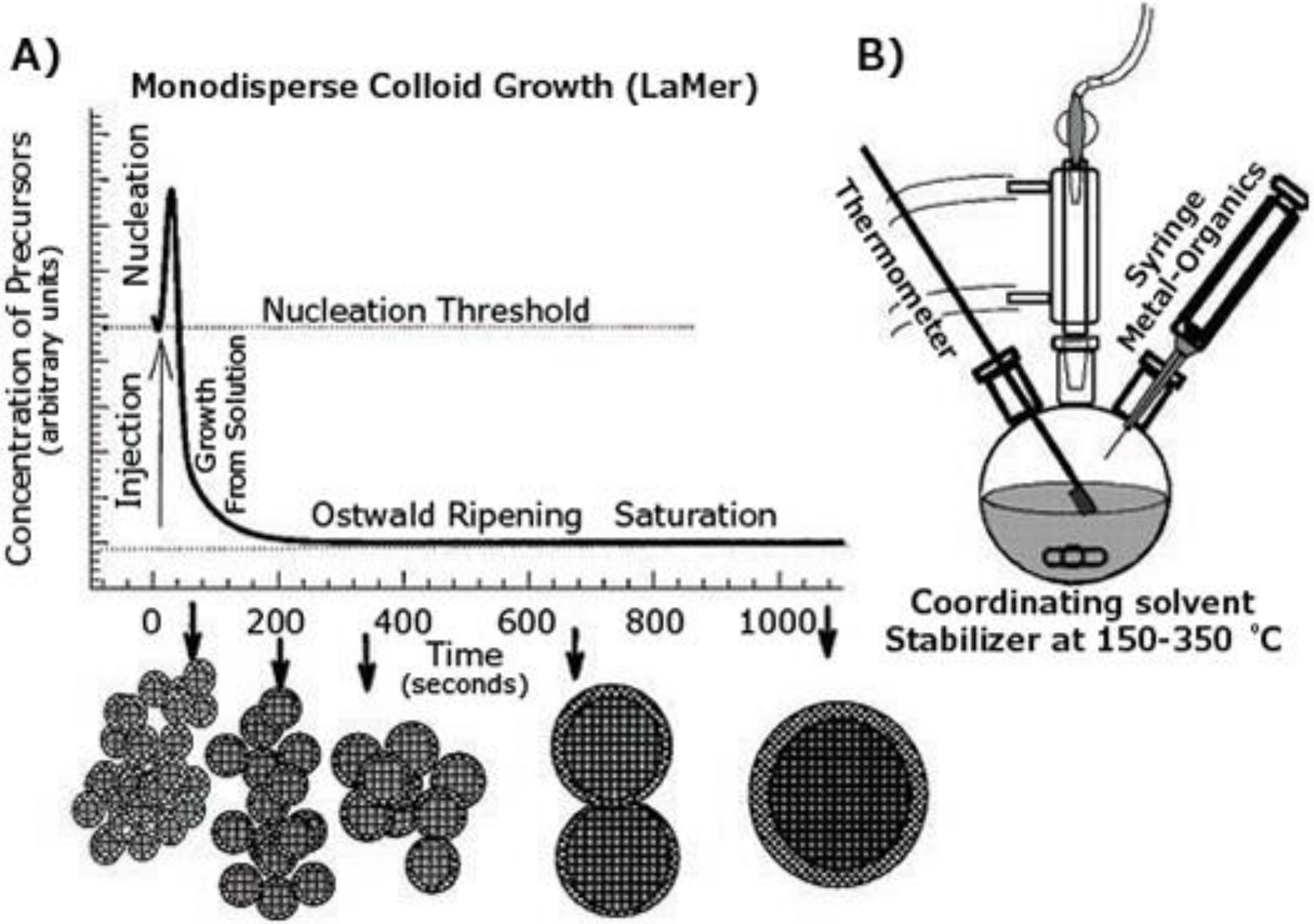


STM

Formation of quantum dots: Colloidal nano-crystals

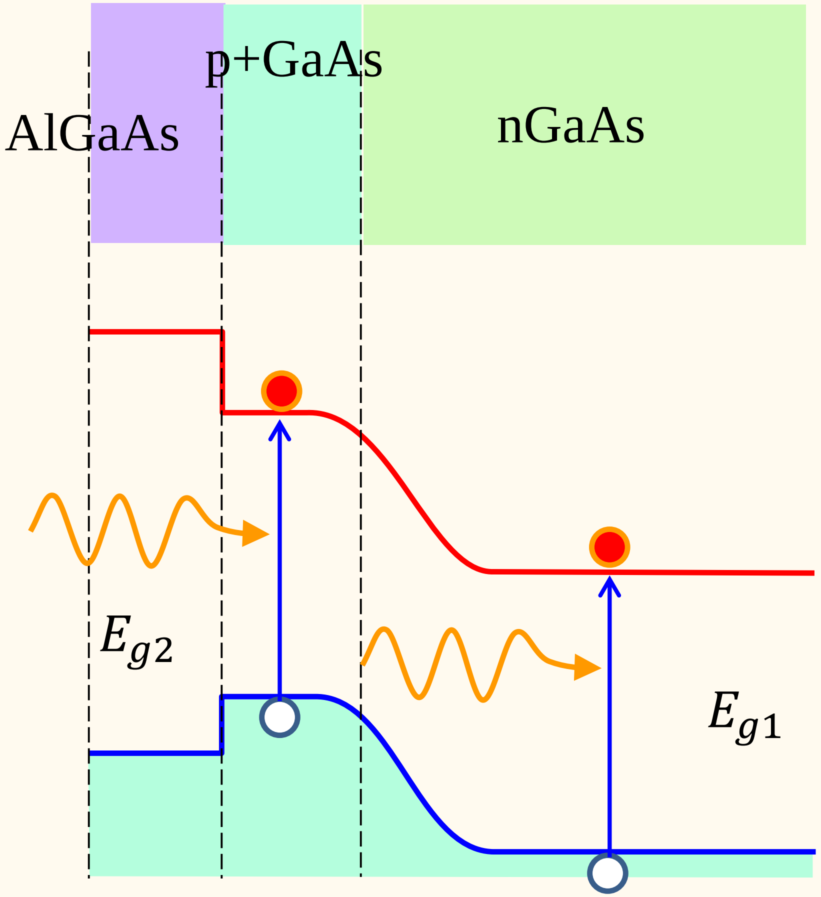






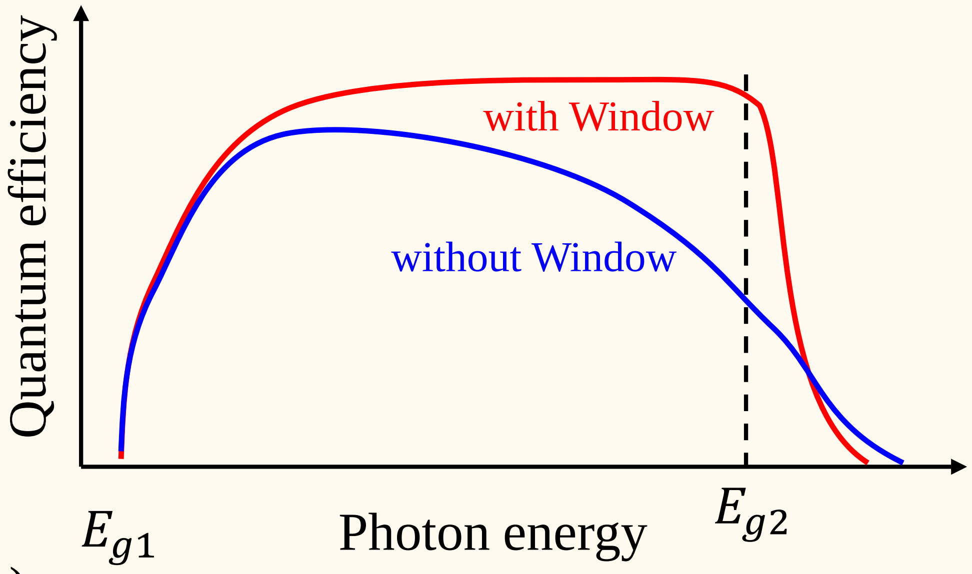
Optical devices with minority carrier confinement

Window layer in solar cells



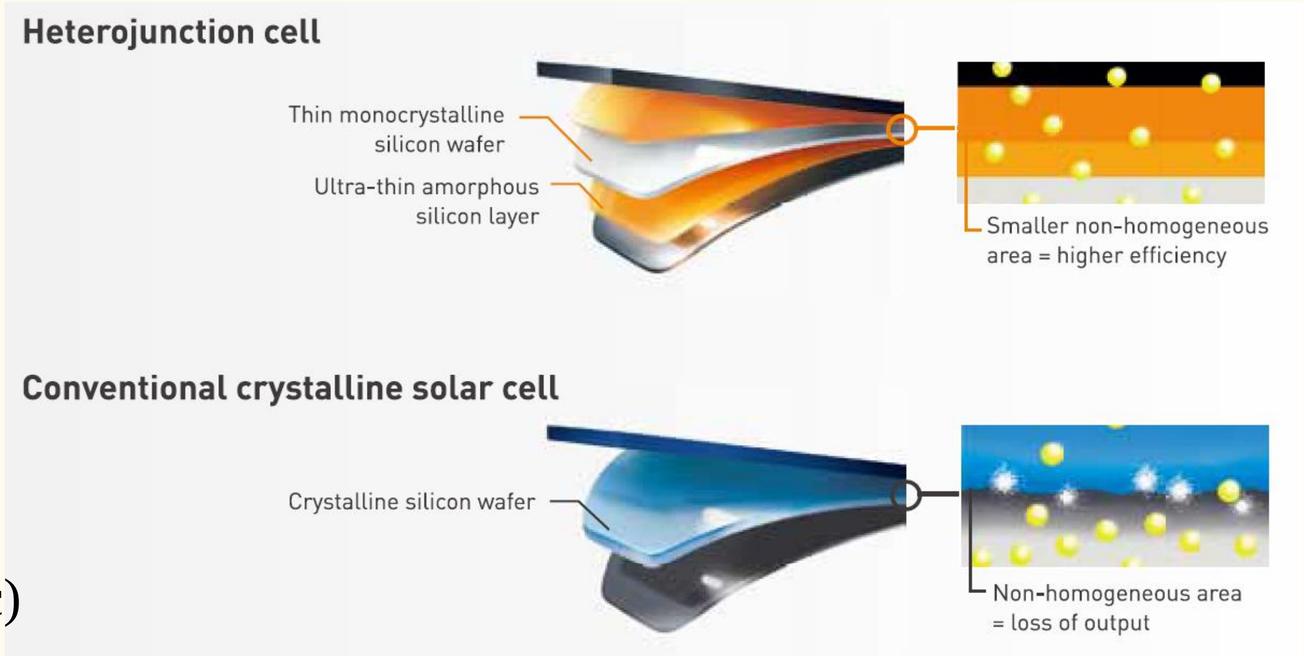
$E_{g2} > E_{g1}$

(a)



(b)

Panasonic HIT



(c)

Light emitting diodes (LEDs)

Emission spectrum $$I(\nu) \propto \nu^2 (h\nu - E_g)^{1/2} \exp\left[\frac{-(h\nu - E_g)}{k_B T}\right]$$

Quantum efficiency $$\eta_q \equiv \frac{R_r}{R} = \frac{\tau_{nr}}{\tau_{nr} + \tau_r} = \frac{\tau_{tot}}{\tau_r}, \qquad \frac{1}{\tau_{tot}} \equiv \frac{1}{\tau_{nr}} + \frac{1}{\tau_r}$$

non-radiative (τ_{nr}) radiative (τ_r)

Minority carrier diffusion $$j_e + j_h = e\left[\frac{D_e n_{p0}}{L_e} + \frac{D_h p_{n0}}{L_h}\right]\left[\exp\left(\frac{eV}{k_B T}\right) - 1\right]$$

Carrier recombination in depletion layer $$j_R = \frac{e n_i w_d}{2\tau_0}\left[\exp\left(\frac{eV}{2k_B T}\right) - 1\right]$$

injection efficiency $$\gamma = \frac{j_e}{j_e + j_h + j_R}$$

Internal quantum efficiency

$$\eta_{iq} = \gamma \eta_q$$

The Nobel Prize in Physics 2014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Isamu Akasaki
Prize share: 1/3


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Hiroshi Amano
Prize share: 1/3


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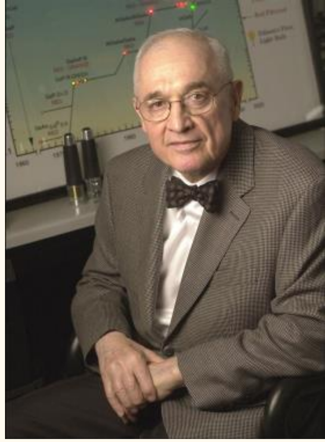
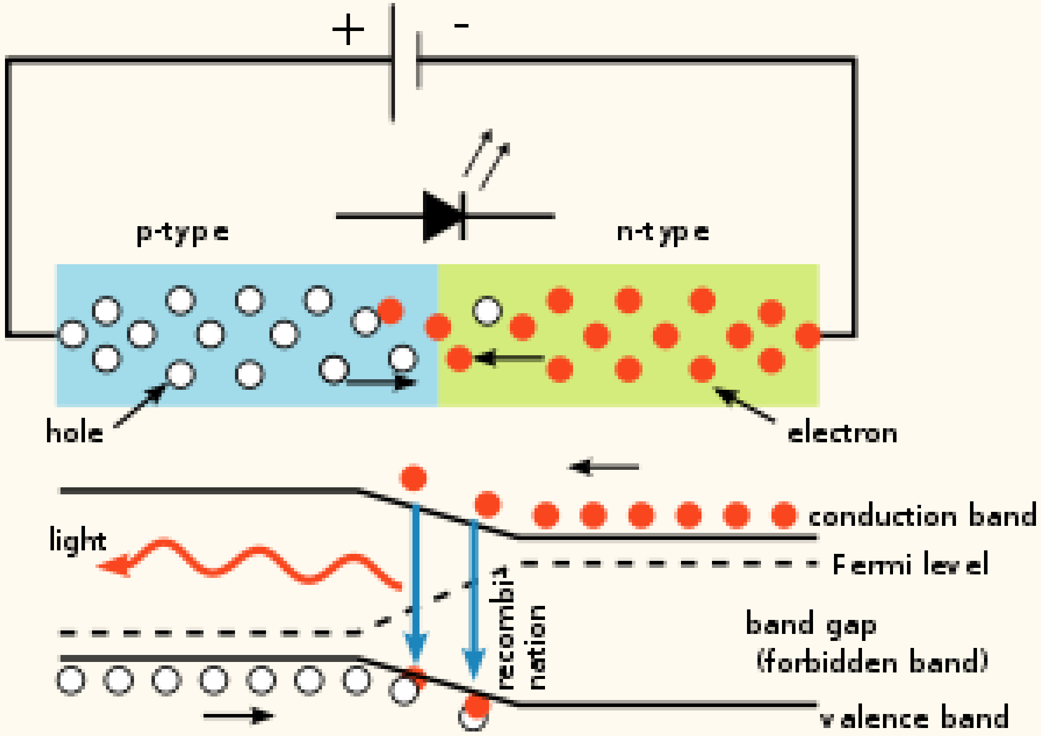
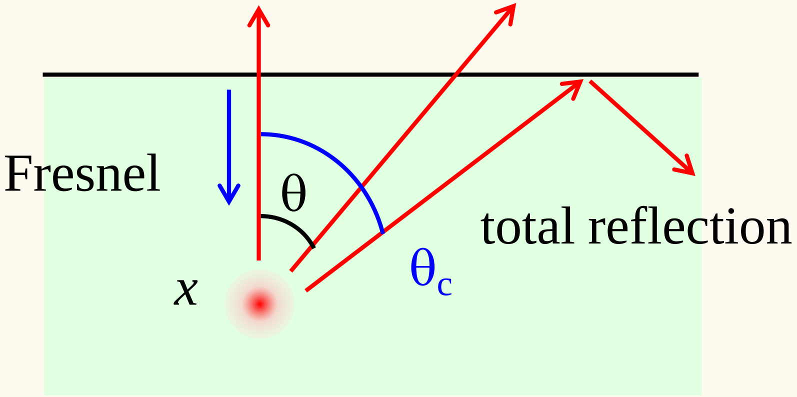

Nick Holonyak Jr.



External quantum efficiency



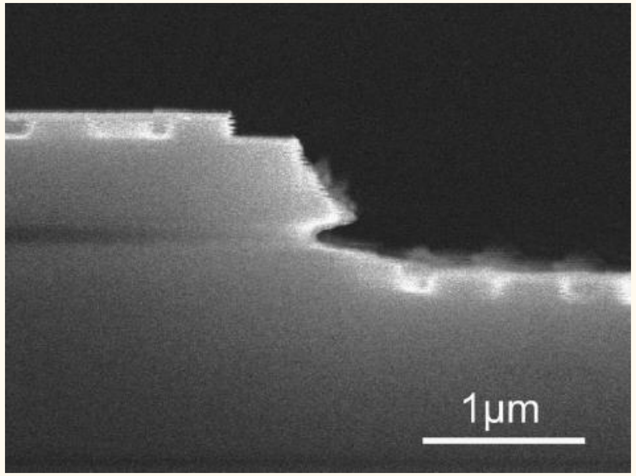
Optical losses — Absorption loss $\zeta_{\mathrm{abs}} = 1 - \exp\left(-\frac{\alpha x}{\cos\theta}\right)$

Fresnel loss $\Gamma = \left(\frac{\bar{n}_2 - \bar{n}_1}{\bar{n}_1 + \bar{n}_2}\right)^2$

Optical efficiency: η_{opt} — Total reflection loss $\theta > \theta_c = \sin^{-1}\frac{\bar{n}_1}{\bar{n}_2}$

External quantum efficiency $\eta_{\mathrm{exq}} = \eta_{\mathrm{opp}}\eta_{\mathrm{iq}}$

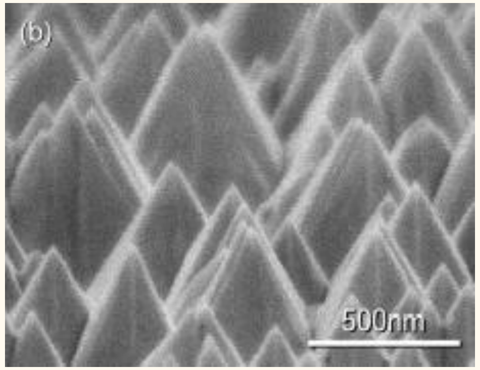
Device example



Windisch *et al*., APL **74**, 2256 (1999).

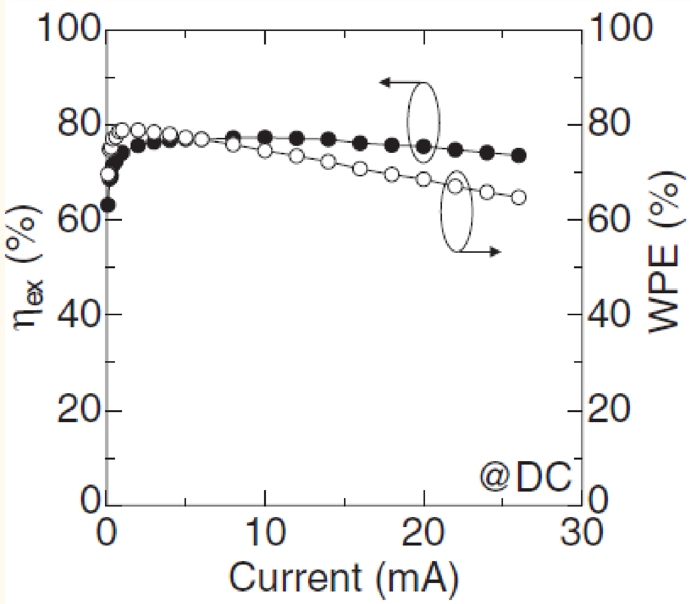
Textured surface AlGaAs/GaAs

η_{exq} >30 %



GaN/InGaN/GaN

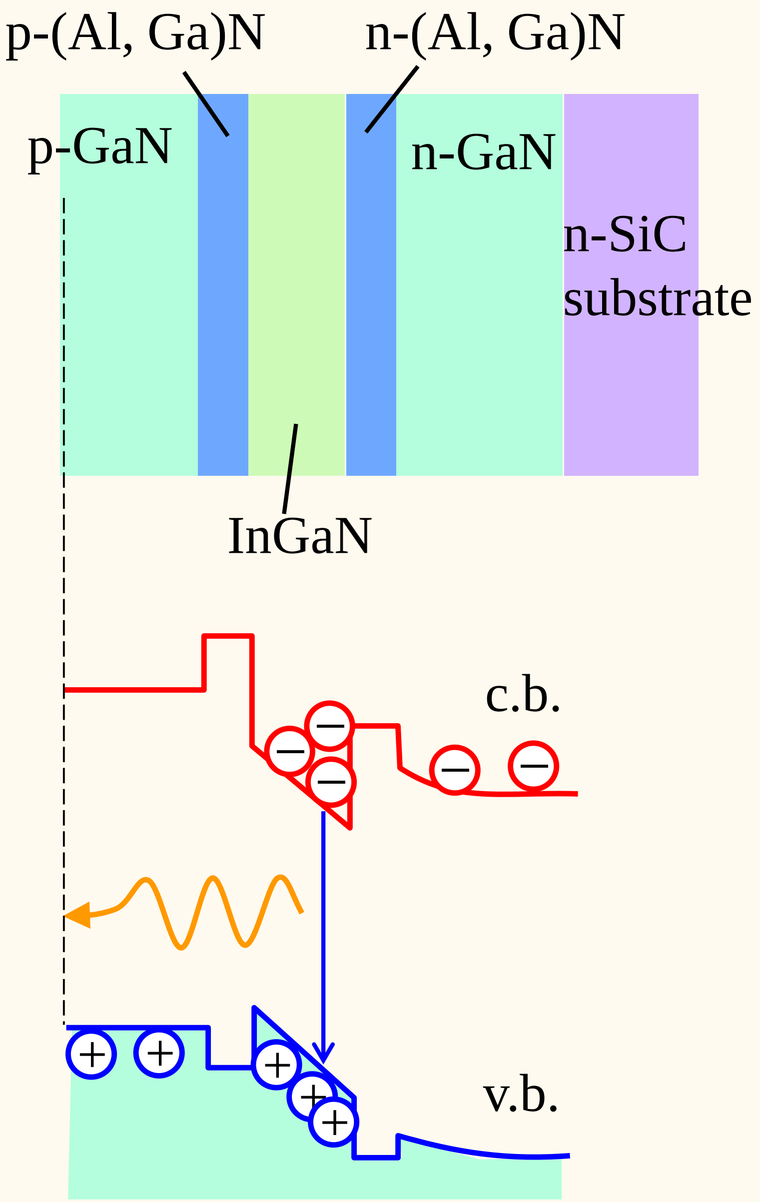
Fujii *et al*., APL **84**, 855 (2004).



InGaN-based YAG

Narukawa *et al*., JJAP **41**, L1431 (2007).

Double heterojunction (DH) LED



Advantages of DH LED

High internal quantum efficiency

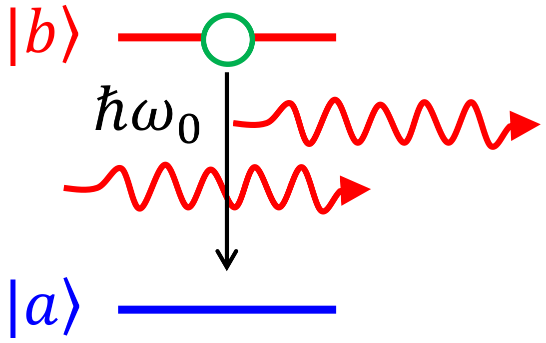
- Narrow active region → high *np* product
- No need for doping in active layer → less concentration of non-radiative recombination center
- Diffusion of minority carrier to surface, recombination centers is reduced.

Low absorption loss

- Energy of emitted photons is lower than the band gaps of the top and the bottom layers.

Laser diode

LASER: Light Amplification with Stimulated Emission of Radiation



(c) stimulated emission

Coherent state: Classical oscillating electromagnetic field

$$\boldsymbol{p} = m\omega_\lambda \boldsymbol{r}_0 \cos(\omega_0 t)$$

$$\vec{e}\cdot\boldsymbol{p} = \frac{\omega_\lambda m}{e}\vec{e}\cdot\boldsymbol{\mu}$$

Probability of stimulated emission

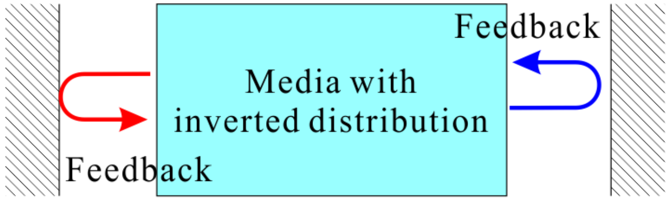
$$P_{ba}(t) = \frac{\omega_\lambda}{\epsilon\epsilon_0\hbar V}|\langle a|\vec{e}\cdot\boldsymbol{\mu}|b\rangle|^2 n_\lambda \frac{t^2}{2}$$

Energy absorption of media from the light (coherent state): $\mathcal{E} = (N_a - N_b)P_{ba}(\tau)\hbar\omega_\lambda$

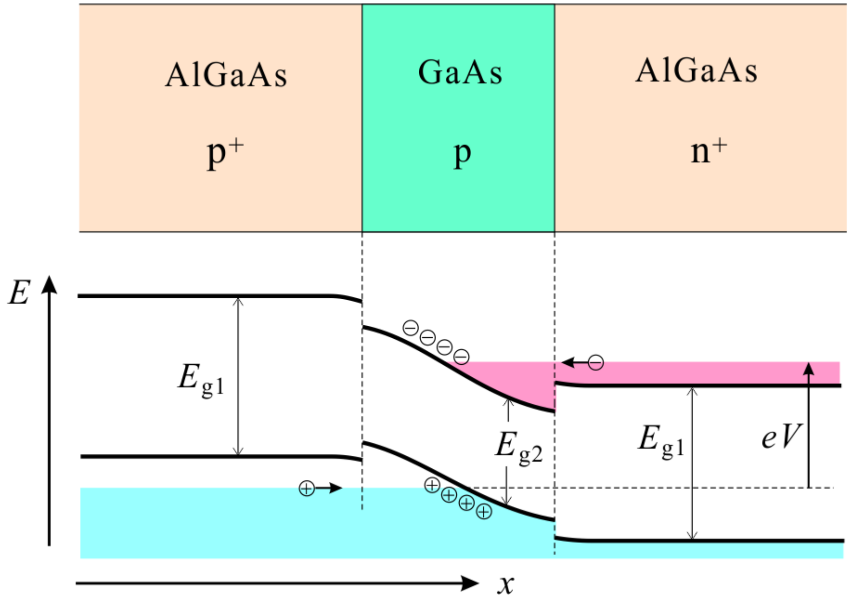
This means if a state with $N_b > N_a$ is realized, $\varepsilon < 0$, *i.e.*, the energy is absorbed from the media to light

Increase of amplitude of the coherent state: Bosonic stimulation

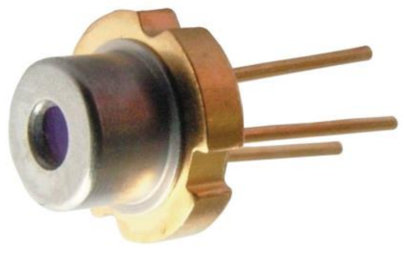
Laser diode



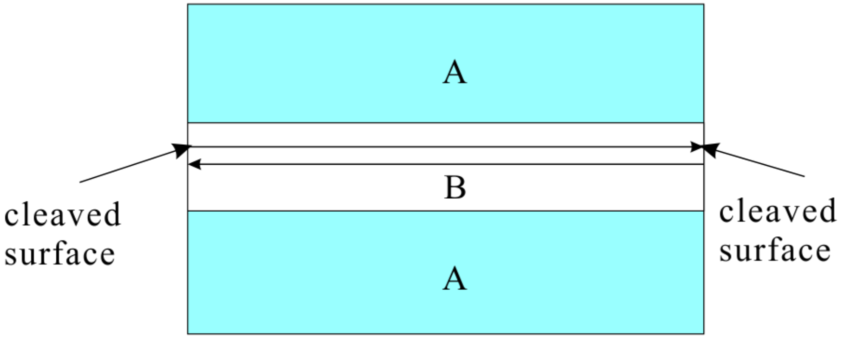
(a)



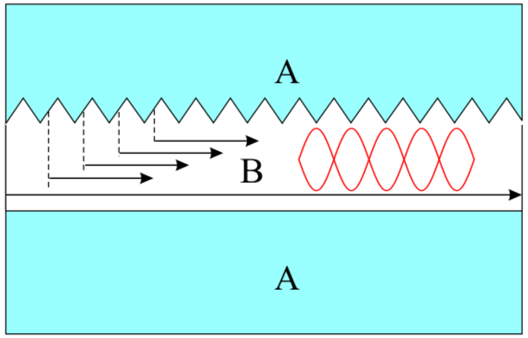
(b)



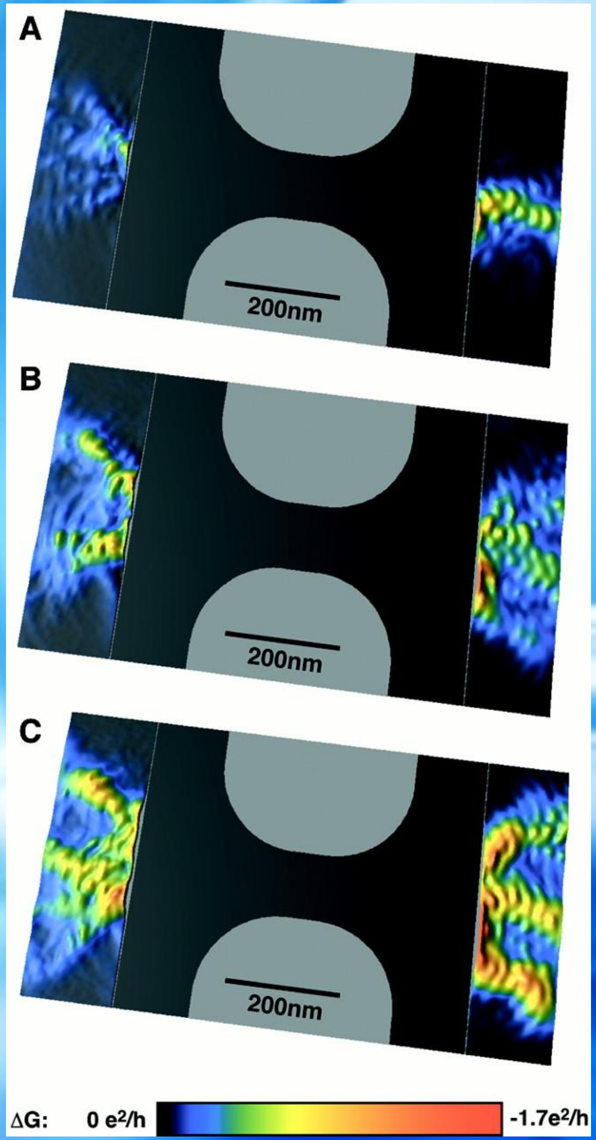
ADL-65074TL-1 - Laser Diode 655nm 7mW



(c) Fabry-Perot type



(d) Distributed Feedback type



M. A. Topinka et al. Science 2000;289:2323-2326

Chapter 8

Basics of Quantum Transport

Quantum entanglement

$|\psi\rangle = |A\rangle + |B\rangle$

$|\varphi\rangle = |1\rangle + |2\rangle$

$\lvert A\rangle$	$\lvert B\rangle$	
$\lvert A\rangle\lvert 1\rangle$		$\lvert 1\rangle$
	$\lvert B\rangle\lvert 2\rangle$	$\lvert 2\rangle$

Direct product $|\Psi\rangle = |\psi\rangle \otimes |\varphi\rangle = |A\rangle|1\rangle + |A\rangle|2\rangle + |B\rangle|1\rangle + |B\rangle|2\rangle$

Maximally entangled state $|\Phi\rangle = |A\rangle|1\rangle + |B\rangle|2\rangle$

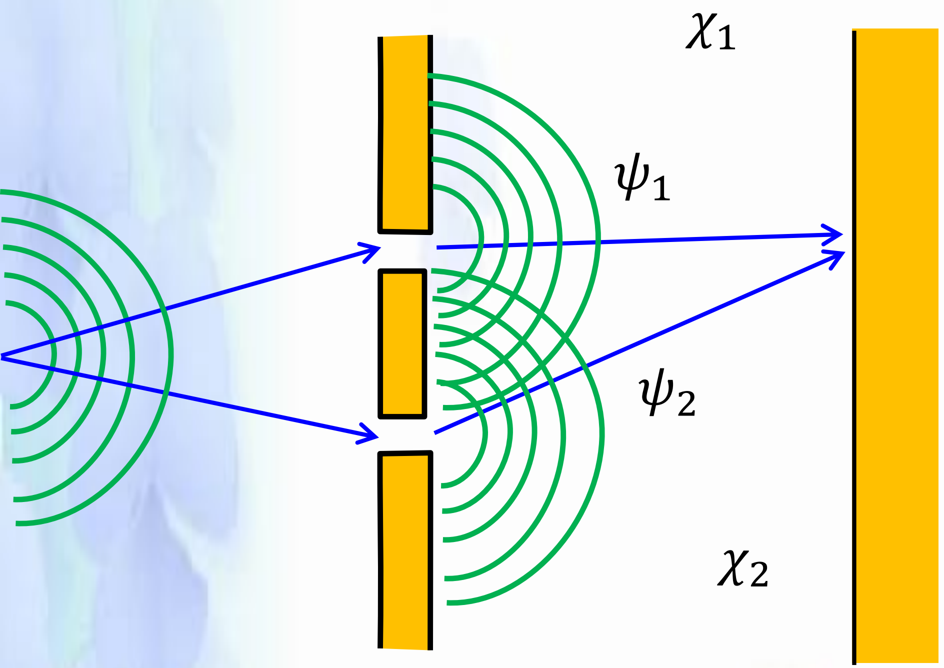
Quantification of Entanglement?

von Neumann entropy (entanglement entropy)

Density matrix $\rho = \sum|\psi\rangle\langle\psi|$

$S = \mathrm{tr}(\rho \ln \rho)$

Boundary between classical and quantum



$$|\psi|^2 = |\psi_1 + \psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2|\cos\theta$$

Environment wavefunction: χ

should associate with electron paths

$$\psi_1 \to \psi_1 \otimes \chi_1, \quad \psi_2 \to \psi_2 \otimes \chi_2$$

Then the interference term is $2|\psi_1||\psi_2|\cos\theta\langle\chi_1|\chi_2\rangle$

$\langle\chi_1|\chi_2\rangle = 1$: Full interference

$\langle\chi_1|\chi_2\rangle = 0$: No interference Particle-Environment maximally entangled

Electron transport: Electron – Phonon inelastic scattering
Electron – Electron inelastic scattering
Electron – Localized spin scattering

Length limit quantum coherence (Coherence length)

Monochromaticity: Thermal length

Energy width: $\Delta E = k_\mathrm{B} T$

Diffusion length: $l = \sqrt{D\tau}$

Phase width: $2\pi \Delta f \tau = 2\pi \dfrac{\Delta E \tau}{h} = 2\pi \dfrac{k_\mathrm{B} T \tau}{h}$ $\rightarrow 2\pi$: $\tau_\mathrm{c} = \dfrac{h}{k_\mathrm{B} T}$

Thermal diffusion length $l_\mathrm{th} = \sqrt{\dfrac{hD}{k_\mathrm{B} T}}$

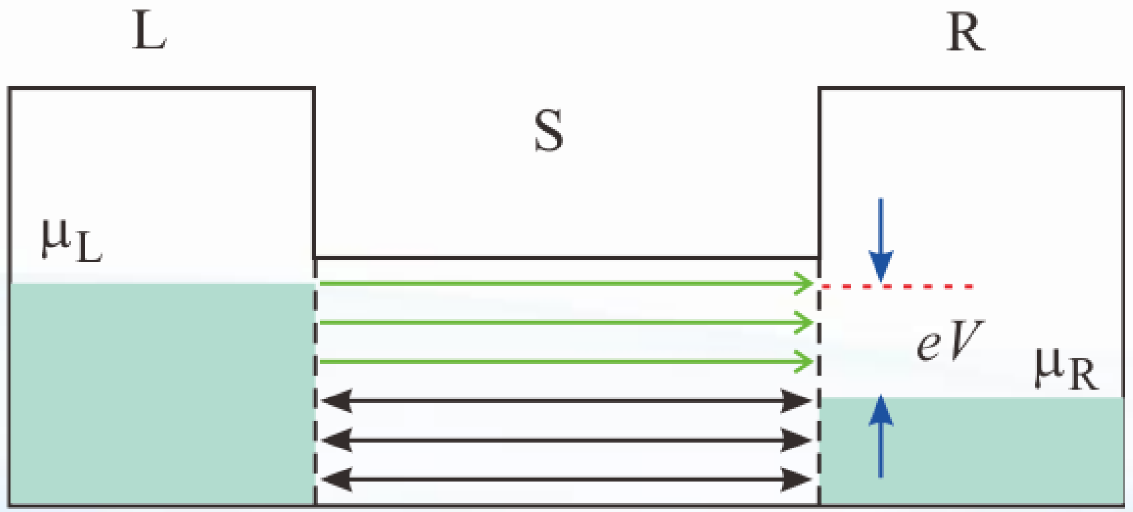
Ballistic thermal length $l_\mathrm{th} = \dfrac{h v_\mathrm{F}}{k_\mathrm{B} T}$

(Some) inelastic scattering time: τ_inel

Ballistic transport: $l_\mathrm{inel} = v_\mathrm{F} \tau_\mathrm{inel}$

Diffusive transport: $l_\mathrm{inel} = \sqrt{D \tau_\mathrm{inel}}$

Conductance quantum



L, R : Particle reservoirs

Thermal equilibrium:
well defined chemical potentials

Instantaneous thermalization:
particles loose quantum coherence

$$j(k) = \frac{e}{L} v_{\mathrm{g}} = \frac{e}{\hbar L} \frac{dE(k)}{dk}$$

L: wavefunction normalization length

$$J = \int_{k_{\mathrm{R}}}^{k_{\mathrm{L}}} j(k) \frac{L}{2\pi} dk = \frac{e}{h} \int_{\mu_{\mathrm{R}}}^{\mu_{\mathrm{L}}} dE = \frac{e}{h}(\mu_{\mathrm{L}} - \mu_{\mathrm{R}}) = \frac{e^2}{h} V$$

$$G = \frac{J}{V} = \frac{e^2}{h} \equiv G_{\mathrm{q}} \ \text{Conductance quantum} \ \left(\frac{2e^2}{h} \equiv G_{\mathrm{q}} \ \text{spin freedom} \right)$$

Conductance quantum as uncertainty relation

Wave packet: $\Delta k \to \Delta x = \dfrac{2\pi}{\Delta k}, \quad v_{\mathrm{g}} = \dfrac{\Delta E}{\hbar \Delta k}$

Fermion statistics: electron charge concentration = $\dfrac{e}{\Delta x} = \dfrac{e\Delta k}{2\pi}$

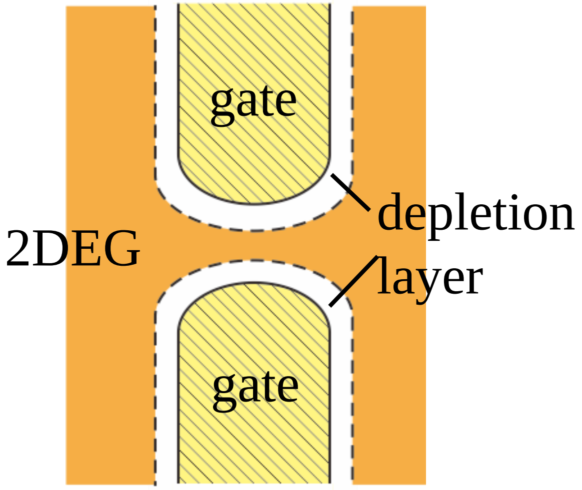
$$J = \frac{e}{\Delta x}\frac{\Delta E}{\hbar \Delta k} = \frac{e^2}{h}V$$

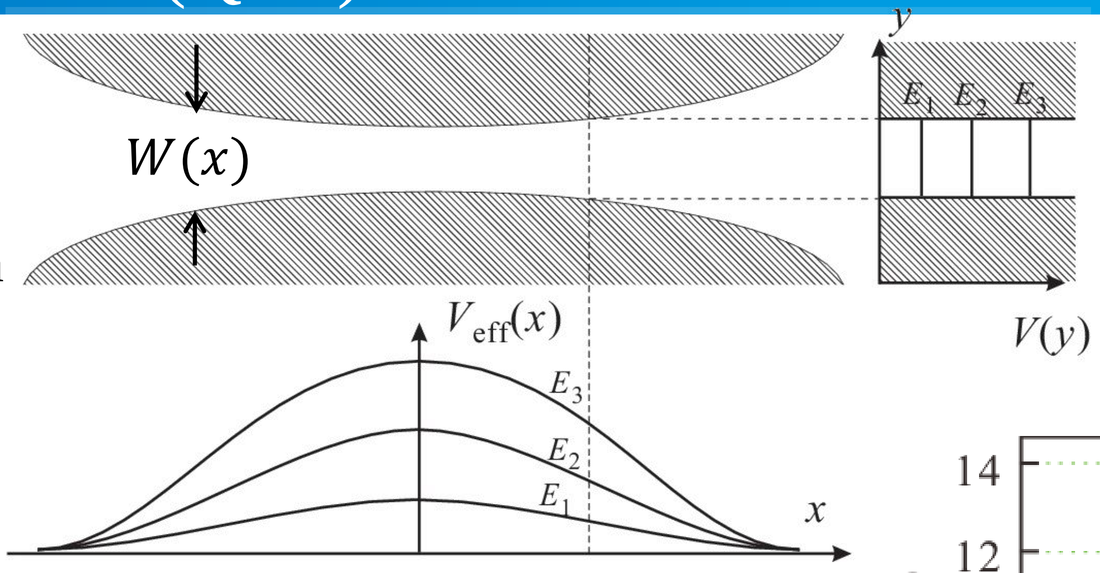
Energy width: $\Delta E = eV$ Wave packet width in time: $\Delta t = \dfrac{h}{\Delta E} = \dfrac{h}{eV}$

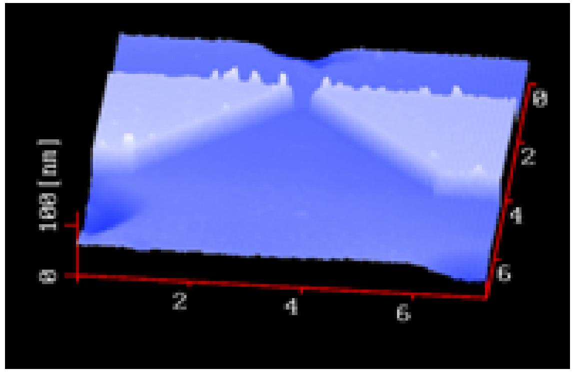
$$J = \frac{e}{\Delta t} = \frac{e^2}{h}V$$

Conductance quantum comes from fermion statistics of electrons

Quantum point contact (QPC)



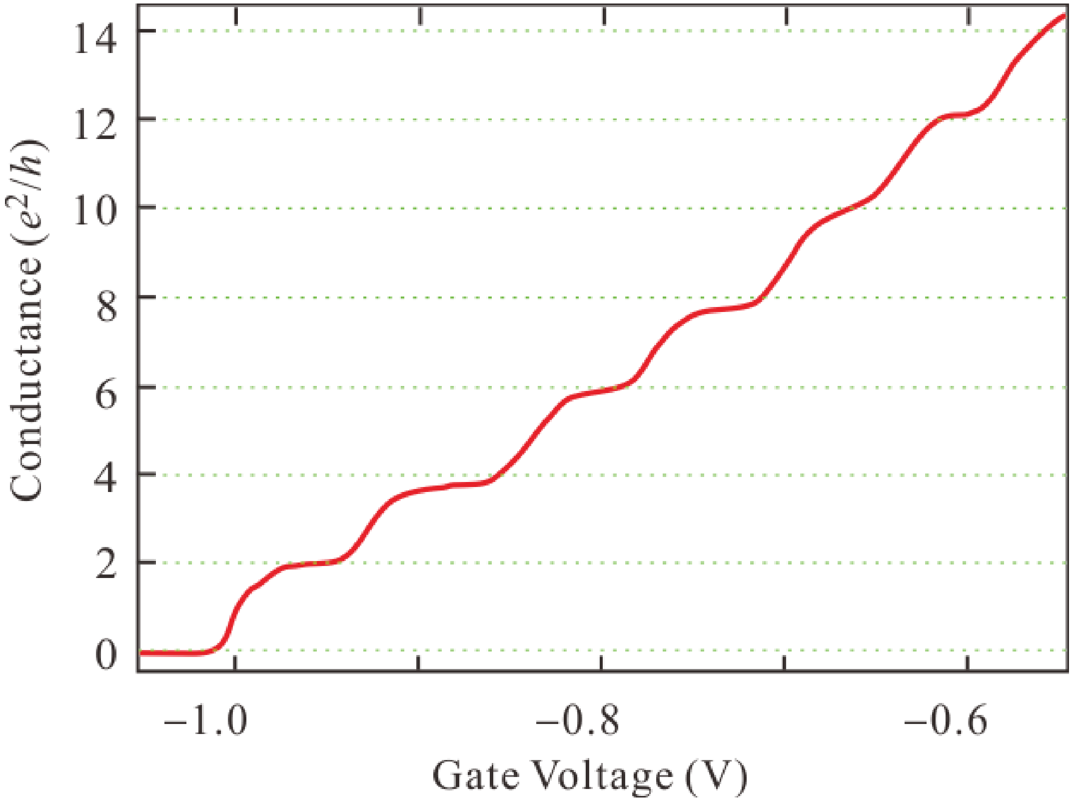




$$H\psi(x,y) = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\varphi_n(y)\phi(x)$$

$$= \varphi_n(y)\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \left(\frac{n\pi}{2W}\right)^2\right)\phi(x) = E\varphi_n(y)\phi(x)$$

$$V_{\text{eff}}(n,x) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2W(x)}\right)^2$$



Transmissible one-dimensional system: Conductance Channel

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.6.23 Lecture 11

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

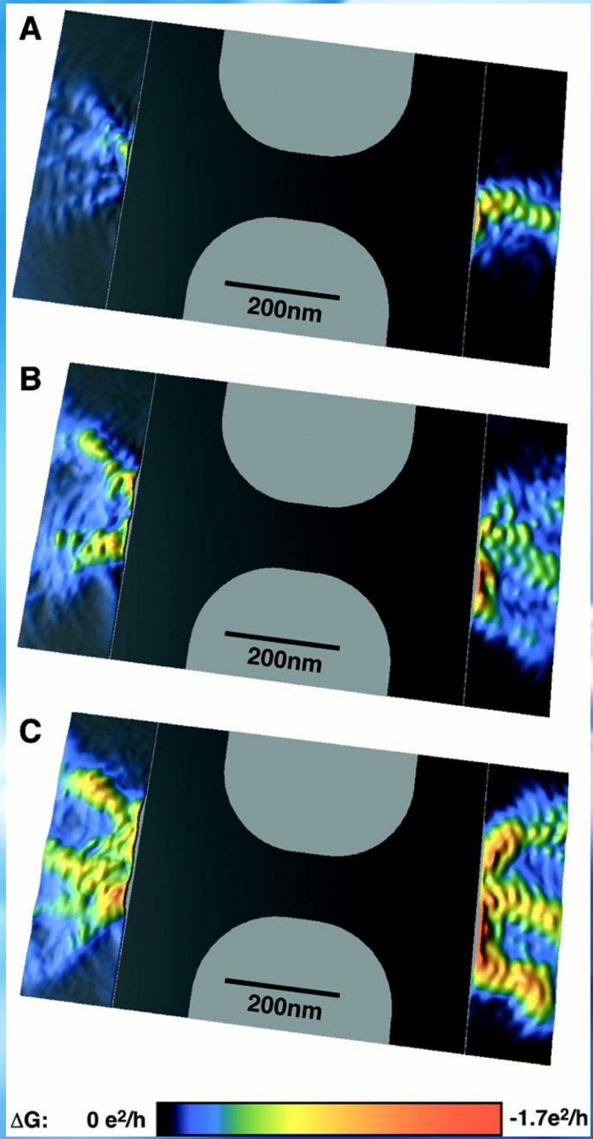
Shingo Katsumoto

Review of last week

- Two-dimensional electrons at heterointerface
- Quantum point contacts, quantum wires
- Core-shell nanowires
- Two dimensional systems → quantum dots
- Self assembled quantum dots
- Colloidal quantum dots
- Optical devices with minority carrier confinement
  Solar cells, DH LEDs, Laser diodes

Chapter 8

Basics of Quantum Transport



M. A. Topinka et al. Science 2000;289:2323-2326

Quantum entanglement

$$|\psi\rangle = |A\rangle + |B\rangle \qquad |\varphi\rangle = |1\rangle + |2\rangle$$

$\|A\rangle$	$\|B\rangle$	
$\|A\rangle\|1\rangle$		$\|1\rangle$
	$\|B\rangle\|2\rangle$	$\|2\rangle$

Direct product $|\Psi\rangle = |\psi\rangle \otimes |\varphi\rangle = |A\rangle|1\rangle + |A\rangle|2\rangle + |B\rangle|1\rangle + |B\rangle|2\rangle$

Maximally entangled state $|\Phi\rangle = |A\rangle|1\rangle + |B\rangle|2\rangle$

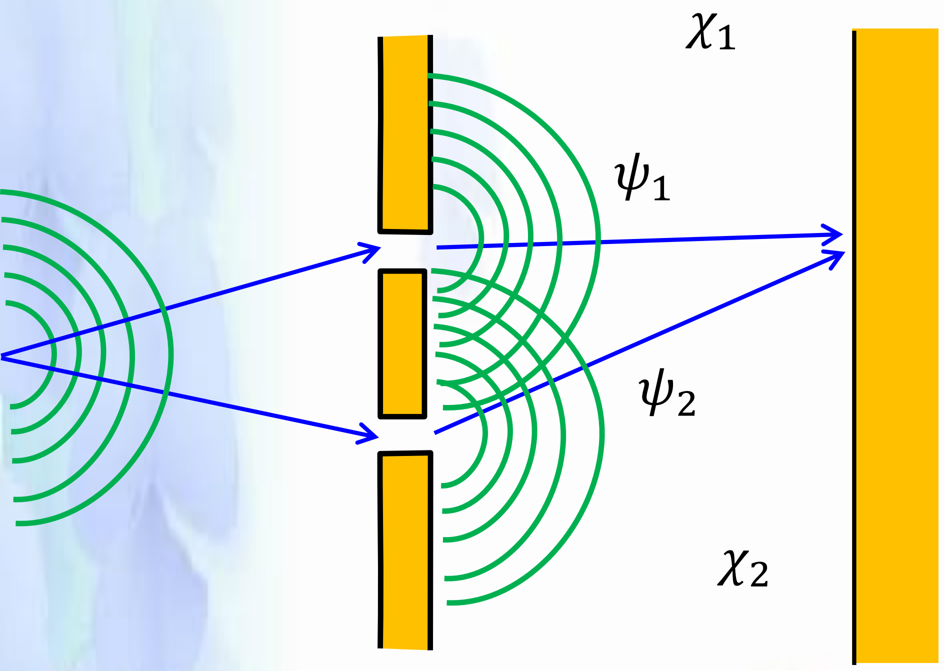
Quantification of Entanglement?

von Neumann entropy (entanglement entropy)

Density matrix $\rho = \sum|\psi\rangle\langle\psi|$

$S = \mathrm{tr}(\rho \ln \rho)$

Boundary between classical and quantum



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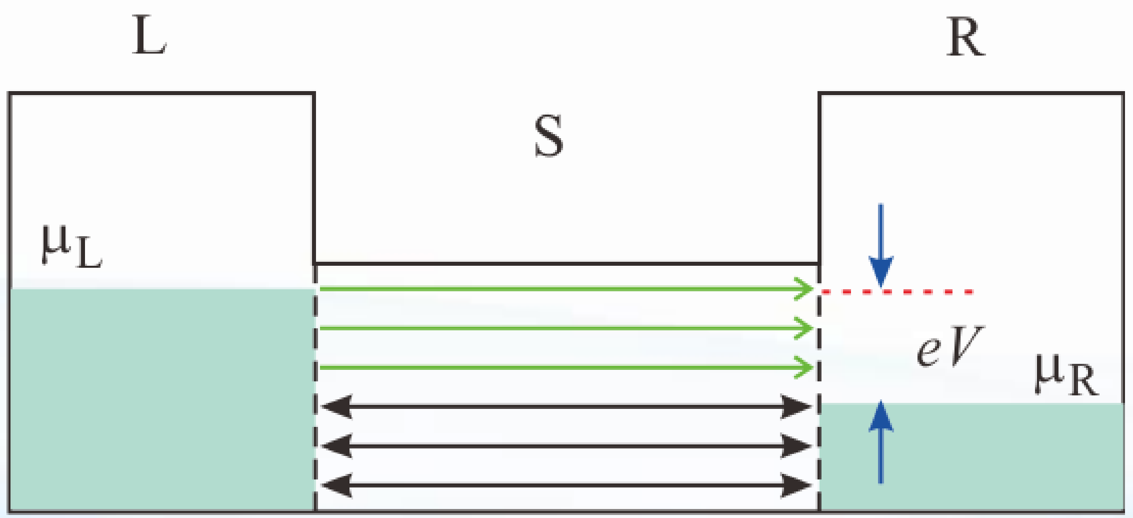
Ballistic thermal length $l_{\rm th} = \frac{hv_{\rm F}}{k_{\rm B}T}$

(Some) inelastic scattering time: $\tau_{\rm inel}$

Ballistic transport: $l_{\rm inel} = v_{\rm F}\tau_{\rm inel}$

Diffusive transport: $l_{\rm inel} = \sqrt{D\tau_{\rm inel}}$

Conductance quantum



L, R : Particle reservoirs

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$$G = \frac{J}{V} = \frac{e^2}{h} \equiv G_{\mathrm{q}} \text{ Conductance quantum } \left(\frac{2e^2}{h} \equiv G_{\mathrm{q}} \text{ spin freedom} \right)$$

Conductance quantum as uncertainty relation

Space coordinate-wavenumber

Wave packet: $\Delta k \rightarrow \Delta x = \frac{2\pi}{\Delta k}, \quad v_g = \frac{\Delta E}{\hbar \Delta k}$

Fermion statistics: electron charge concentration $= \frac{e}{\Delta x} = \frac{e\Delta k}{2\pi}$

$$J = en_{\text{electron}} v_g = \frac{e}{\Delta x}\frac{\Delta E}{\hbar \Delta k} = \frac{e^2}{h} V$$

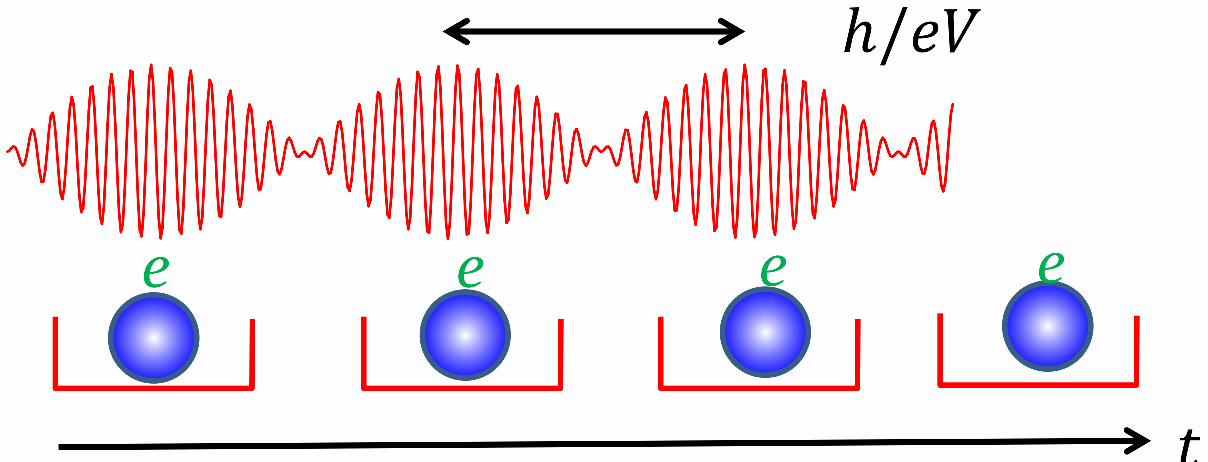
Energy-time

Energy width: $\Delta E = eV$

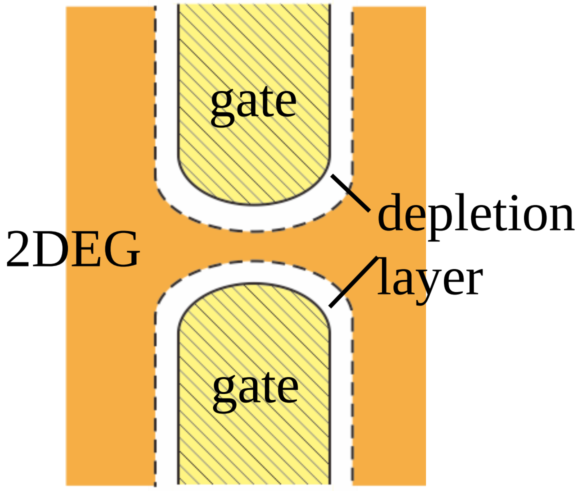
Wave packet width in time: $\Delta t = \frac{h}{\Delta E} = \frac{h}{eV}$

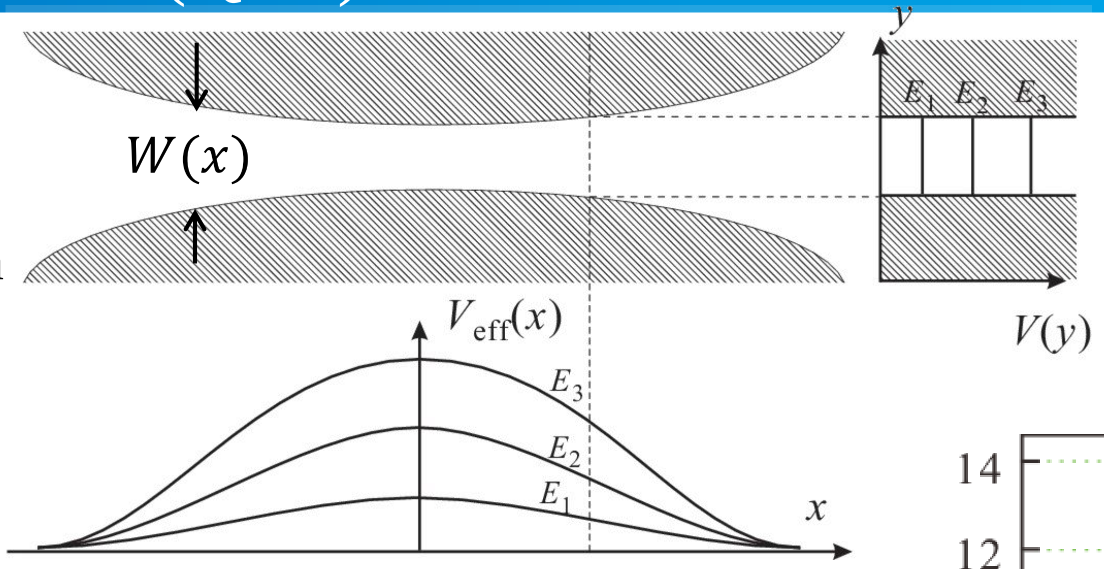
Fermion anti-bunching effect: $J = \frac{e}{\Delta t} = \frac{e^2}{h} V$

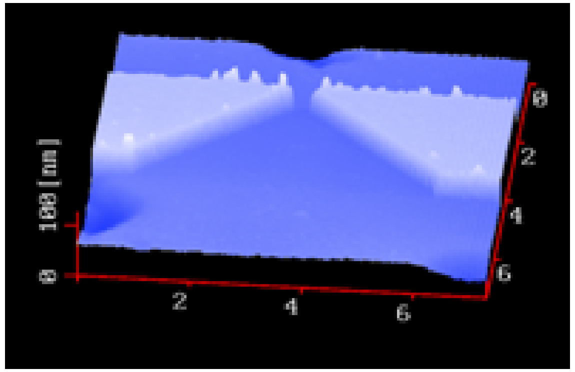
Conductance quantum comes from fermion statistics of electrons

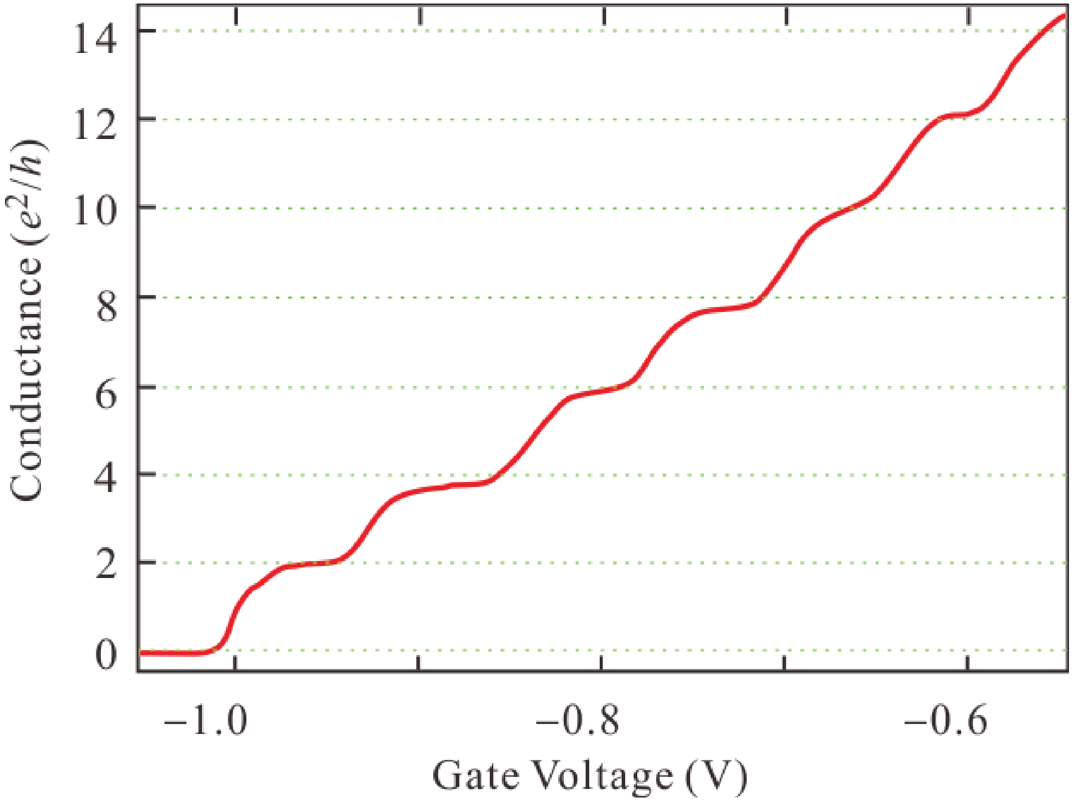


Quantum point contact (QPC)









$$H\psi(x,y) = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\varphi_n(y)\phi(x)$$

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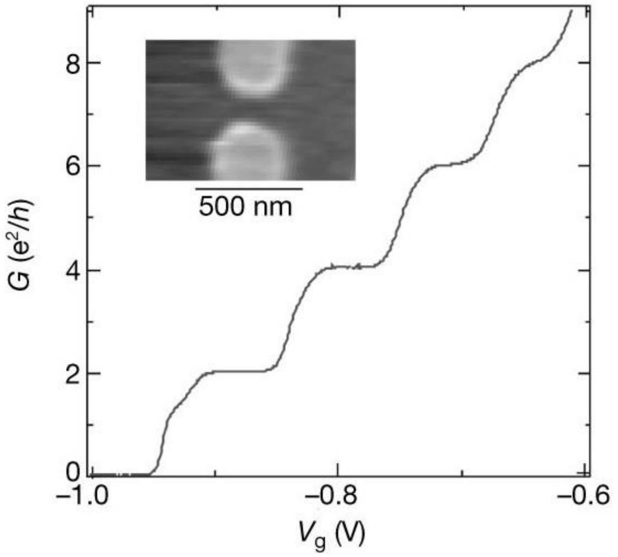
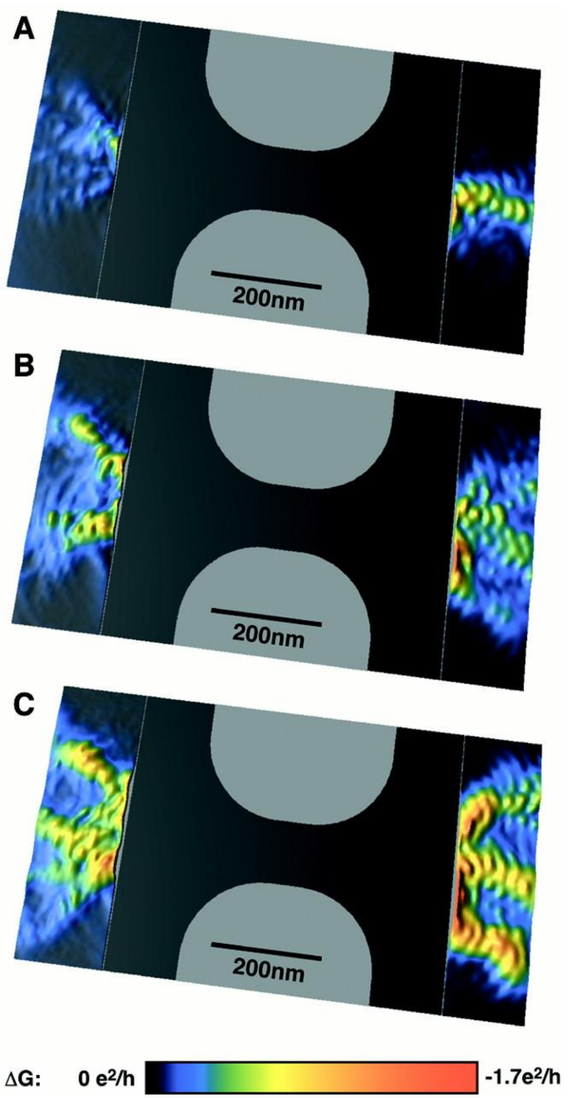
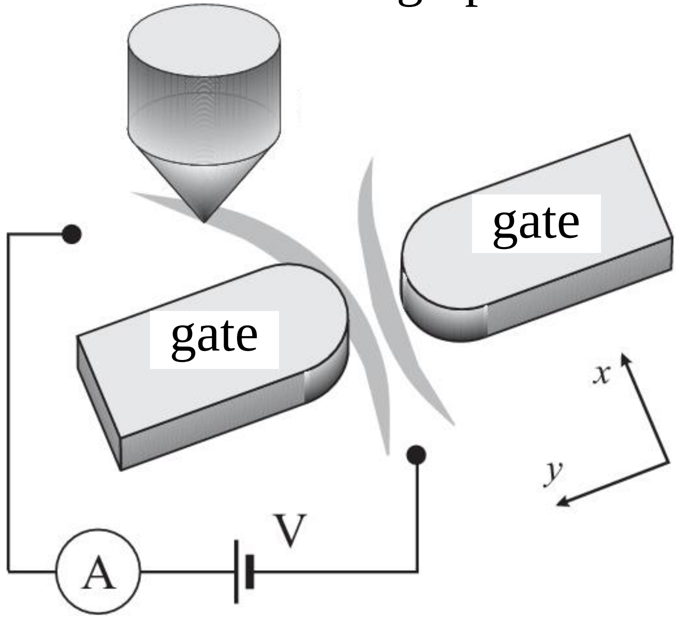
Transmissible one-dimensional system: Conductance Channel

Scanning tip conductance measurement







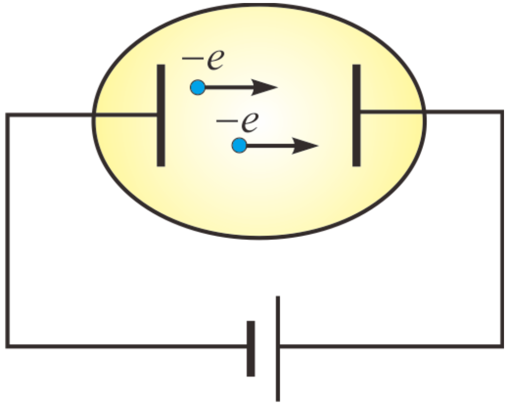
Tip image potential scatters electrons

→ conductance shifts from quantized value

Scattering amplitude ∝ $|\psi|^2$

M. A. Topinka et al.,
Nature **410**, 183 (2001)

Shot noise reduction on the conductance plateaus



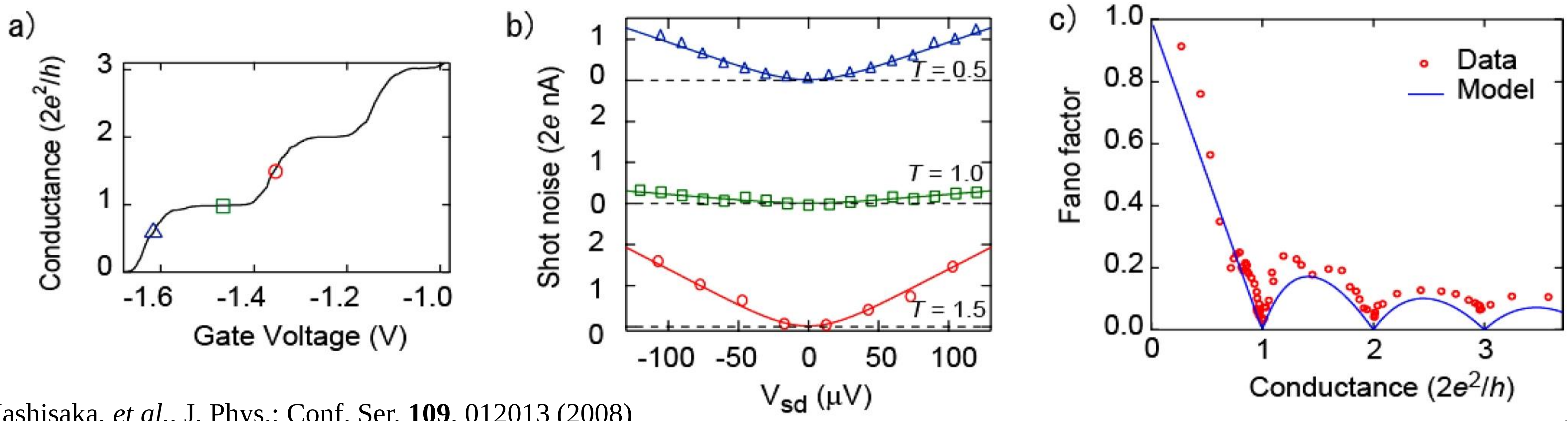
Flow of single electron: Time domain: δ-function approximation

$$J_e(t) = e\delta(t-t_0) = e\int_{-\infty}^{\infty} e^{2\pi i f(t-t_0)}df = 2e\int_0^{\infty}\cos[2\pi f(t-t_0)]df$$

Current fluctuation density for infinitesimal band df $\delta J = d\sqrt{\langle J_e^2\rangle} = \frac{2e}{\sqrt{2}}df = \sqrt{2}edf$

$$\overline{\langle\delta j^2\rangle} = (j_p + j_q e^{i\phi})(j_p + j_q e^{-i\phi}) = j_p^2 + j_q^2 + 2j_p j_q\cos\phi = j_p^2 + j_q^2 = 2\times(\sqrt{2}e)^2 df$$

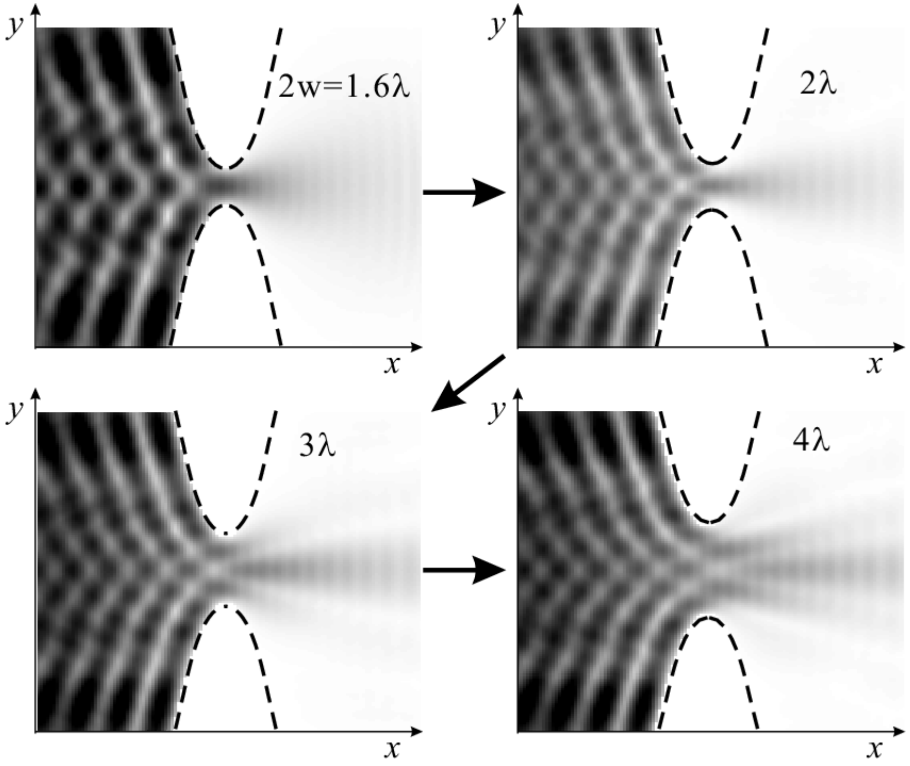
Flow of *N*-electrons $\overline{\langle\delta J^2\rangle} = N\times 2e^2 df = 2e\bar{J}df \quad (\bar{J} = eN)$: Poissonian noise



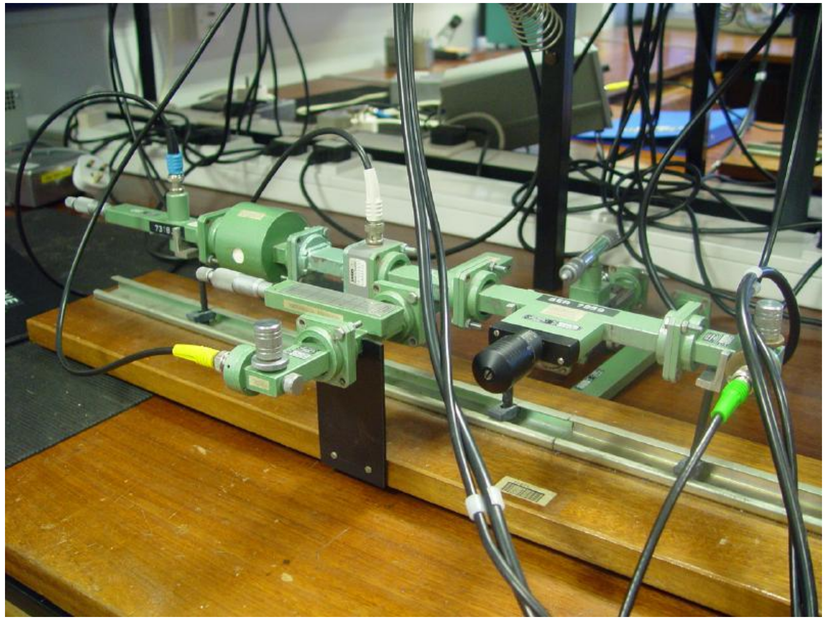
M. Hashisaka, *et al.*, J. Phys.: Conf. Ser. **109**, 012013 (2008)

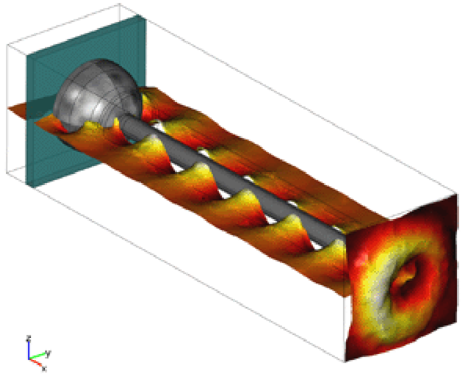
Microwave and electron waveguides

Quantum point contact



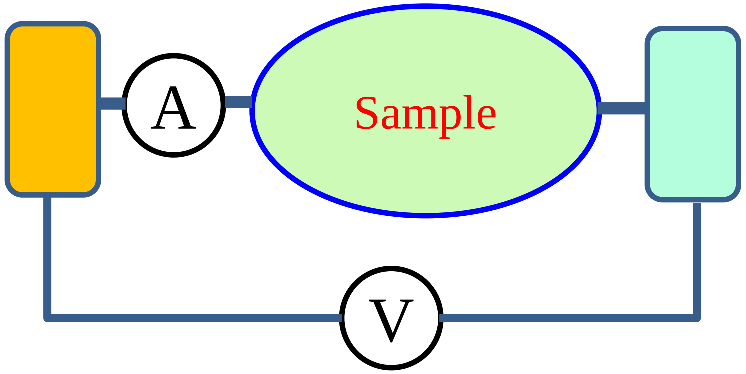
Microwave waveguide

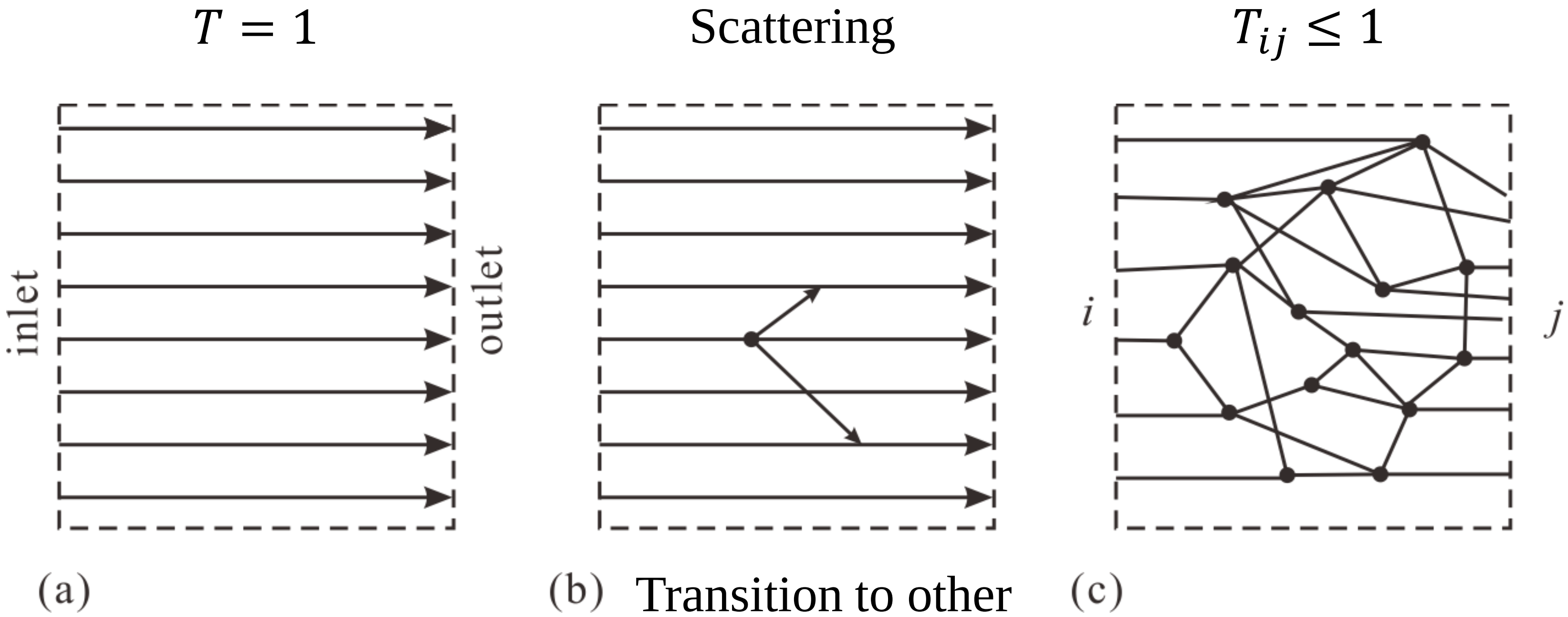




Quantum point contacts or quantum wires can be viewed as "electron waveguides."

Landauer formula for two-terminal conductance





$$G = 2\frac{e^2}{h}\sum_{i,j} T_{ij}$$

Electron spin

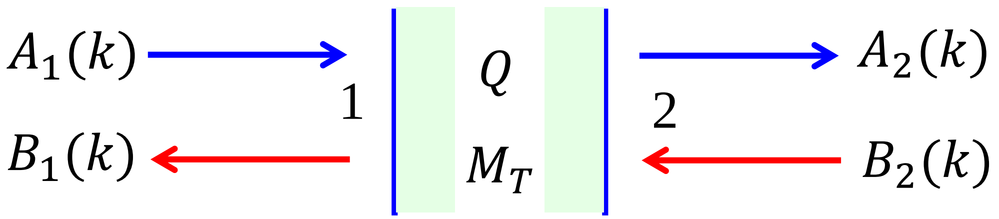
Fermion antibunching

Waveguide connection

Rolf Landauer
1927 - 1999

Scattering matrix (S-matrix)

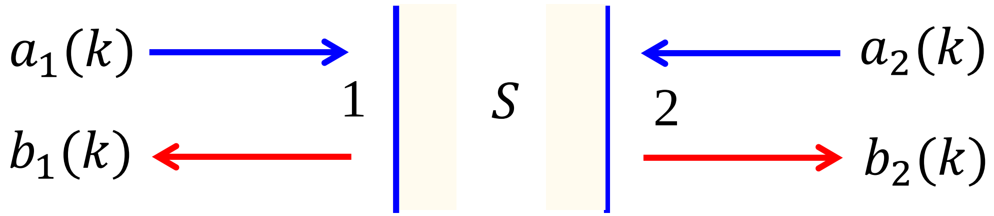
T-matrix



Transfer matrix: M_T

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \equiv M_T \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

S-matrix



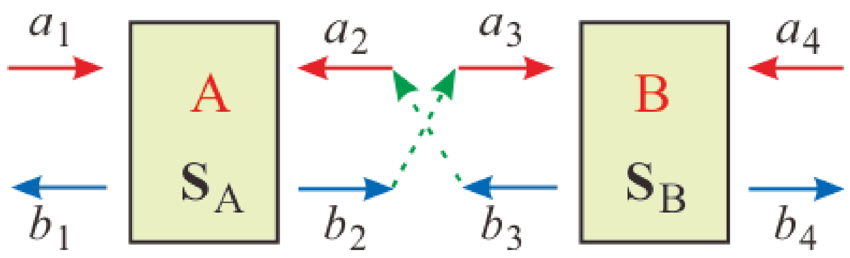
incoming

outgoing

$$\begin{pmatrix} b_1(k) \\ b_2(k) \end{pmatrix} = S \begin{pmatrix} a_1(k) \\ a_2(k) \end{pmatrix} = \begin{pmatrix} r_{\mathrm{L}} & t_{\mathrm{R}} \\ t_{\mathrm{L}} & r_{\mathrm{R}} \end{pmatrix} \begin{pmatrix} a_1(k) \\ a_2(k) \end{pmatrix}$$

Complex probability density flux $a_i(k) = \sqrt{v_{\mathrm{Fi}}}\psi_{ai}(k_{\mathrm{F}})$

Series connection of S-matrix



$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = S_A \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} r_{\mathrm{L}}^{(\mathrm{A})} & t_{\mathrm{R}}^{(\mathrm{A})} \\ t_{\mathrm{L}}^{(\mathrm{A})} & r_{\mathrm{R}}^{(\mathrm{A})} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix},$$

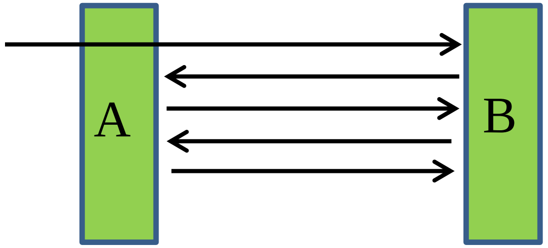
$$\begin{pmatrix} b_3 \\ b_4 \end{pmatrix} = S_B \begin{pmatrix} a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} r_{\mathrm{L}}^{(\mathrm{B})} & t_{\mathrm{R}}^{(\mathrm{B})} \\ t_{\mathrm{L}}^{(\mathrm{B})} & r_{\mathrm{R}}^{(\mathrm{B})} \end{pmatrix} \begin{pmatrix} a_3 \\ a_4 \end{pmatrix}$$

$$b_2 = a_3, \quad a_2 = b_3$$

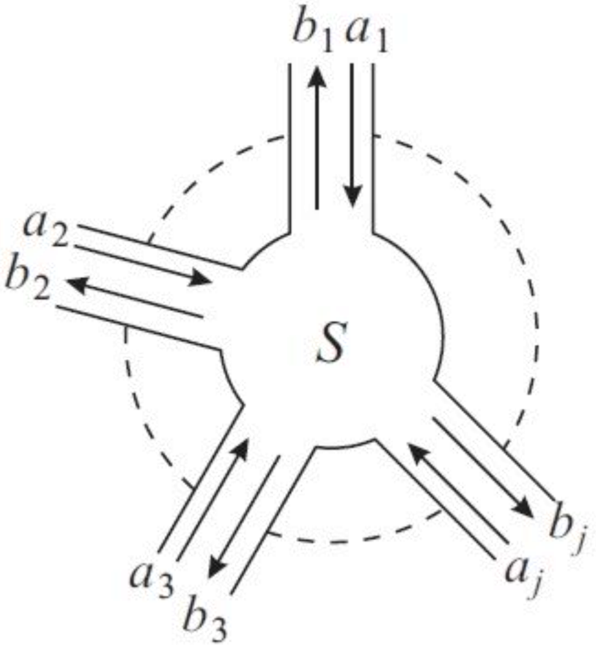
$$S_{\mathrm{AB}} = \begin{pmatrix} r_{\mathrm{L}}^{(\mathrm{A})} + t_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})} \left(I - r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})}\right)^{-1} t_{\mathrm{L}}^{(\mathrm{A})} & t_{\mathrm{R}}^{(\mathrm{A})} \left(I - r_{\mathrm{L}}^{(\mathrm{B})} r_{\mathrm{R}}^{(\mathrm{A})}\right)^{-1} t_{\mathrm{R}}^{(\mathrm{B})} \\ t_{\mathrm{L}}^{(\mathrm{B})} \left(I - r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})}\right)^{-1} t_{\mathrm{L}}^{(\mathrm{A})} & r_{\mathrm{R}}^{(\mathrm{B})} + t_{\mathrm{L}}^{(\mathrm{B})} \left(I - r_{\mathrm{R}}^{(\mathrm{A})} r_{\mathrm{L}}^{(\mathrm{B})}\right)^{-1} r_{\mathrm{R}}^{(\mathrm{A})} t_{\mathrm{R}}^{(\mathrm{B})} \end{pmatrix}$$

S-matrix

$$\left(I - r_{\rm R}^{\rm (A)} r_{\rm L}^{\rm (B)}\right)^{-1} = I + r_{\rm R}^{\rm (A)} r_{\rm L}^{\rm (B)} + (r_{\rm R}^{\rm (A)} r_{\rm L}^{\rm (B)})^2 + (r_{\rm R}^{\rm (A)} r_{\rm L}^{\rm (B)})^3 + \cdots$$



Multi-channel



$$\boldsymbol{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_i \\ \vdots \\ b_n \end{pmatrix} = \begin{pmatrix} S_{11} & \cdots & S_{1i} & \cdots & S_{1n} \\ \vdots & \ddots & & & \vdots \\ S_{i1} & & S_{ii} & & S_{in} \\ \vdots & & & \ddots & \vdots \\ S_{n1} & \cdots & S_{ni} & \cdots & S_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_i \\ \vdots \\ a_n \end{pmatrix} = \mathrm{S}\boldsymbol{a}$$

Reciprocity $S_{ij} = S_{ji}$ (time-reversal symmetry)

Unitarity $\displaystyle\sum_j S_{ji} S_{jk}^* = \delta_{ik}$

Onsager reciprocity

$$\left[\frac{(i\hbar\nabla + e\boldsymbol{A})^2}{2m} + V\right]\psi = E\psi$$ Complex conjugate and $\boldsymbol{A} \to -\boldsymbol{A}$

Lars Onsager
1903-1976

$$\left[\frac{(i\hbar\nabla + e\boldsymbol{A})^2}{2m} + V\right]\psi^* = E\psi^*$$ $\{\psi^*(-B)\} = \{\psi(B)\}$

Scattering solution: Sc$\{a \to b\}$ $\mathrm{Sc}\{\boldsymbol{a}(B) \to \boldsymbol{b}(B)\} \in \{\psi(B)\}, \quad i.e., \quad \boldsymbol{b}(B) = S(B)\boldsymbol{a}(B)$

$$\boldsymbol{b}^*(B) = S^*(B)\boldsymbol{a}^*(B)$$

$$\mathrm{Sc}\{\boldsymbol{b}^*(-B) \to \boldsymbol{a}^*(-B)\} \in \{\psi^*(-B)\} = \{\psi(B)\} \quad i.e. \quad \boldsymbol{a}^*(-B) = S(B)\boldsymbol{b}^*(-B)$$

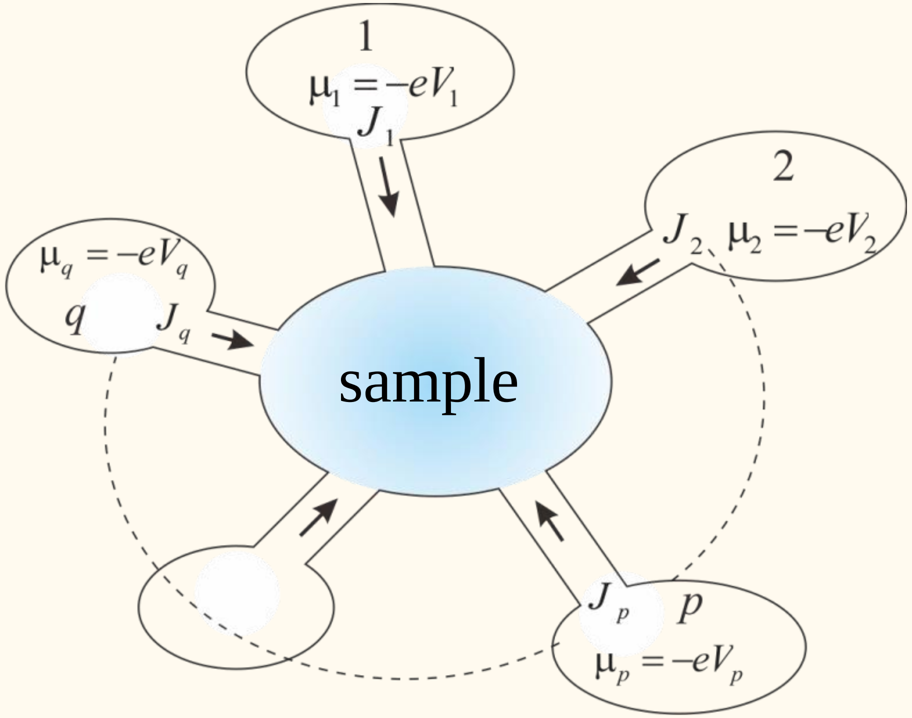
$$\boldsymbol{b}^*(B) = S^{-1}(-B)\boldsymbol{a}^*(B)$$

$$S^*(B) = S^{-1}(-B) = S^\dagger(-B) \quad (\quad \text{unitarity} \quad SS^\dagger = S^\dagger S = I)$$

$$S(B) = {}^tS(-B) \qquad\qquad S_{ij}(B) = S_{ji}(-B)$$

Landauer-Büttiker formula

Makus Büttiker
1950-2013



$$J_p = -\frac{2e}{h}\sum_q [T_{q\leftarrow p}\mu_p - T_{p\leftarrow q}\mu_q]$$

$$\mathscr{T}_{pq} \equiv T_{p\leftarrow q} \quad (p \neq q), \qquad \mathscr{T}_{pp} \equiv -\sum_{q\neq p} T_{q\leftarrow p}$$

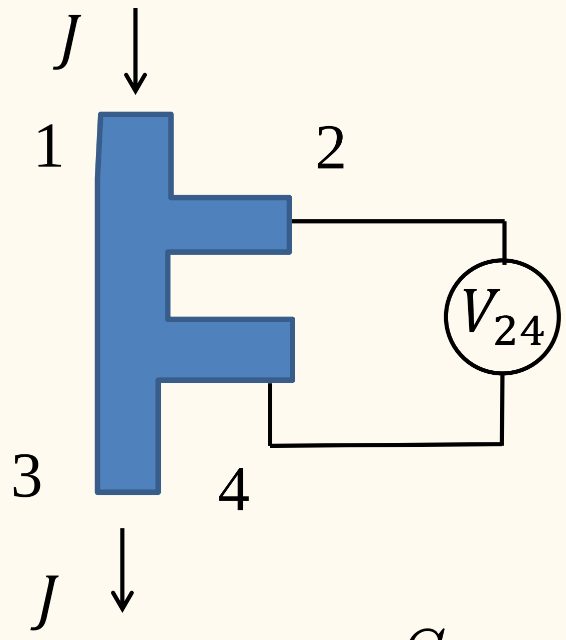
$$\boldsymbol{J} =^t (J_1, J_2, \cdots), \boldsymbol{\mu} =^t (\mu_1, \mu_2, \cdots)$$

$$\boldsymbol{J} = \frac{2e}{h}\mathscr{T}\boldsymbol{\mu}$$

$$V_q = \frac{\mu_q}{-e}, \qquad G_{pq} \equiv \frac{2e^2}{h} T_{p\leftarrow q} \ \text{ then } \ J_p = \sum_q [G_{qp}V_p - G_{pq}V_q]$$

$$\sum_q J_q = 0 \qquad \sum_q [G_{qp} - G_{pq}] = 0 \qquad G_{qp}(B) = G_{pq}(-B)$$

Landauer-Büttker formula: Application to 4-terminal measurement



$$\alpha_{11} = 2G_q[-\mathscr{T}_{11} - S^{-1}(\mathscr{T}_{14} + \mathscr{T}_{12})(\mathscr{T}_{41} + \mathscr{T}_{21})]$$
$$\alpha_{12} = 2G_q S^{-1}(\mathscr{T}_{12}\mathscr{T}_{34} - \mathscr{T}_{14}\mathscr{T}_{32})$$
$$\alpha_{21} = 2G_q S^{-1}(\mathscr{T}_{21}\mathscr{T}_{43} - \mathscr{T}_{23}\mathscr{T}_{41})$$
$$\alpha_{22} = 2G_q[-\mathscr{T}_{22} - S^{-1}(\mathscr{T}_{21} - \mathscr{T}_{23})(\mathscr{T}_{32} + \mathscr{T}_{12})]$$

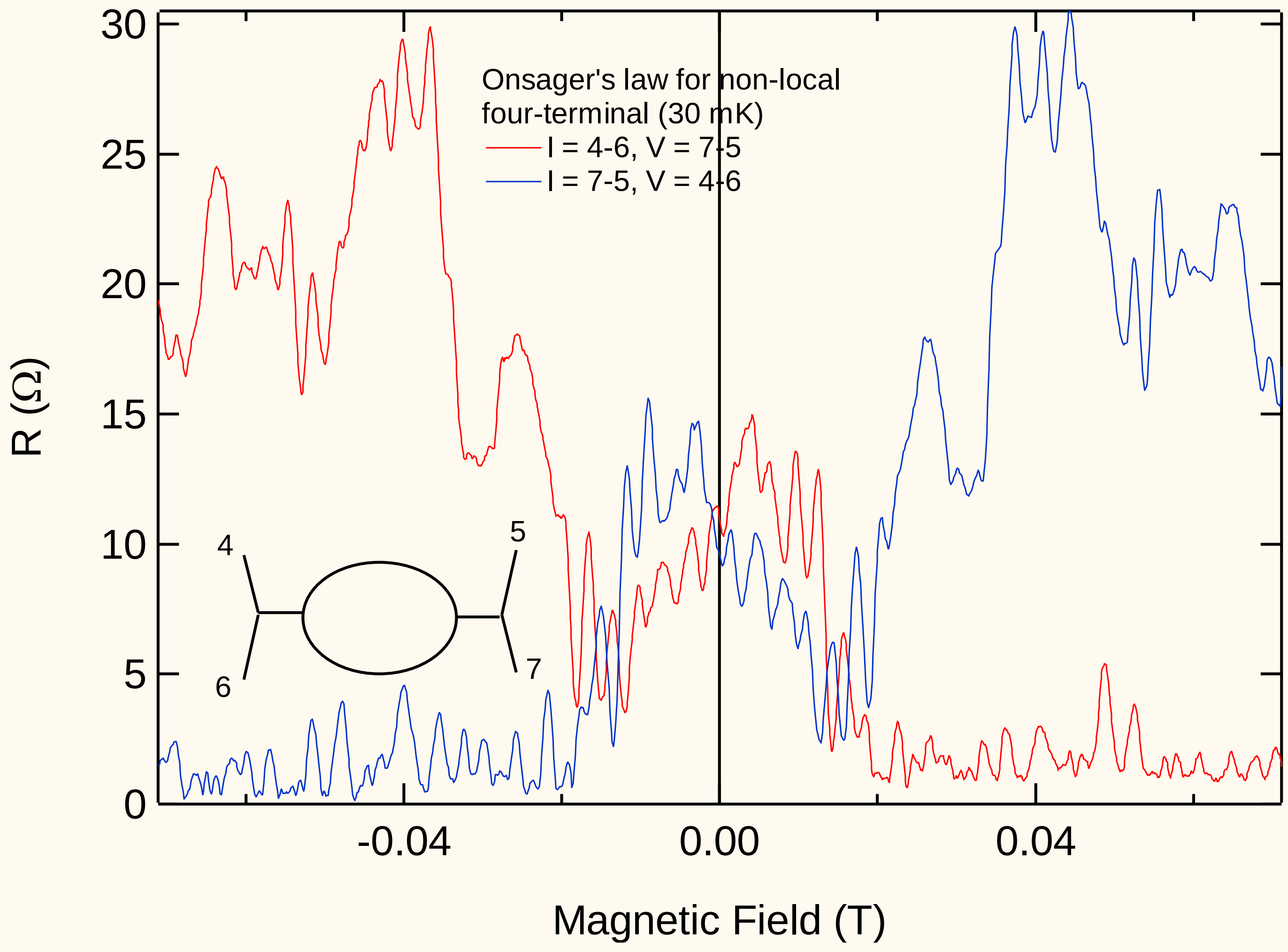
$$S = \mathscr{T}_{12} + \mathscr{T}_{14} + \mathscr{T}_{32} + \mathscr{T}_{34} = \mathscr{T}_{21} + \mathscr{T}_{41} + \mathscr{T}_{23} + \mathscr{T}_{43}$$

$$\mathcal{R}_{13,24} = \frac{V_2 - V_4}{J_1} = \frac{\alpha_{21}}{\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}}$$

$$\mathcal{R}_{mn,kl}(B) = -\mathcal{R}_{kl,mn}(-B)$$ Onsager reciprocity

Onsager reciprocity in AB ring

$$\mathcal{R}_{ij,kl}(B) = \mathcal{R}_{kl,ij}(-B)$$



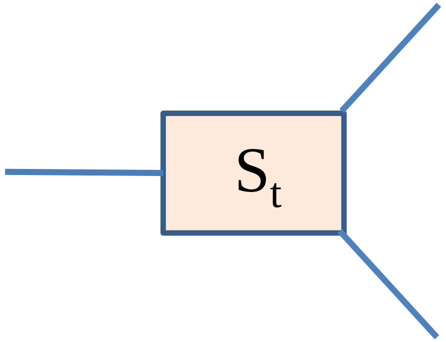
Magnetoresistance: Universal conductance fluctuation including AB oscillation

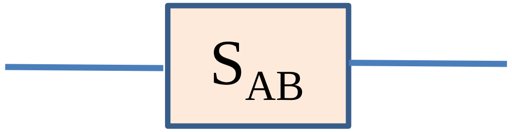
S-matrix: Application to Aharonov-Bohm ring

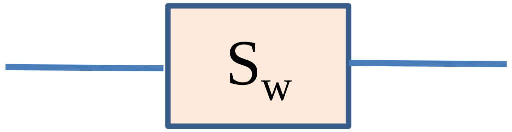
$$S_t = \begin{pmatrix} 0 & -1/\sqrt{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 1/2 & -1/2 \\ -1/\sqrt{2} & -1/2 & 1/2 \end{pmatrix}$$

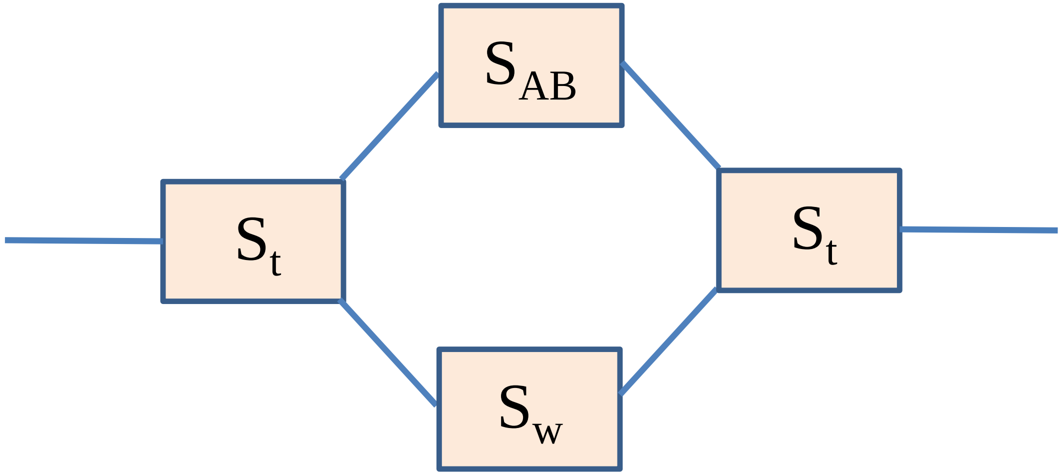
$$S_{\mathrm{AB}} = \begin{pmatrix} 0 & e^{i\theta_{\mathrm{AB}}} \\ e^{-i\theta_{\mathrm{AB}}} & 0 \end{pmatrix}, \qquad \theta \equiv 2\pi\frac{\phi}{\phi_0} = \frac{e}{\hbar}\phi$$

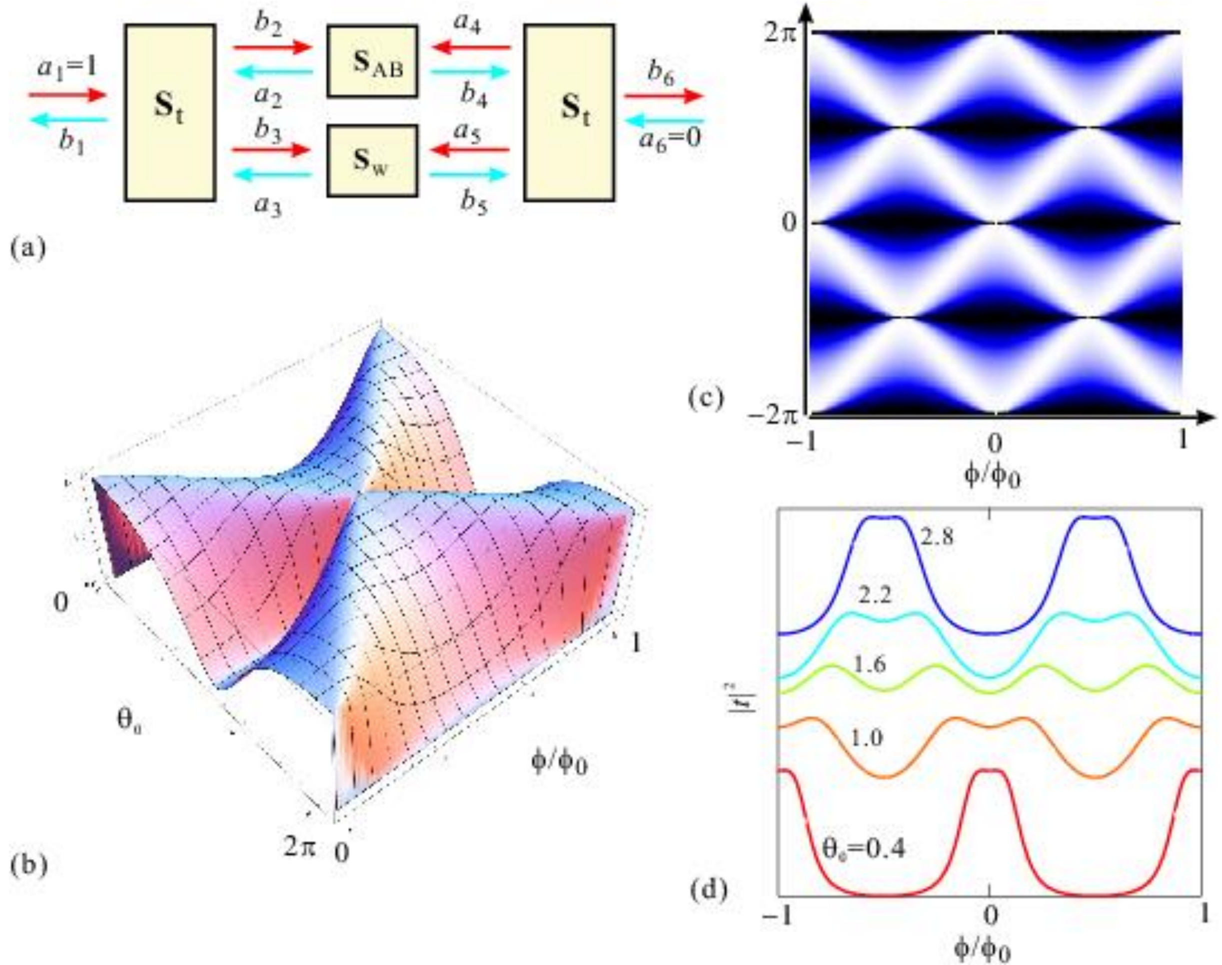
$$S_{\mathrm{w}} = \begin{pmatrix} 0 & e^{i\theta_0} \\ e^{i\theta_0} & 0 \end{pmatrix}$$











$$t = \frac{4\sin\theta_0}{1 + e^{i\theta_{\mathrm{AB}}}\left(e^{i\theta_{\mathrm{AB}}} + e^{i\theta_0} - 3e^{-i\theta_0}\right)}$$

Bunching and anti-bunching of particles

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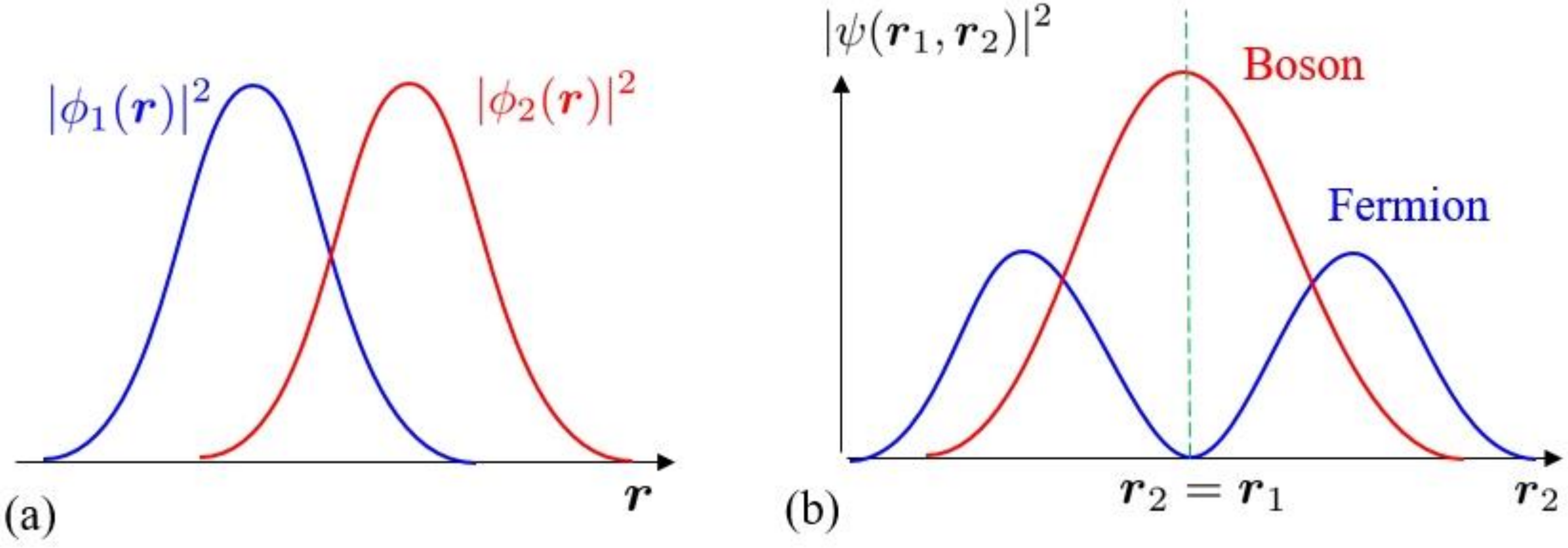
Probability of finding two-particles at the same position

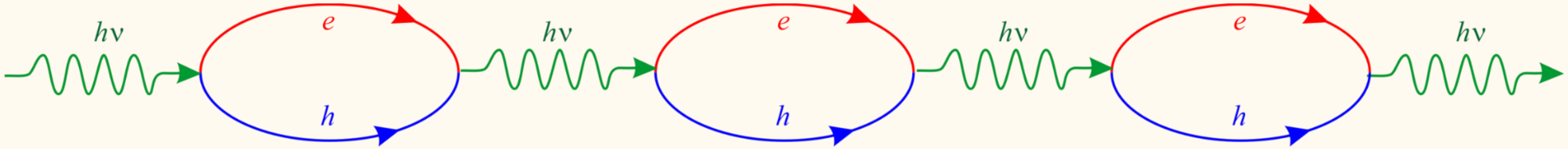
$$|\psi(\boldsymbol{r}_1, \boldsymbol{r}_1)|^2 = \begin{cases} 2|\phi_1(\boldsymbol{r}_1)|^2|\phi_2\boldsymbol{r}_1|^2 & \text{(boson)}, \\ 0 & \text{(fermion)} \end{cases}$$

Boson: bunching, bosonic stimulation → laser oscillation, Bose-Einstein Condensation



Waveguide for exciton-polariton

exciton-polariton



Chain of photon-exciton (photon-dressed exciton)

1 cycle ~ few fs

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photon→ cavity photon

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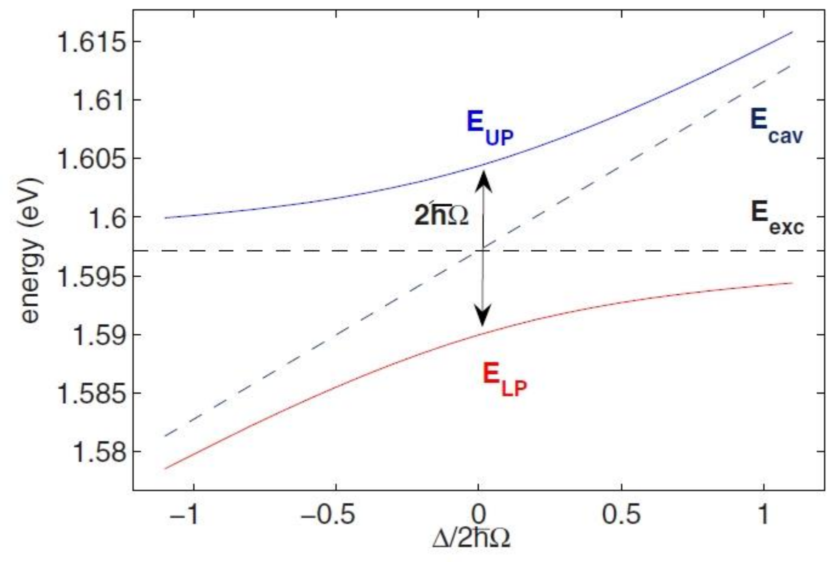
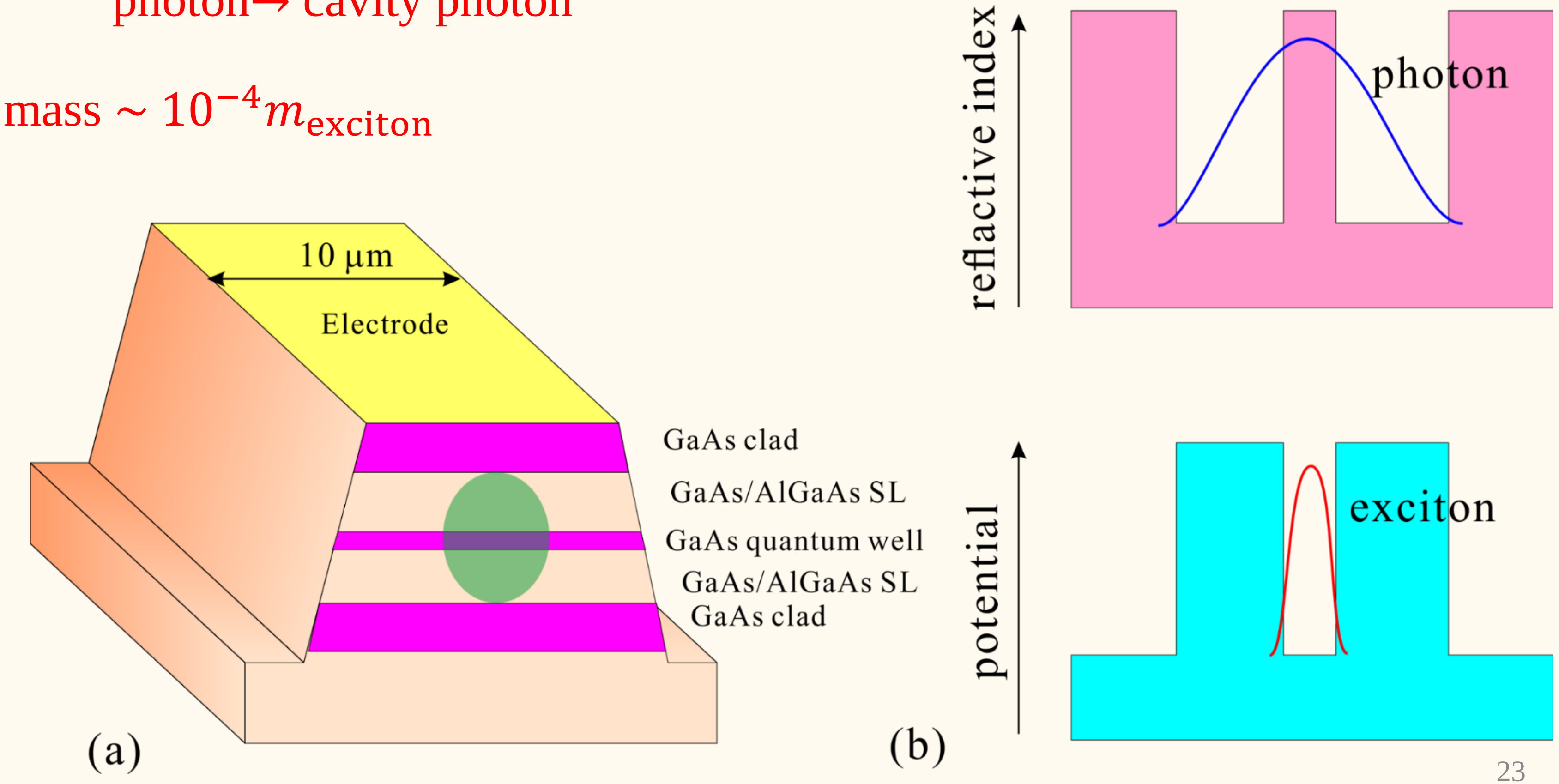


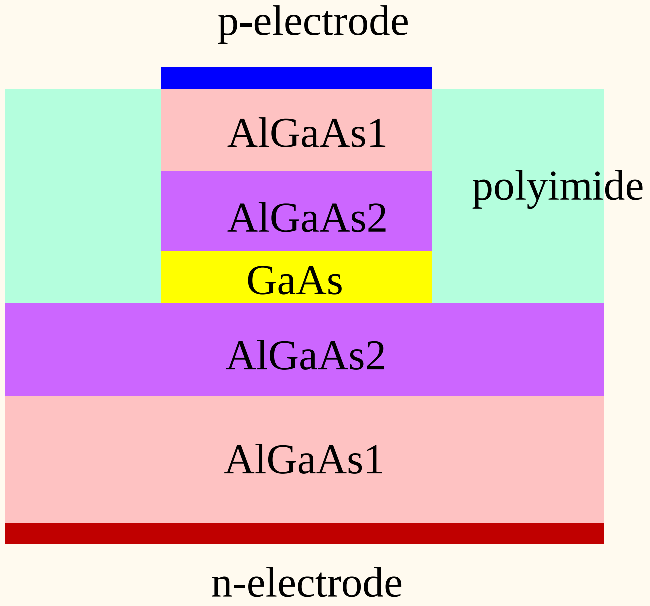


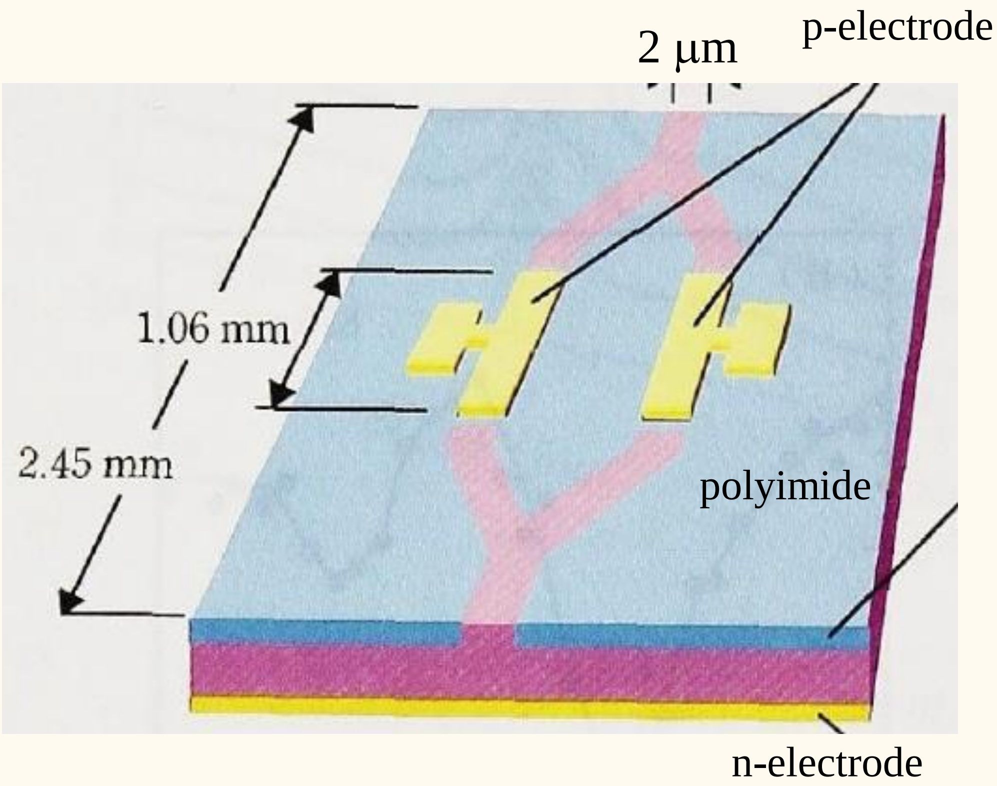
Mach-Zehnder interferometer (voltage-type)

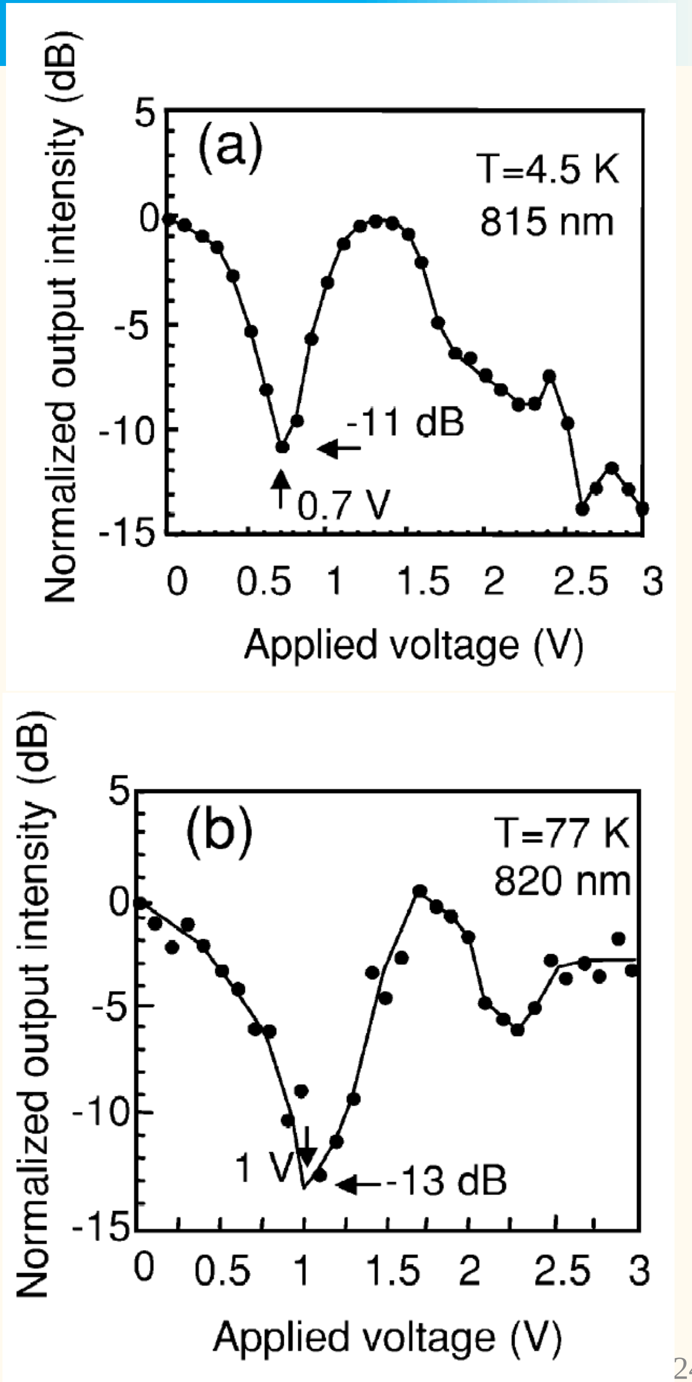
Kinetic phase shift with electric field: $\Delta\varphi = L\left[\frac{\sqrt{2mE_k}}{\hbar} - \frac{\sqrt{2m(E_k-\delta E)}}{\hbar}\right]$

δE: energy shift due to the depletion of quantum well

junction-FET type waveguide







Katsuyama, Hosomi, Micro. Eng. **63**, 23 (2002).

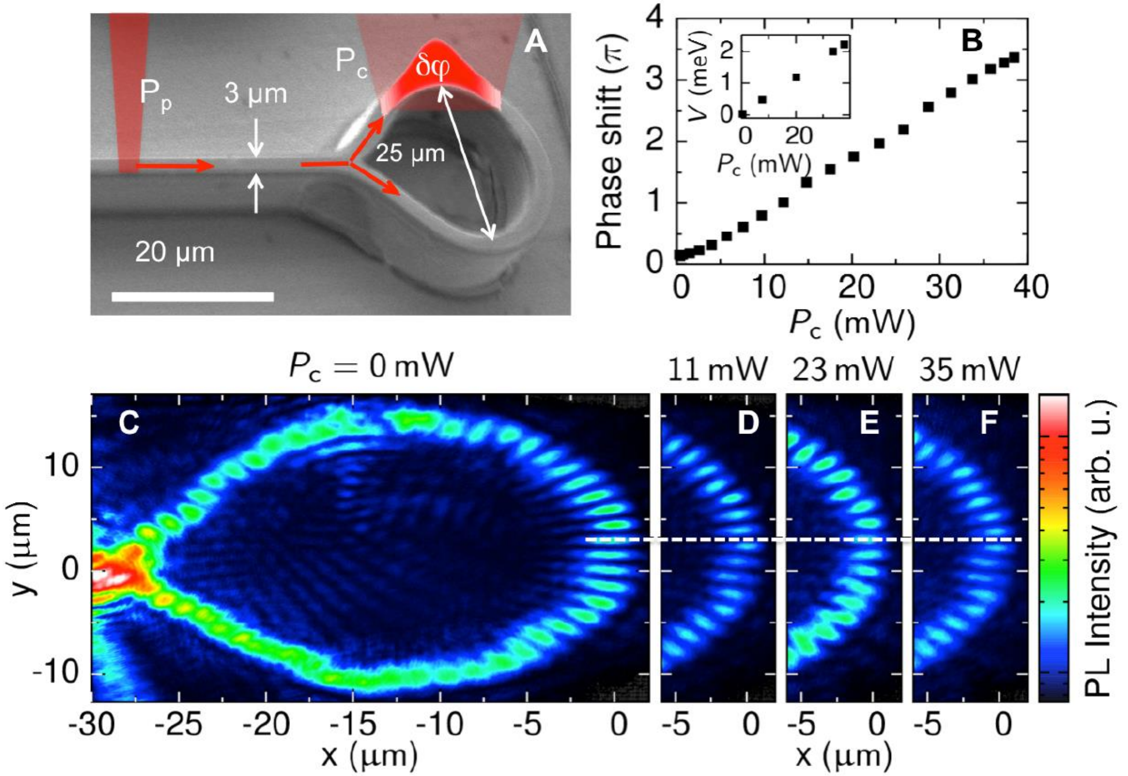
Voltage control of optical output through interference

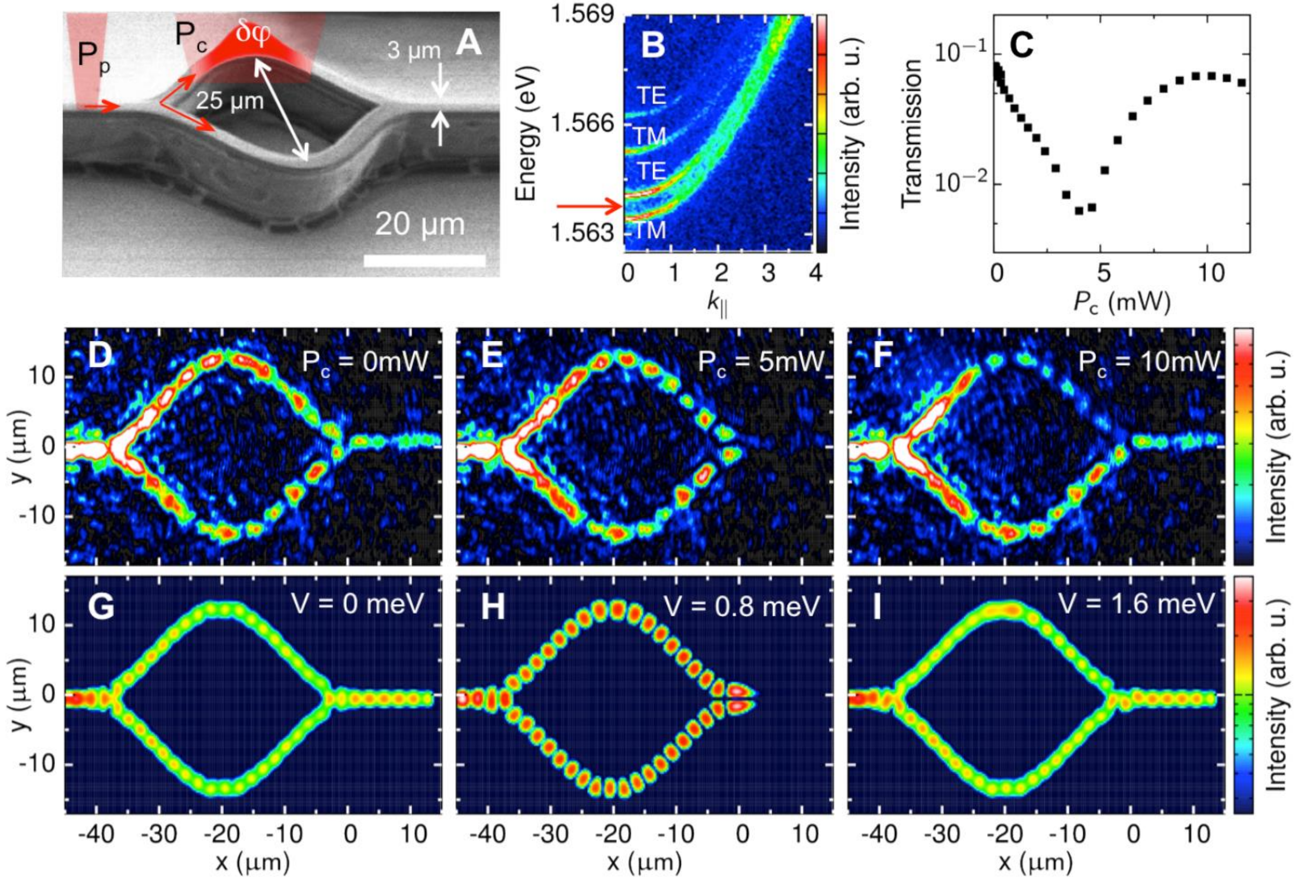
Mach-Zehnder interferometer 2 (optical control)

Kinetic phase shift with electric field: $\Delta\varphi = L\left[\frac{\sqrt{2mE_k}}{\hbar} - \frac{\sqrt{2m(E_k-\delta E)}}{\hbar}\right]$

δE: energy shift due to the barrier by optically excited carriers (quasi-Fermi levels)

Sturm *et al.*, Nature Comm. **5**, 3278 (2014)





Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.6.30 Lecture 12

10:25 – 11:55

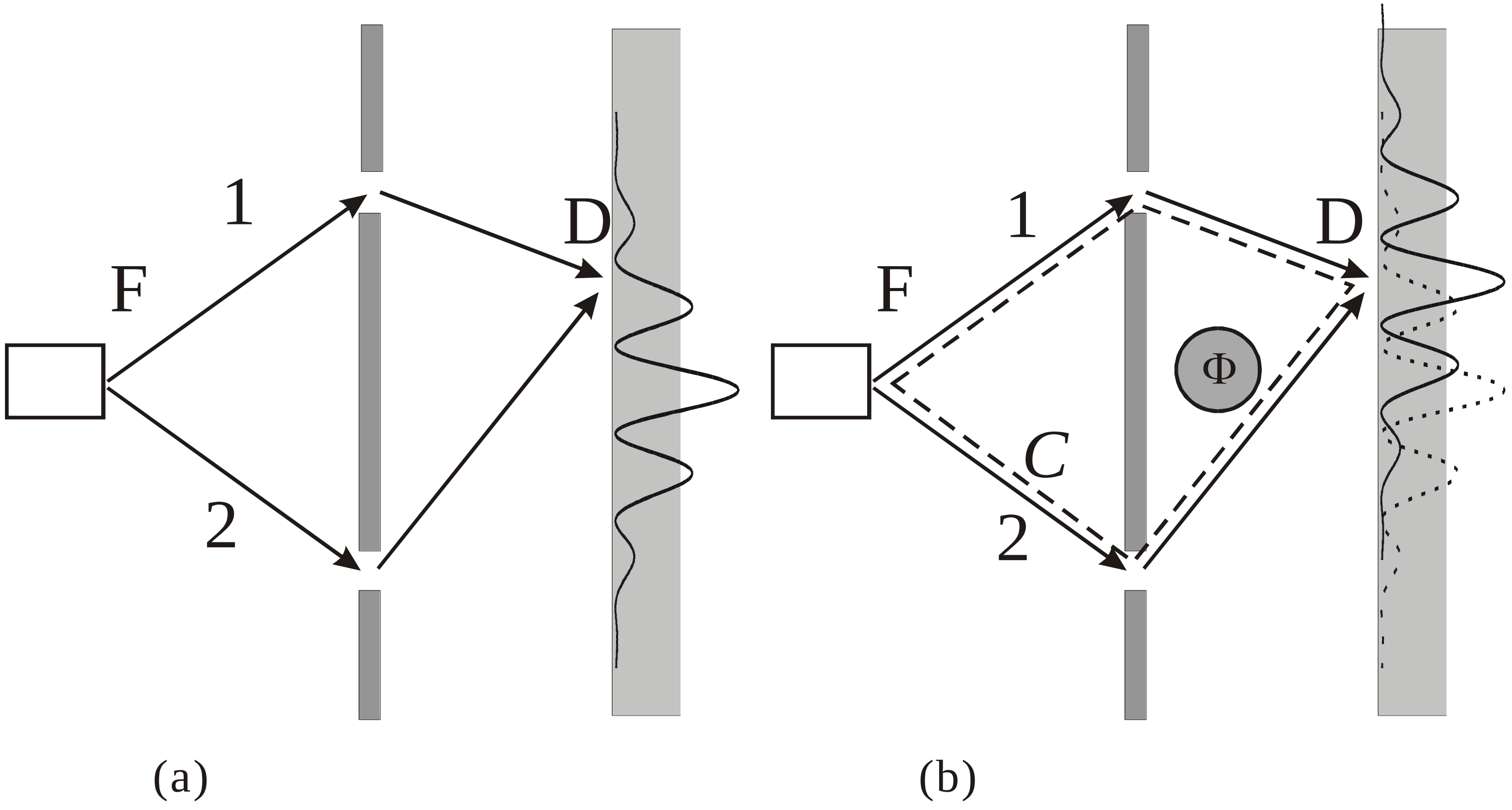
Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

Chapter 8 Basics of Quantum Transport

- Boundary between classical and quantum (coherence length)
- Conductance quantum
- Quantum point contact
- Landauer formula for two-terminal conductance
- Scattering matrix (S-matrix)
- Onsager reciprocity
- Landauer-Büttker formula for multi-terminal conductance

Aharonov-Bohm effect

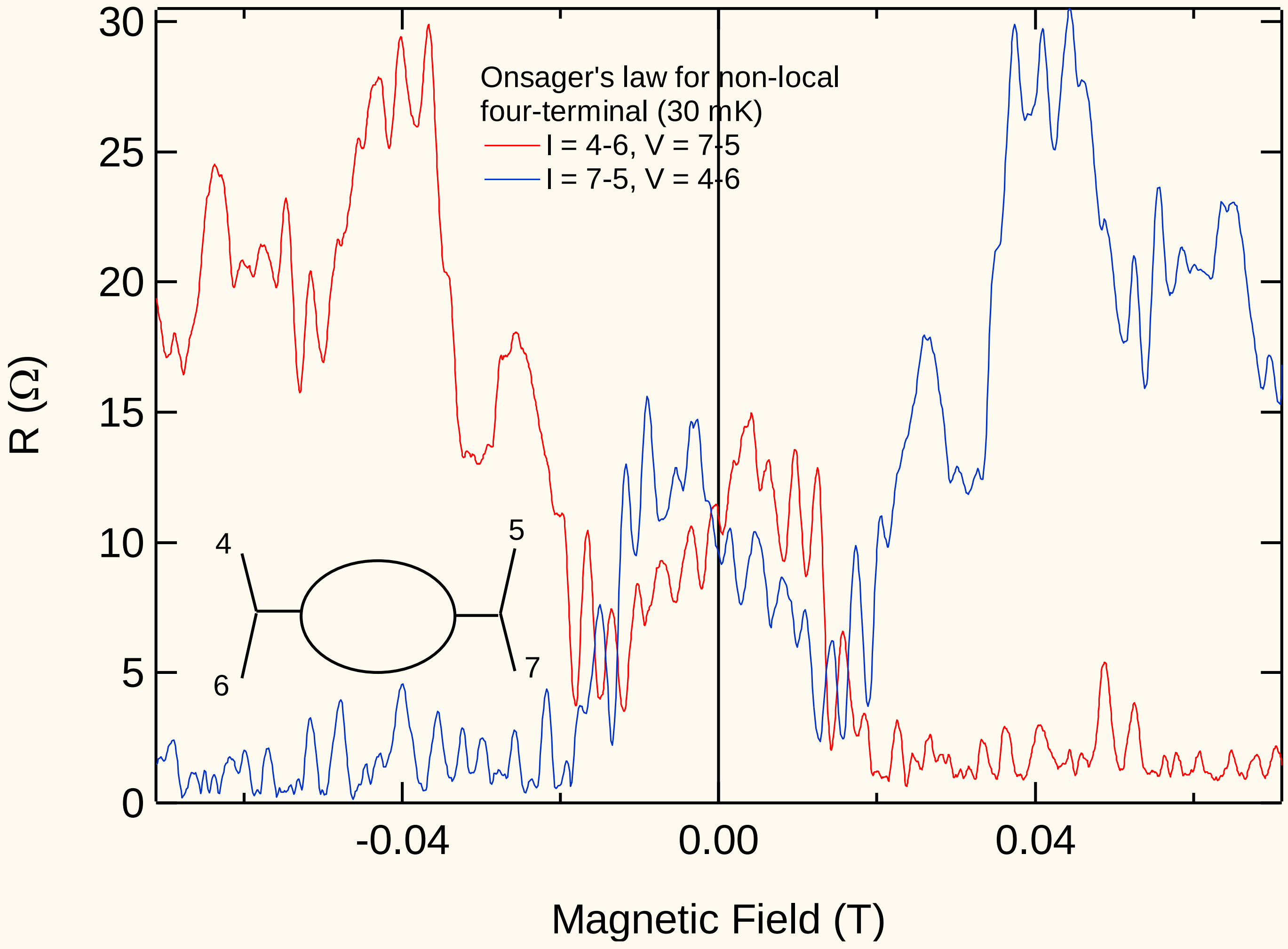


$$\boldsymbol{p} = m\boldsymbol{v} + e\boldsymbol{A} \qquad p = \hbar k = \frac{h}{\lambda}$$

$$\Delta\theta = \frac{e}{\hbar}\oint_C \Delta\boldsymbol{A}\cdot \mathrm{d}\boldsymbol{s} = \frac{e}{\hbar}\int_S \boldsymbol{B}\cdot \mathrm{d}\boldsymbol{n} = 2\pi\frac{\Phi}{\Phi_0} \qquad \Phi_0 \equiv \frac{h}{e}$$

Onsager reciprocity in AB ring

$$\mathcal{R}_{ij,kl}(B) = \mathcal{R}_{kl,ij}(-B)$$



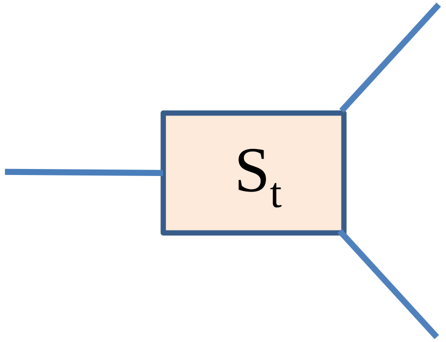
In the case of two-terminal measurement

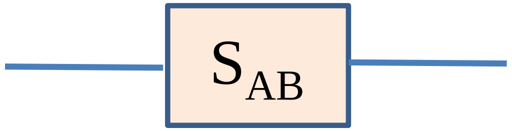
$$R(B) = R(-B)$$

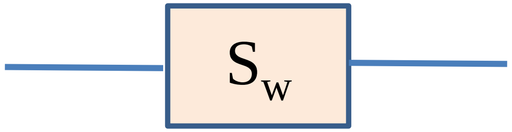
Magnetoresistance: Universal conductance fluctuation including AB oscillation

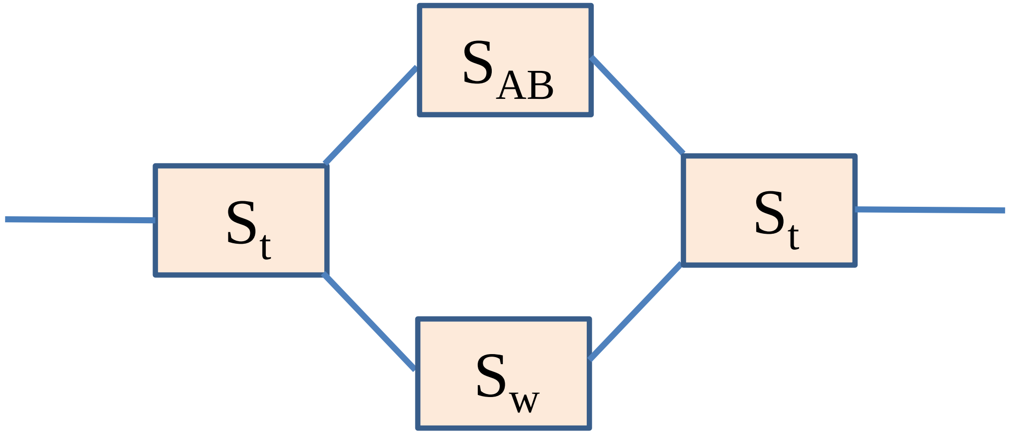
S-matrix: Application to Aharonov-Bohm ring

$$S_t = \begin{pmatrix} 0 & -1/\sqrt{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & 1/2 & -1/2 \\ -1/\sqrt{2} & -1/2 & 1/2 \end{pmatrix} \qquad S_{\mathrm{AB}} = \begin{pmatrix} 0 & e^{i\theta_{\mathrm{AB}}} \\ e^{-i\theta_{\mathrm{AB}}} & 0 \end{pmatrix}, \qquad \theta \equiv 2\pi \frac{\phi}{\phi_0} = \frac{e}{\hbar}\phi \qquad S_{\mathrm{w}} = \begin{pmatrix} 0 & e^{i\theta_0} \\ e^{i\theta 0} & 0 \end{pmatrix}$$









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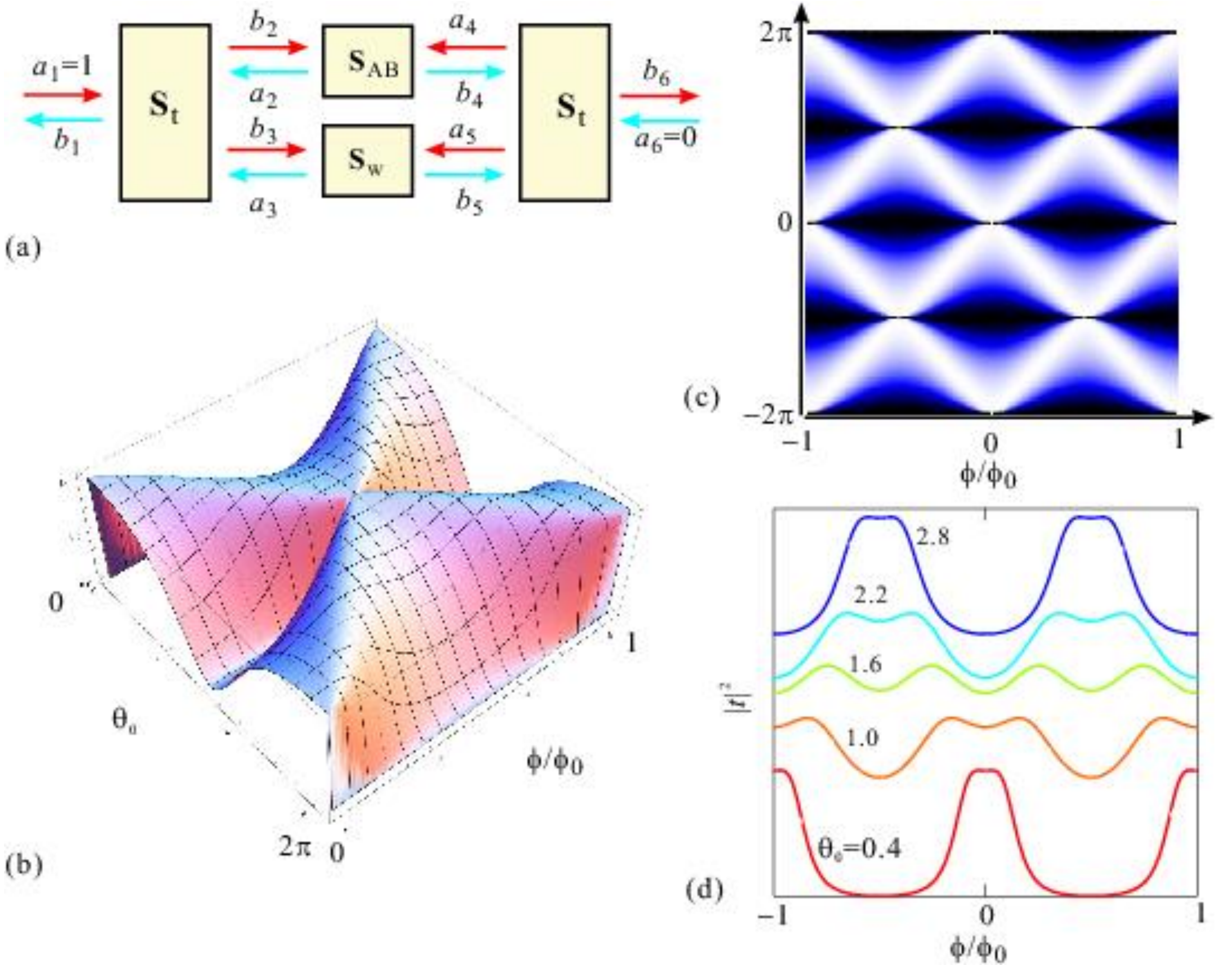
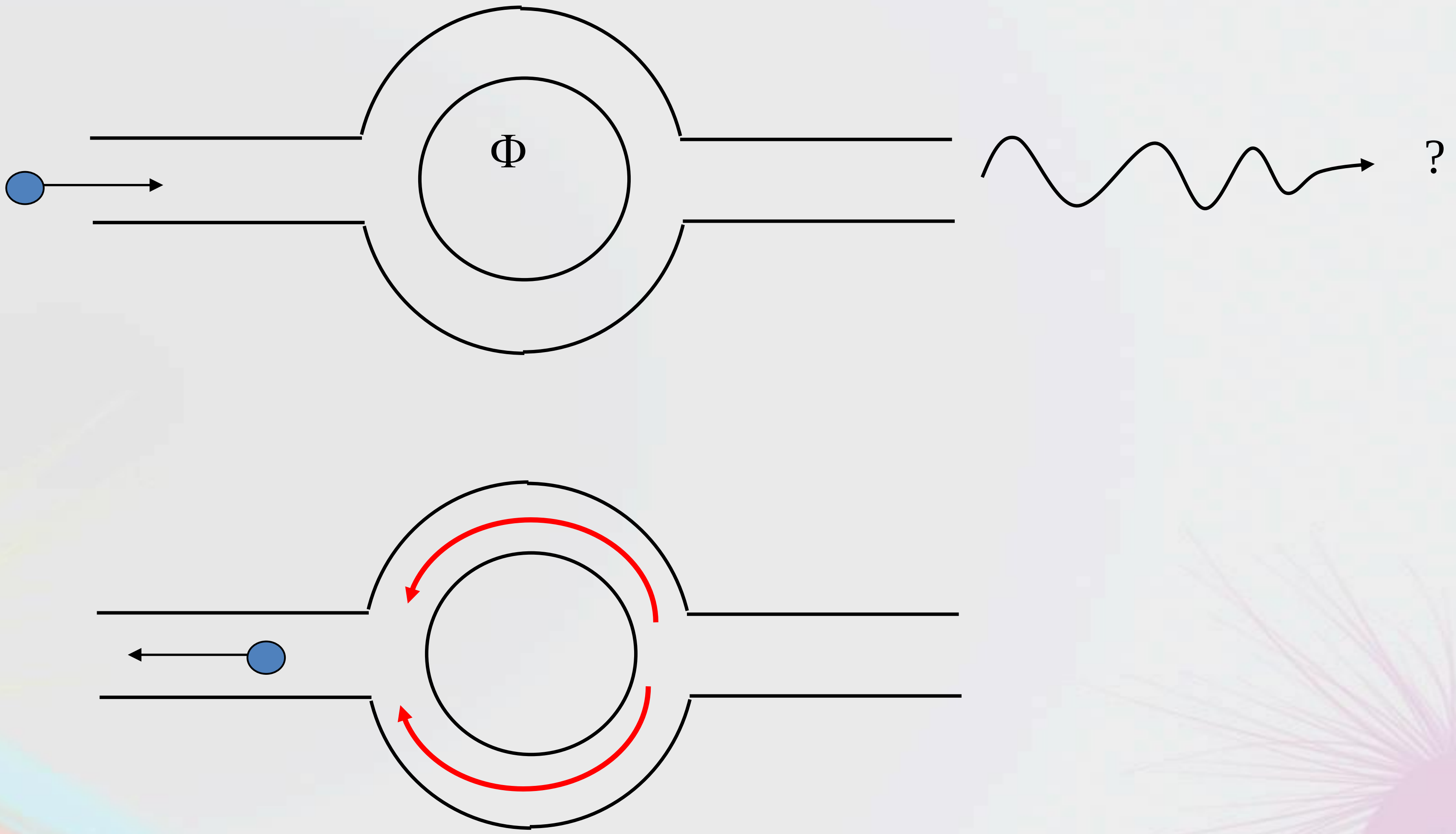


Disappearance of electrons?



Bunching and anti-bunching of particles

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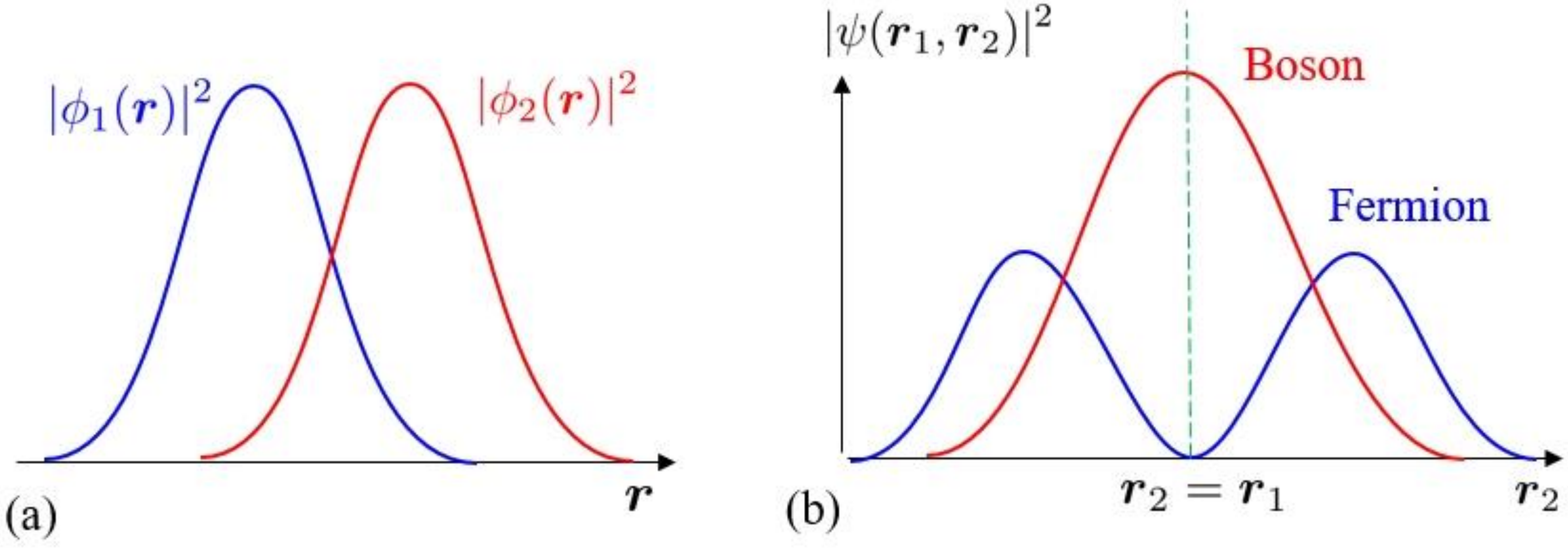
Boson: bunching, bosonic stimulation → laser oscillation, Bose-Einstein Condensation

Fermion: anti-bunching, conductance quantization, shot noise reduction



Waveguide for exciton-polariton

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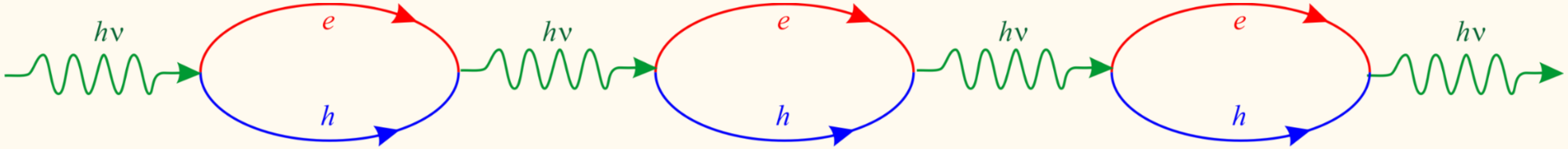

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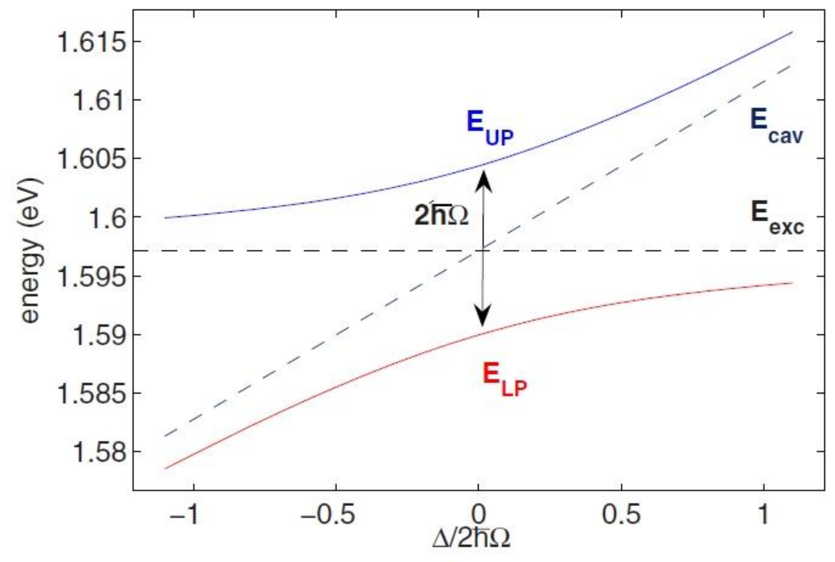
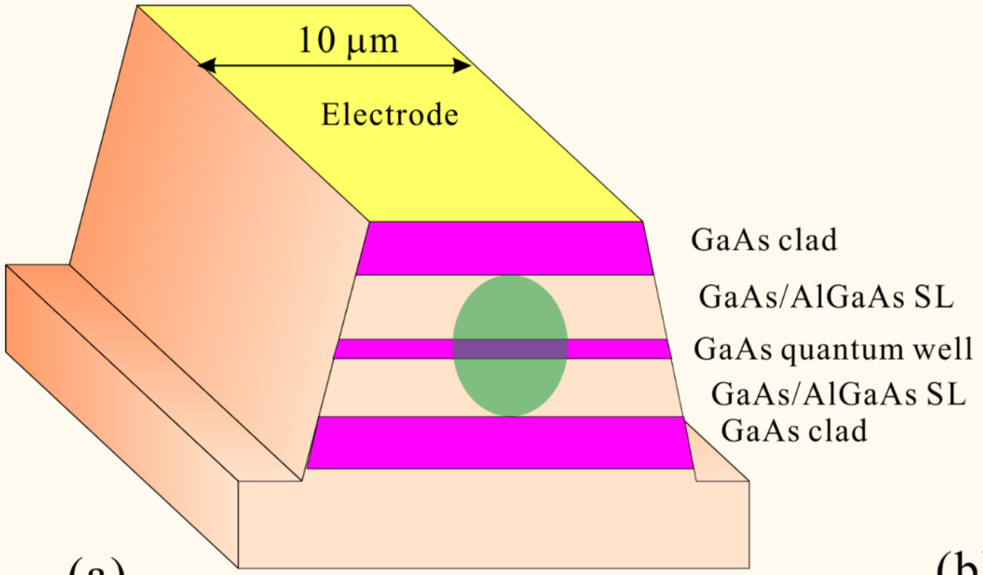
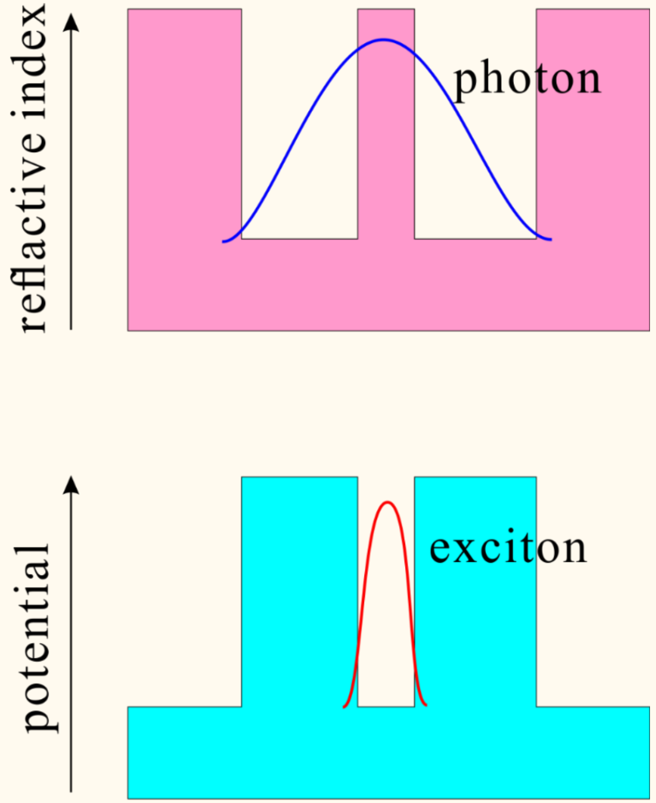




(a)



(b)

Mach-Zehnder interferometer (voltage-type)

Kinetic phase shift with electric field: $\Delta\varphi = L\left[\frac{\sqrt{2mE_k}}{\hbar} - \frac{\sqrt{2m(E_k - \delta E)}}{\hbar}\right]$

δE: energy shift due to the depletion of quantum well

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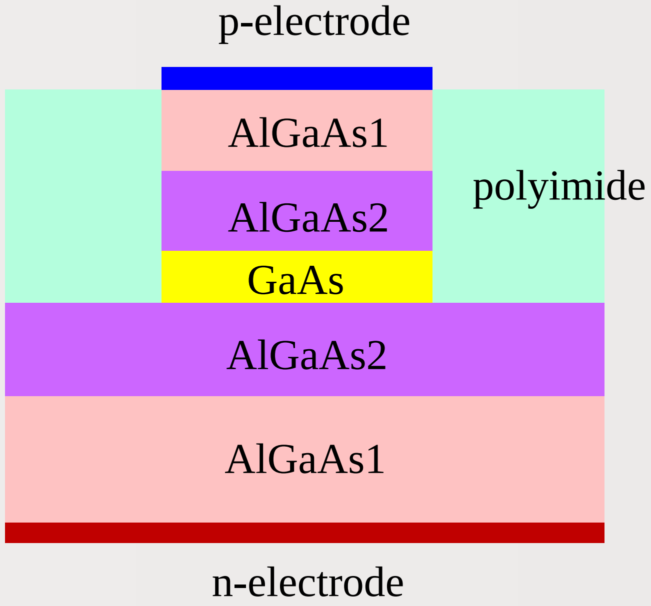
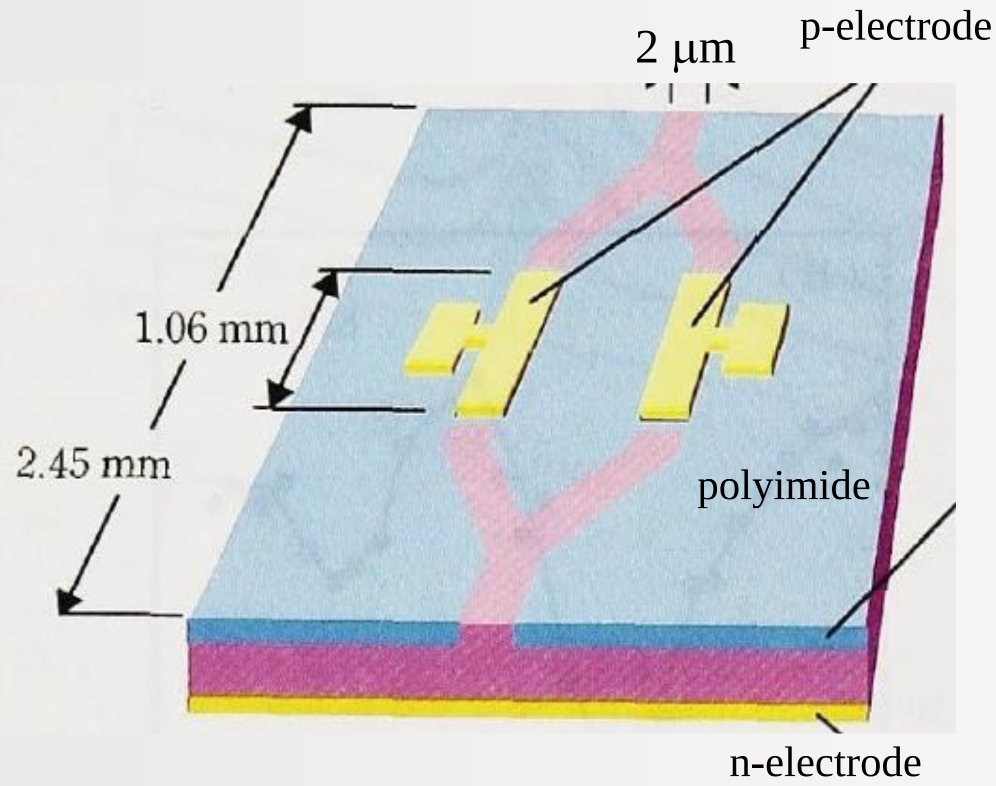
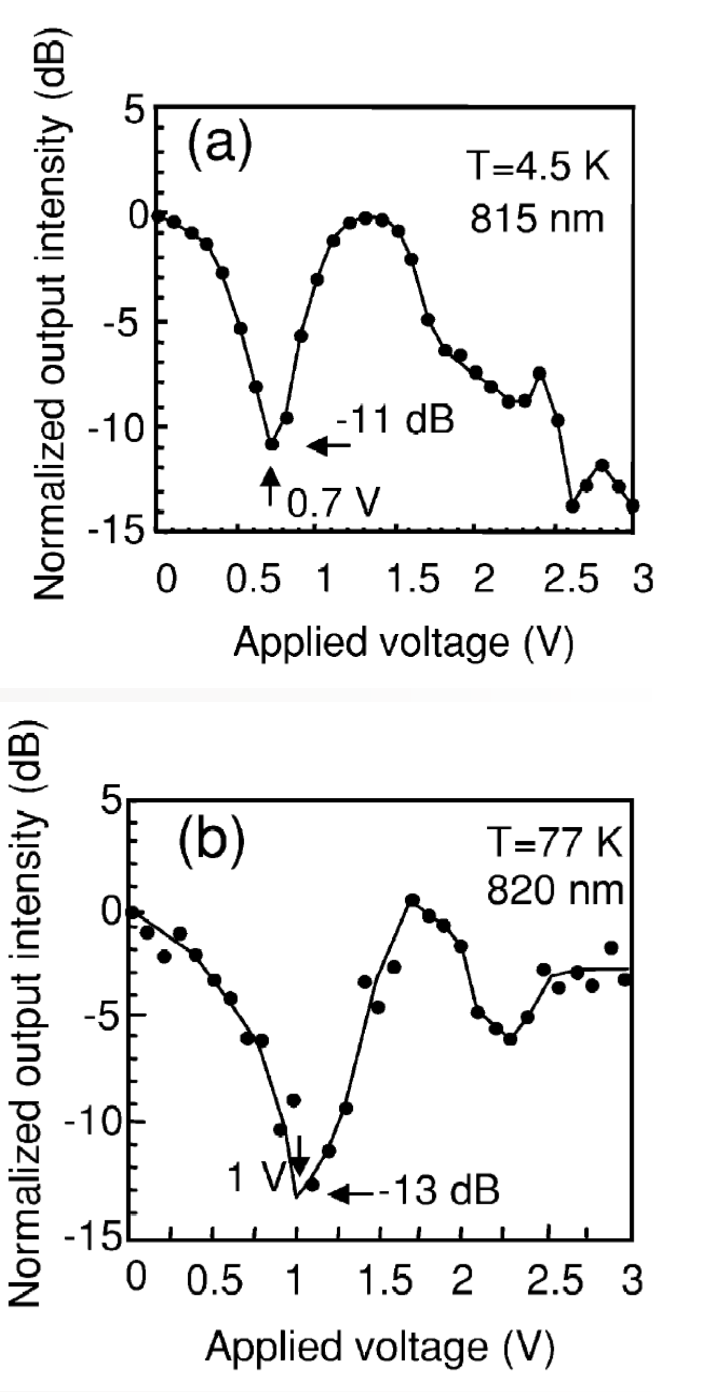




Katsuyama, Hosomi, Micro. Eng. **63**, 23 (2002).

Voltage control of optical output through interference



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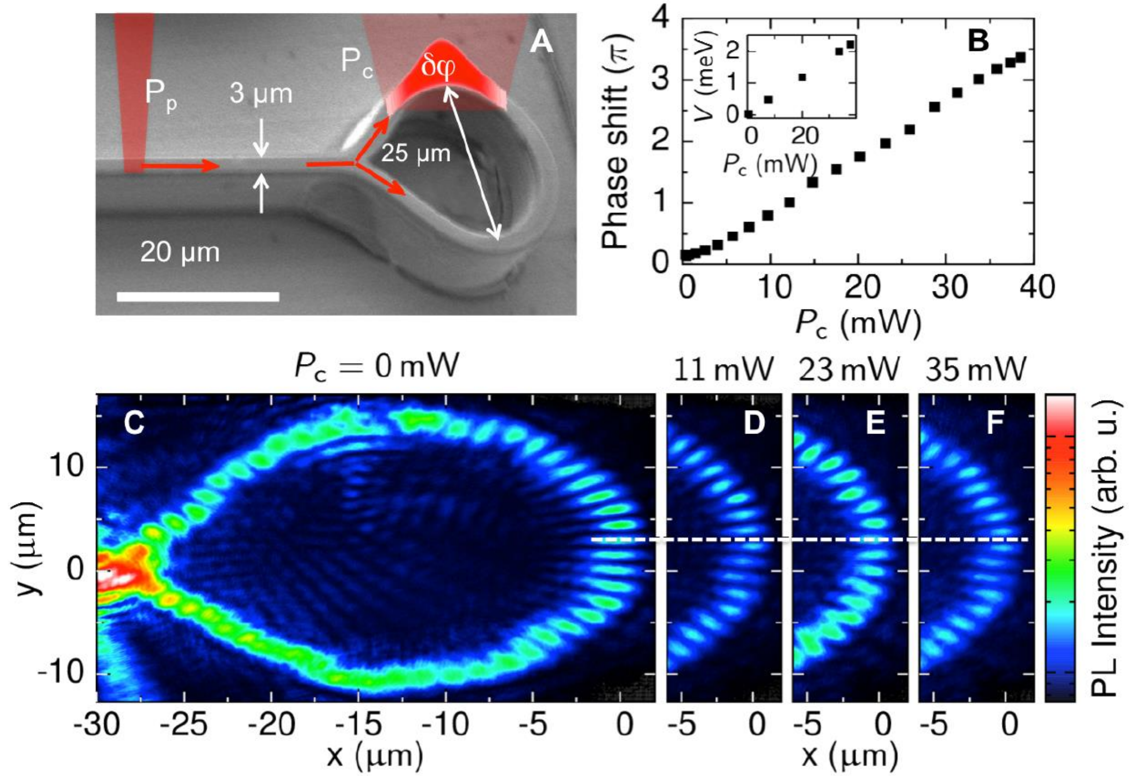
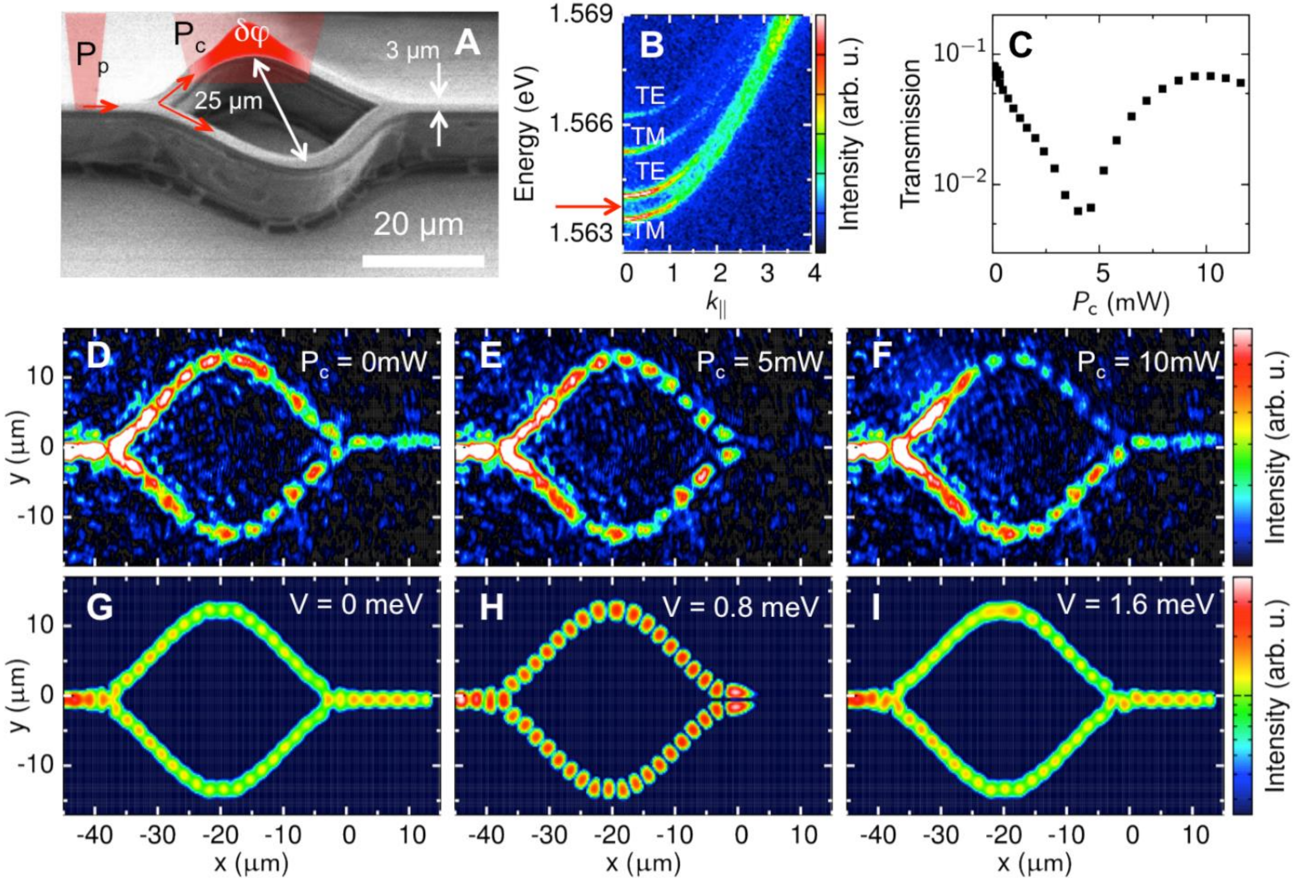
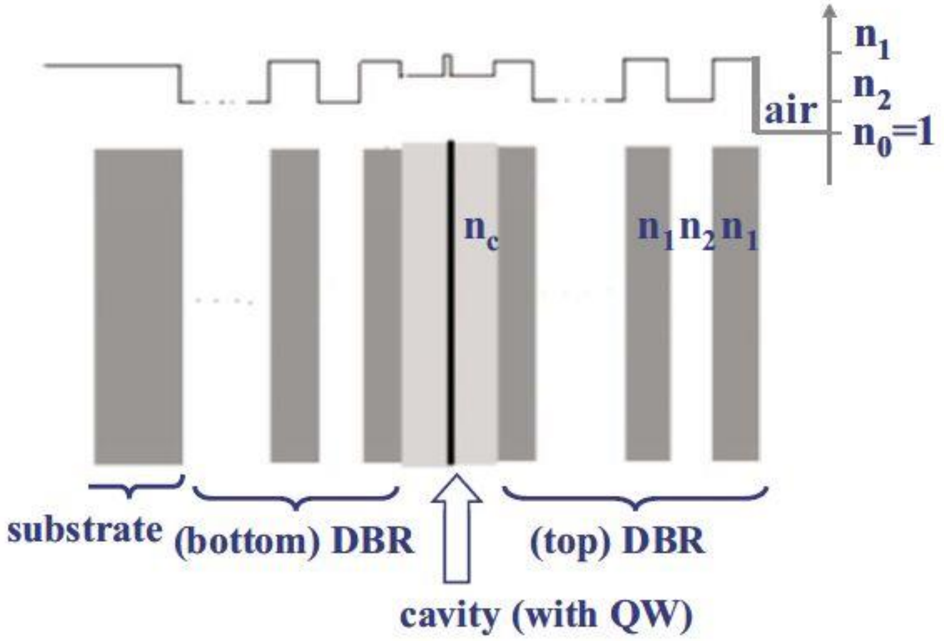
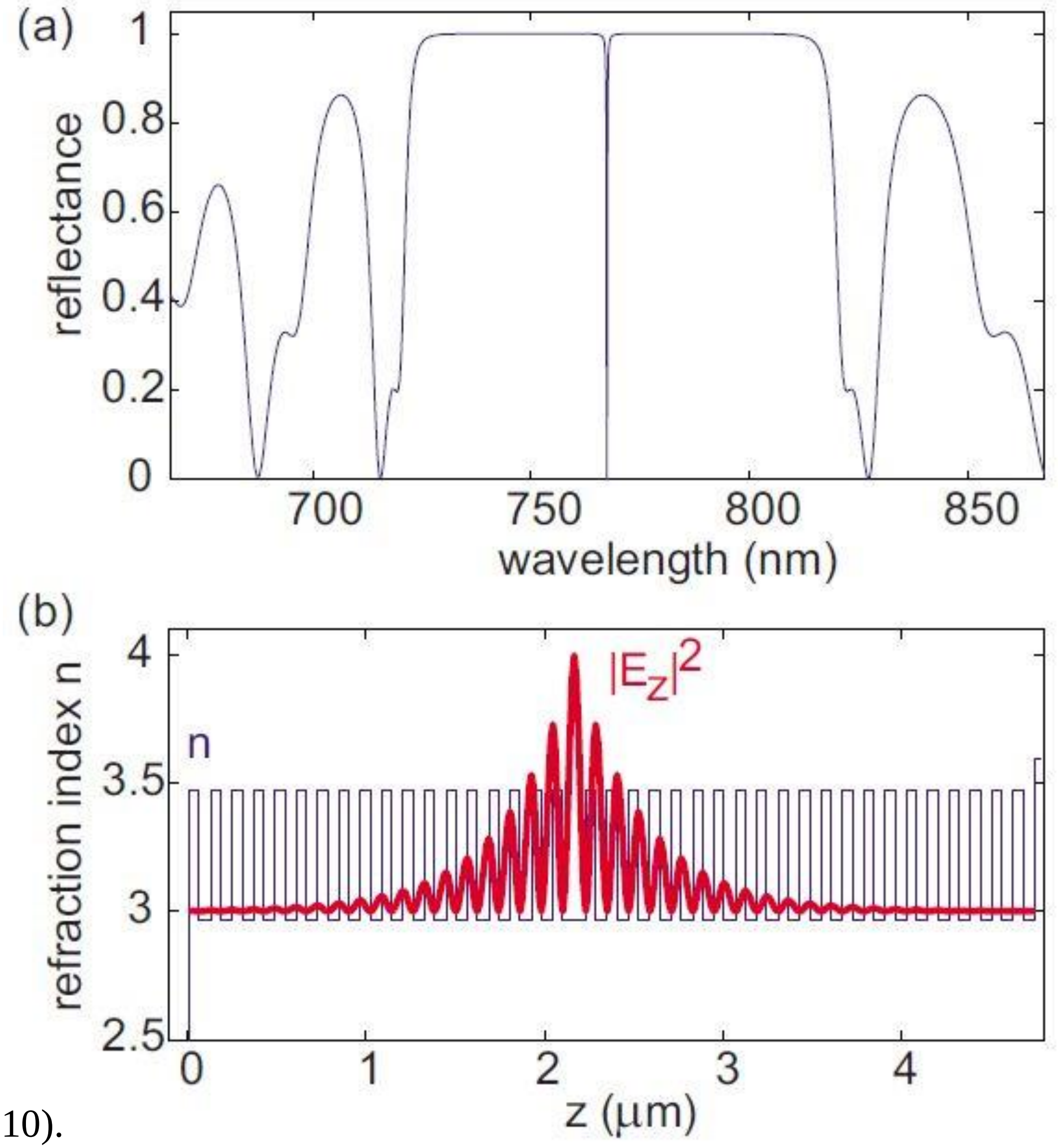
Sturm *et al.*, Nature Comm. **5**, 3278 (2014)





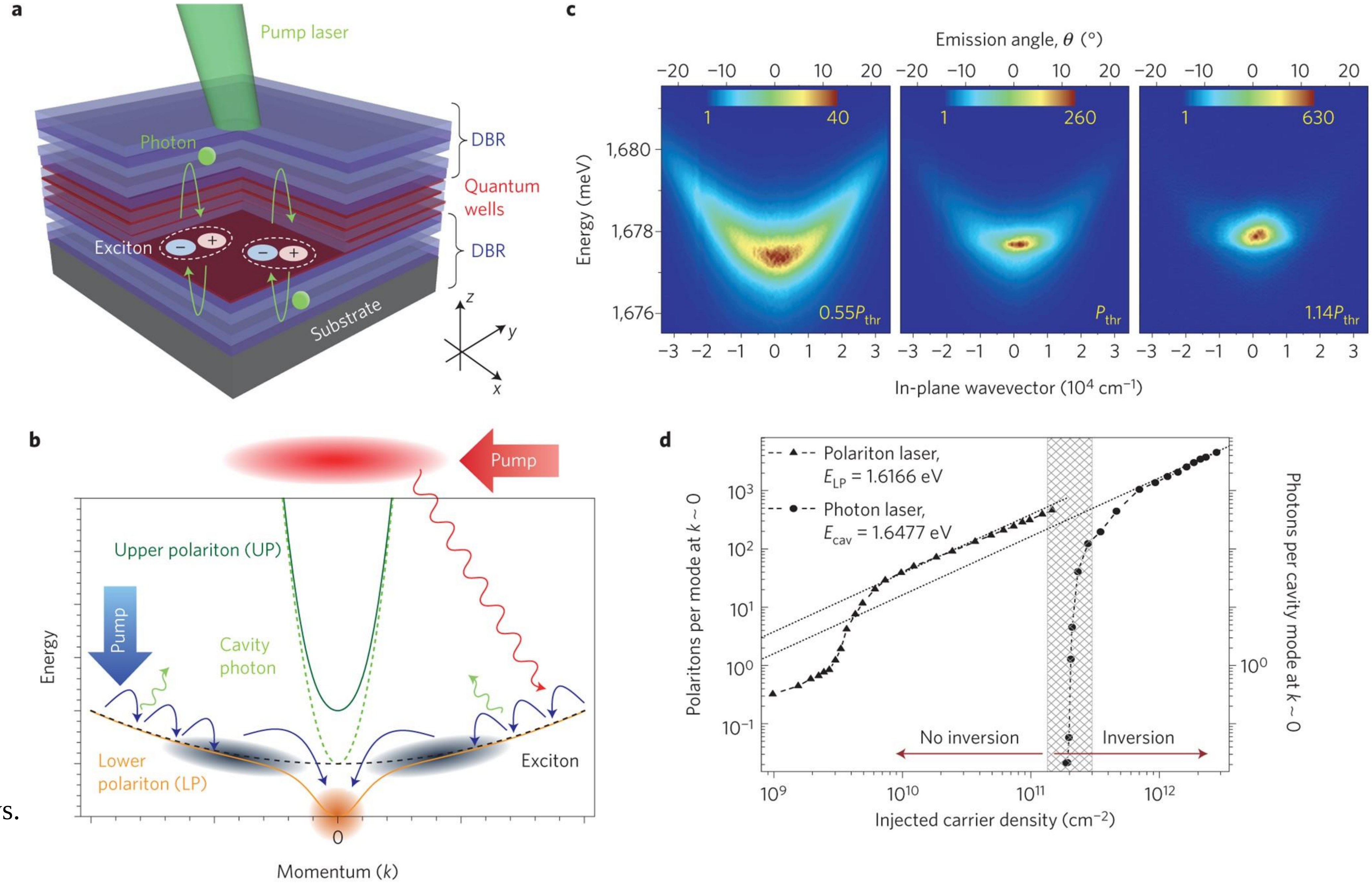




$$T = \frac{(1-R_1)(1-R_2)}{[1-\sqrt{R_1R_2}]^2 + 4\sqrt{R_1R_2}\sin^2(\phi/2)}$$

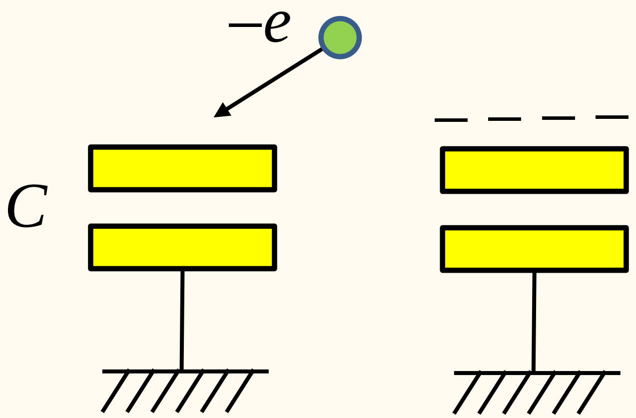
Deng, Haug, Yamamoto, Rev. Mod. Phys. **82**, 1489 (2010).

Exciton-polariton condensation2



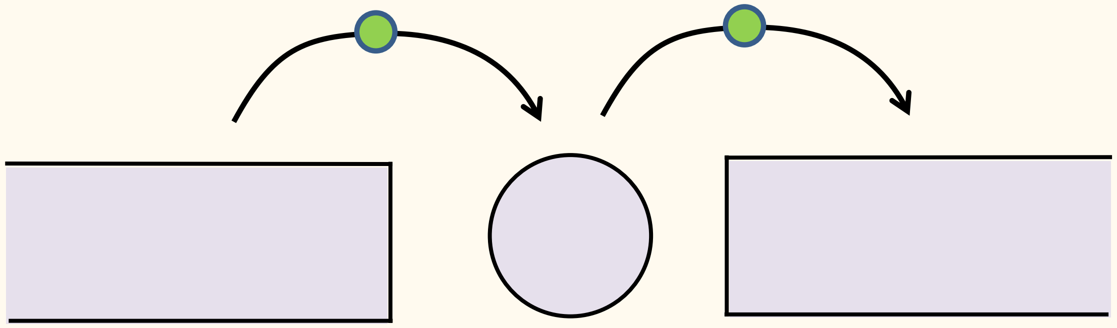
Byrnes, Kim, Yamamoto, Nat. Phys. **10**, 803 (2014),

Single electron effect

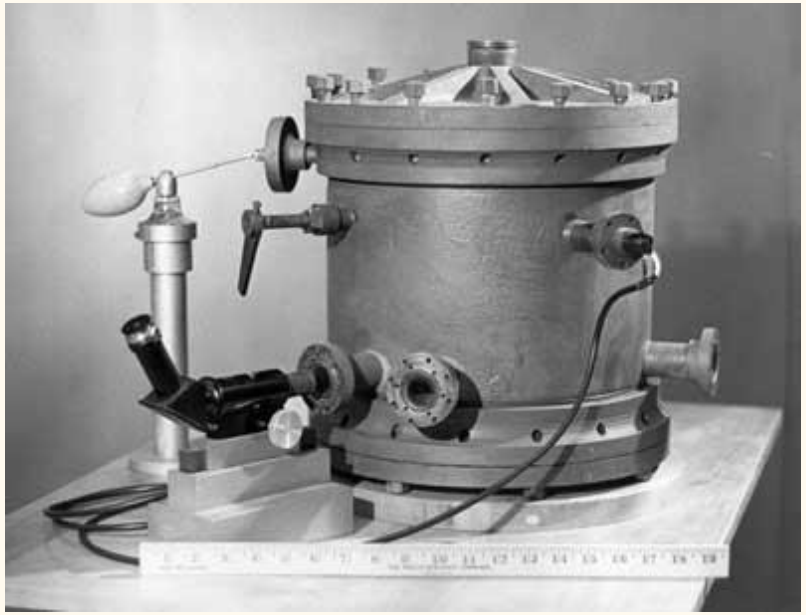


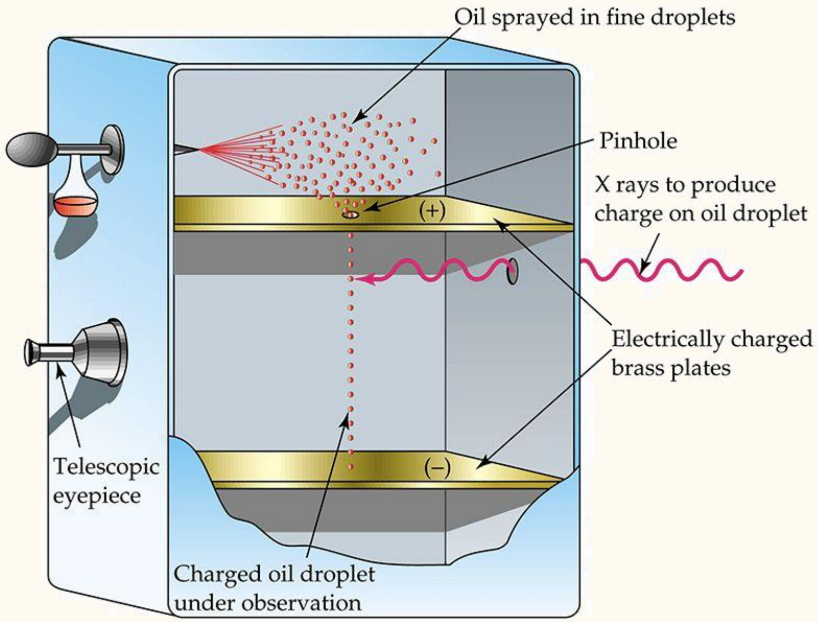
$$E_c = \frac{e^2}{2C} > k_B T$$

Coulomb blockade

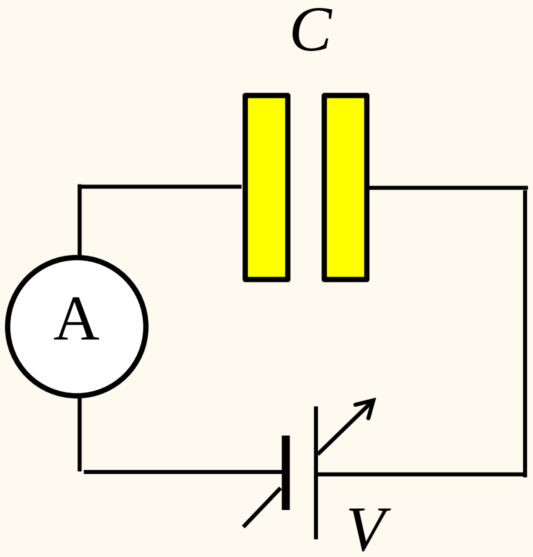


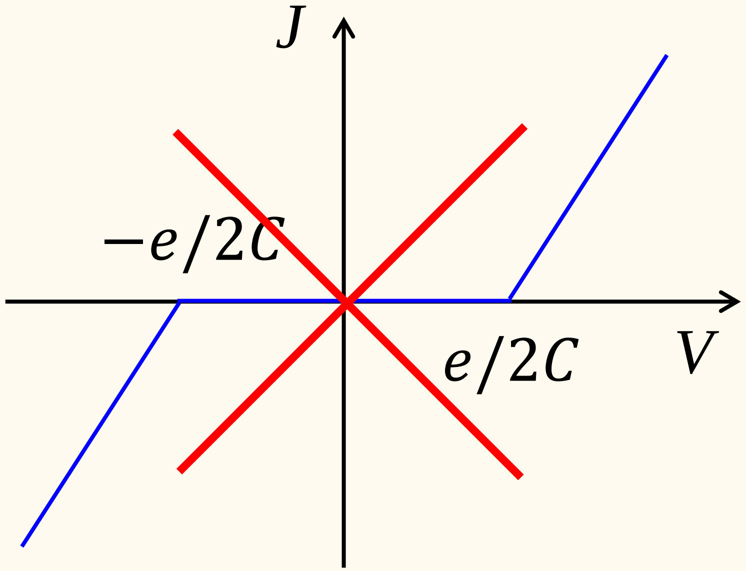
Millikan's oil droplet experiment





Role of power sources





Power sources: Automatically supply energy.

Energy → Enthalpy $\quad H = U - PV$

Constant interaction model, capacitor model

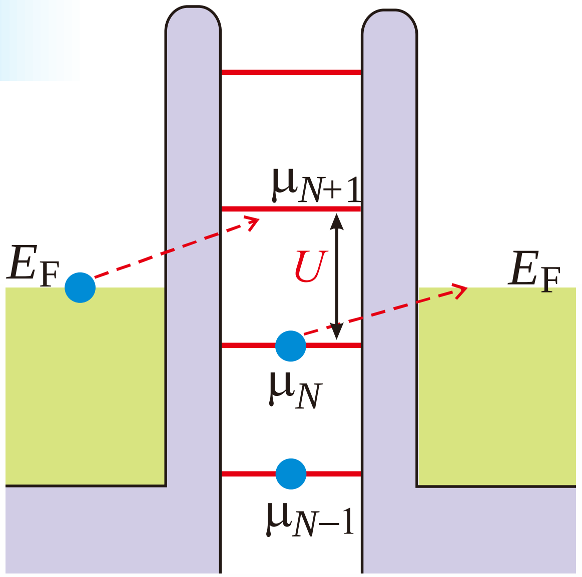
Constant interaction: U

Electron number: N
Interaction energy

$$E_{cN} = {}_N C_2 U = \frac{N(N-1)U}{2} = \frac{U(N-1/2)^2}{2} - \frac{U}{8}$$

Chemical potential

$$\Delta E_+(N) = (N-1)U$$



Charge relations

$$Q_1 + Q_2 = -eN, \quad Q_1 = CV_d,$$
$$Q_2 = C_g(V_d - V_g)$$

Electrostatic energy

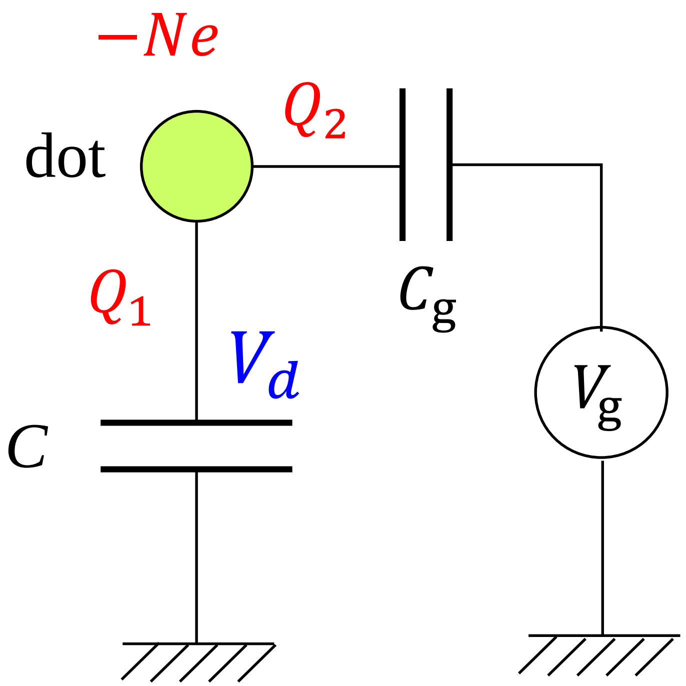
$$E = \frac{1}{2}CV_d^2 + \frac{1}{2}C_g(V_d - V_g)^2$$

Enthalpy

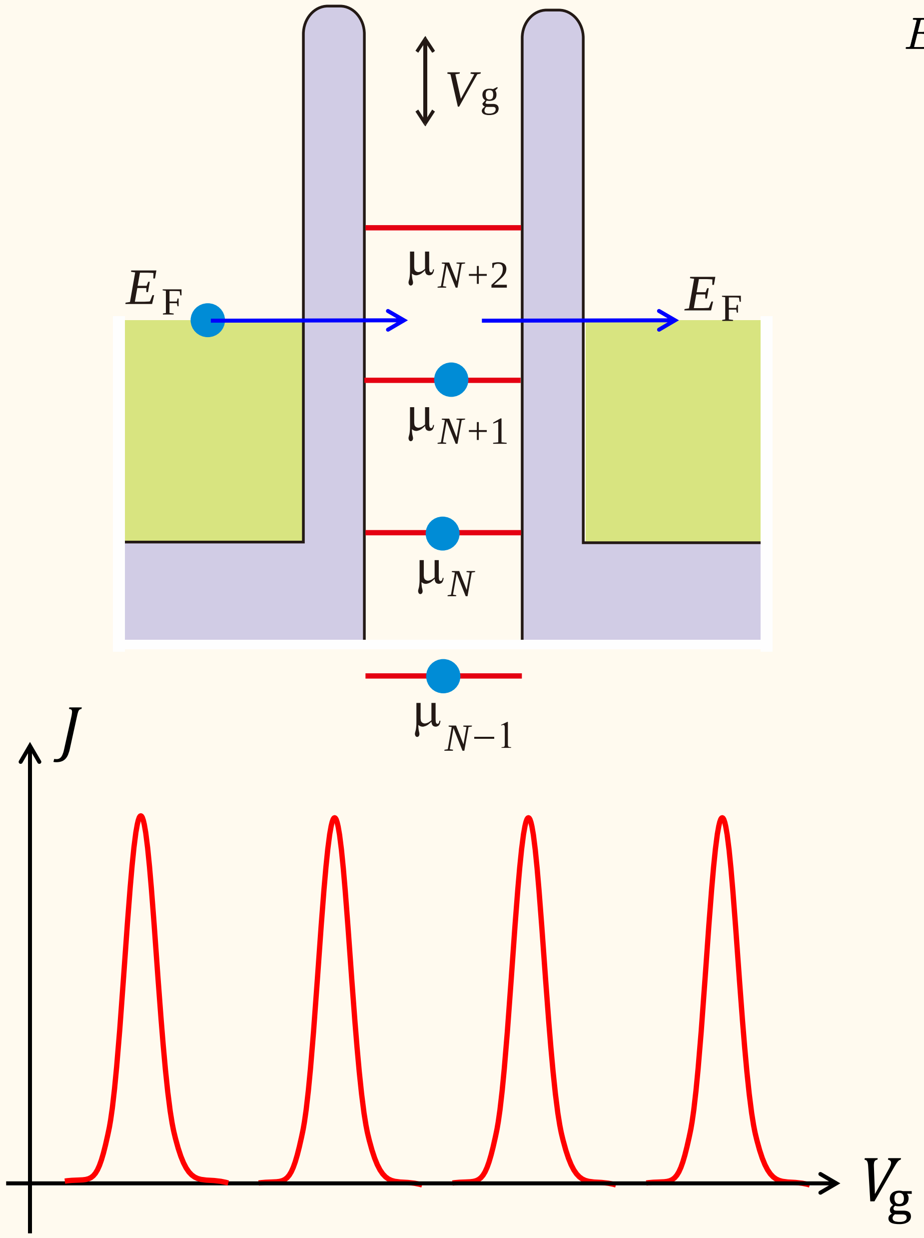
$$H(N, V_g) = \frac{(Ne - C_gV_g)^2}{2(C + C_g)} \equiv \frac{(Ne - C_gV_g)^2}{2C_s}$$

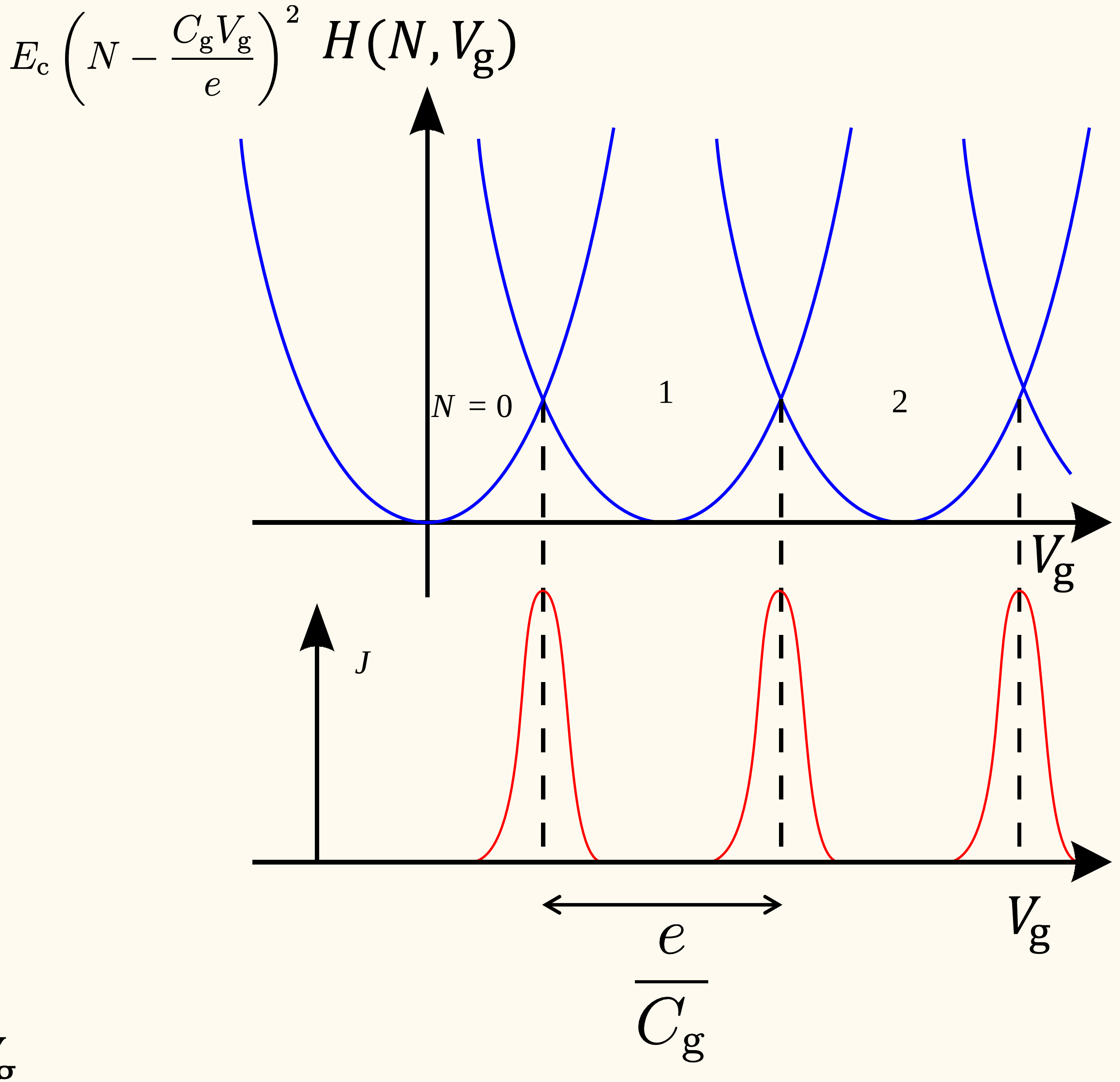
Chemical potential

$$\mu_N \approx \frac{dH}{dN} = \frac{e(Ne - C_gV_g)}{C_s} = 2E_c\left(N - \frac{C_gV_g}{e}\right)$$

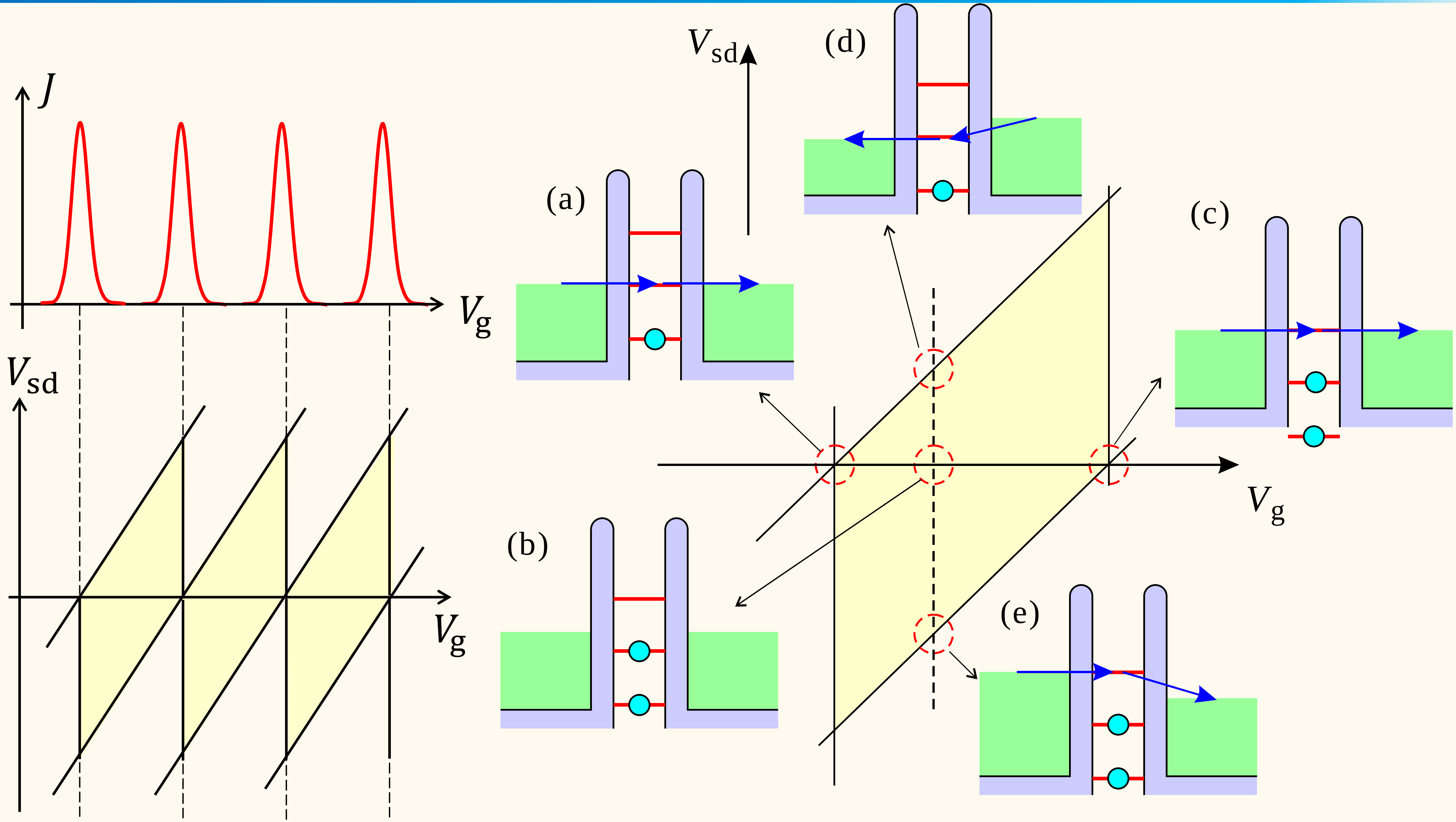


Coulomb oscillation

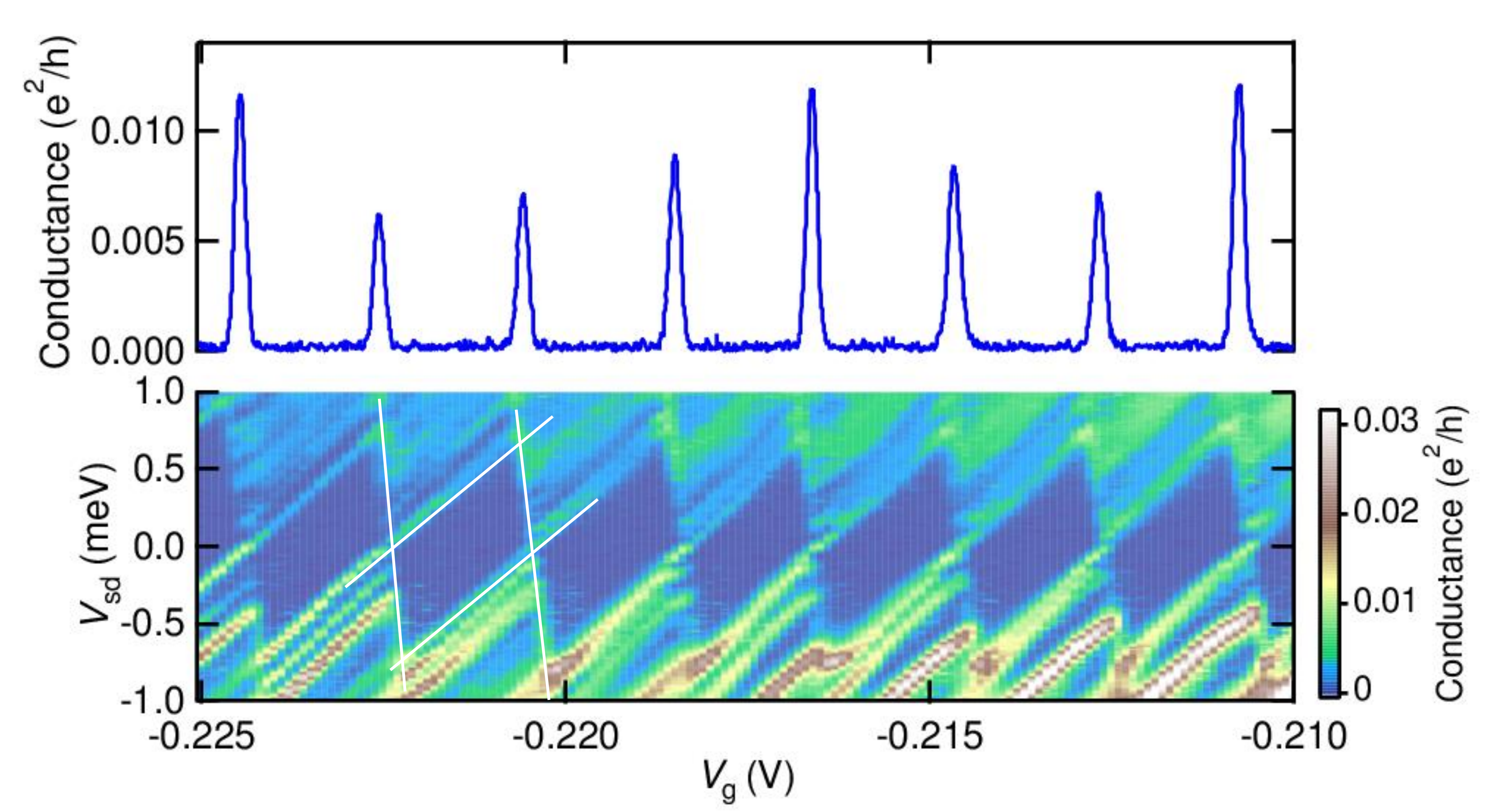




Coulomb diamond

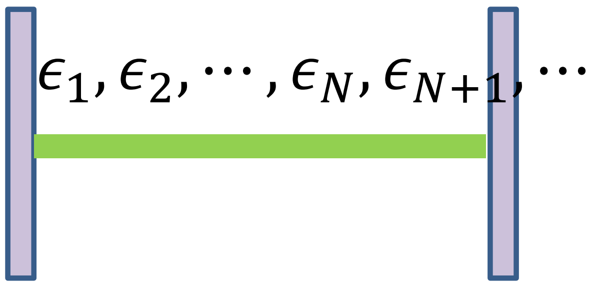


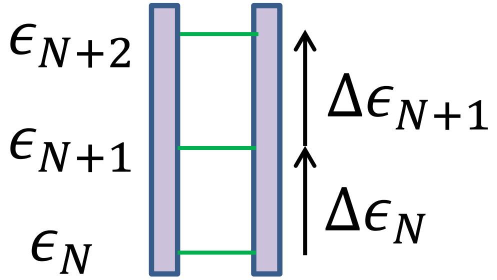
Coulomb oscillation and diamonds

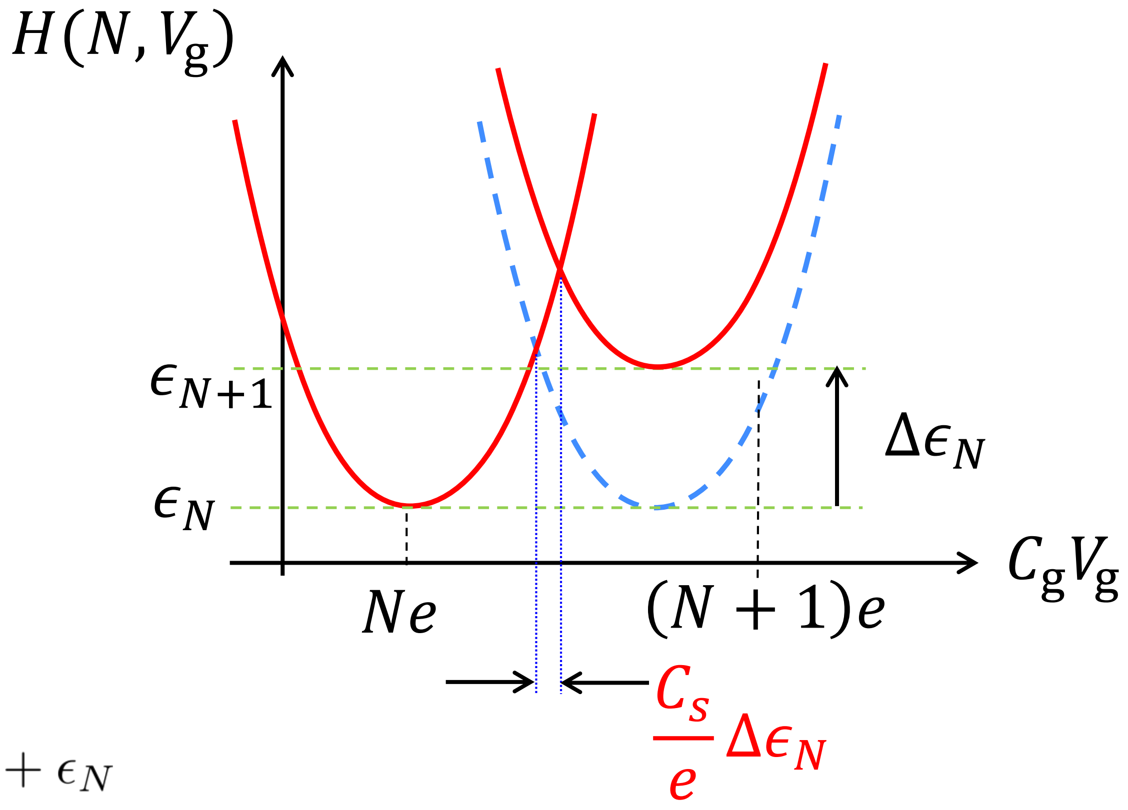


Quantum confinement

Zero-dimensional confinement to a quantum dot gives shifts in Coulomb peak positions.







Enthalpy shift by quantum confinement

$$H(N) = \frac{(Ne - C_g V_g)^2}{2C_s} + \epsilon_N$$

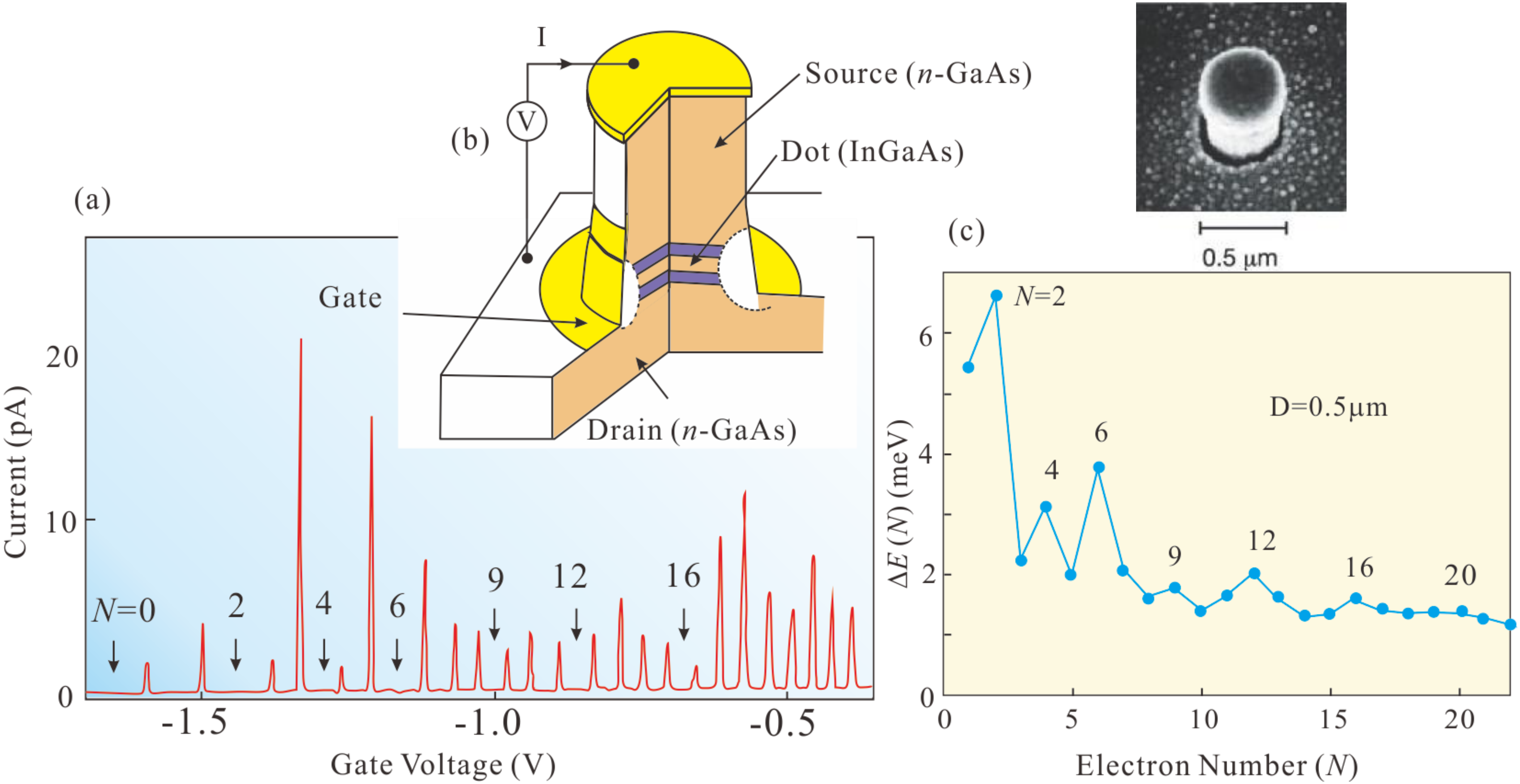
Chemical potential shift

$$\Delta H(N, N+1) = H(N+1) - H(N)$$
$$= \frac{e}{C_s}\left\{\left(N + \frac{1}{2}\right)e - C_g V_g\right\} + \Delta\epsilon_N$$
$$\Delta\epsilon_N \equiv \epsilon_{N+1} - \epsilon_N$$

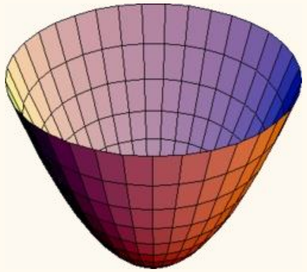
Shift in gate voltage

$$V_{gX}(N, N+1) = \frac{1}{C_g}\left\{\left(N + \frac{1}{2}\right)e + \frac{C_s}{e}\Delta\epsilon_N\right\}$$

Quantum confinement effect in a vertical quantum dot



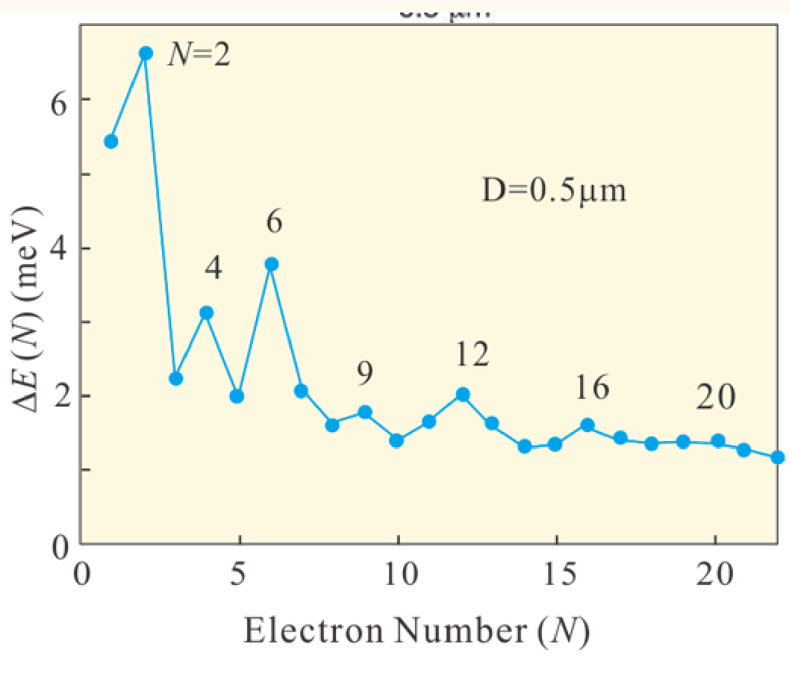
Two-dimensional harmonic potential

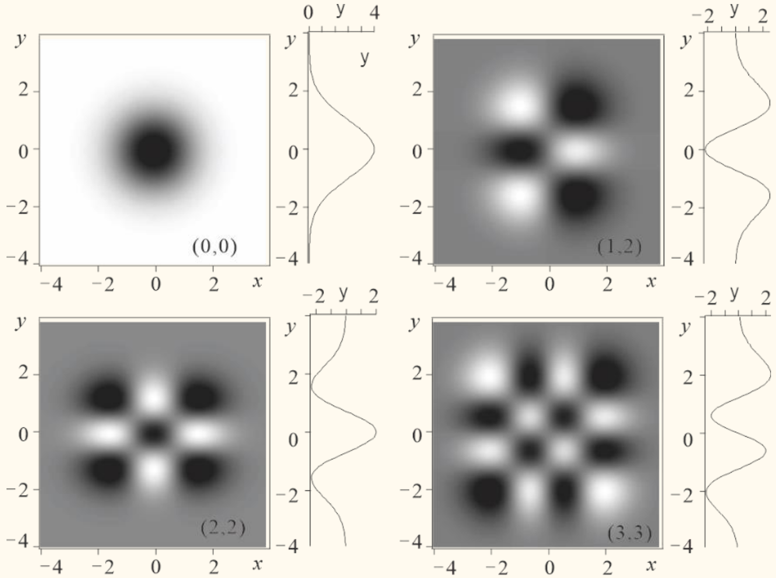


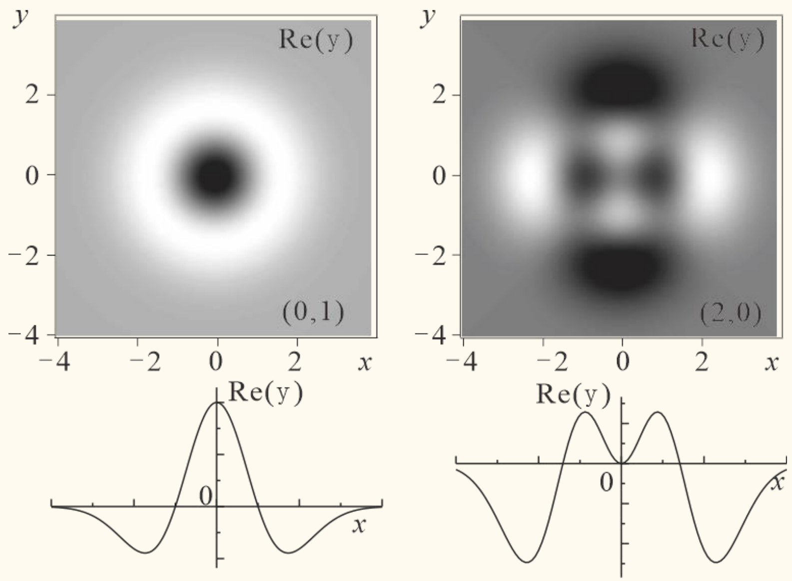
Potential shape: $V(x,y) = \frac{m\omega}{2}(x^2+y^2)$

Easy solutions from 1d harmonic potential $\psi_{n_x n_y} = A\exp\left[-\frac{m\omega(x^2+y^2)}{2\hbar}\right] H_{n_x}\left[\sqrt{\frac{m\omega}{\hbar}}x\right] H_{n_y}\left[\sqrt{\frac{m\omega}{\hbar}}y\right]$

Eigen energies: $E(n_x,n_y) = (n_x+n_y+1)\hbar\omega = (n_t+1)\hbar\omega \quad n_x+n_y \equiv n_t = 0,1,2,\cdots$







For fixed n_t $\quad n_x = 0,1,2,\cdots,n_t$ $\qquad n_t+1$ degeneracy

With spin degeneracy: 2, 4, 6, 8, ⋯

$N = 2, 6, 12, 20, \cdots, (n+1)(n+2), \cdots$

Quantum dot in magnetic field

Hamiltonian with $\boldsymbol{B} = (0, 0, B)$

$$\mathscr{H} = \frac{(\boldsymbol{p} + e\boldsymbol{A})^2}{2m} + \frac{m}{2}\omega^2(x^2 + y^2) \quad \boldsymbol{A} = \left(-\frac{By}{2}, \frac{Bx}{2}, 0\right)$$

Expansion of the kinetic energy term

$$\frac{(\boldsymbol{p} + e\boldsymbol{A})^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{ie\hbar B}{2m}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{e^2B^2}{8m}(x^2 + y^2)$$

Definition of cyclotron frequency and composite harmonic confinement potential frequency

$$\omega_{\mathrm{c}} = \frac{eB}{m} \quad \Omega \equiv \sqrt{\omega^2 + (\omega_{\mathrm{c}}/2)^2}$$

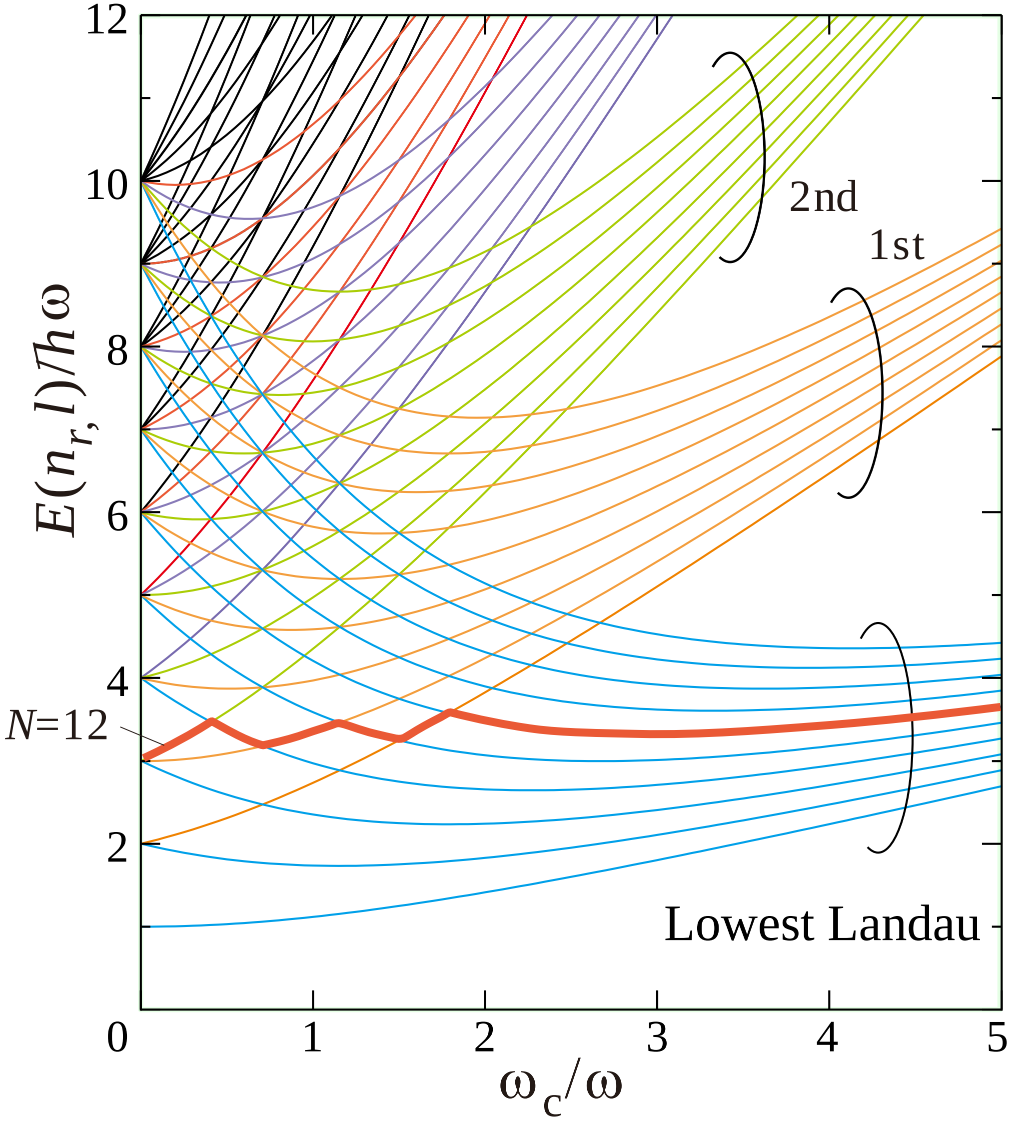
The Hamiltonian is rewritten as

$$\mathscr{H} = \frac{\hbar^2\nabla^2}{2m} + \frac{\Omega}{2m}(x^2 + y^2) + \frac{\omega_{\mathrm{c}}\hat{L}_z}{2} = \mathscr{H}_\Omega + \frac{\omega_{\mathrm{c}}\hat{L}_z}{2}$$

Fock-Darwin state eigen energies

$$E(n_r, l) = \hbar\Omega(2n_r + |l| + 1) + \hbar\omega_{\mathrm{c}}l/2$$

Quantum dot in magnetic field



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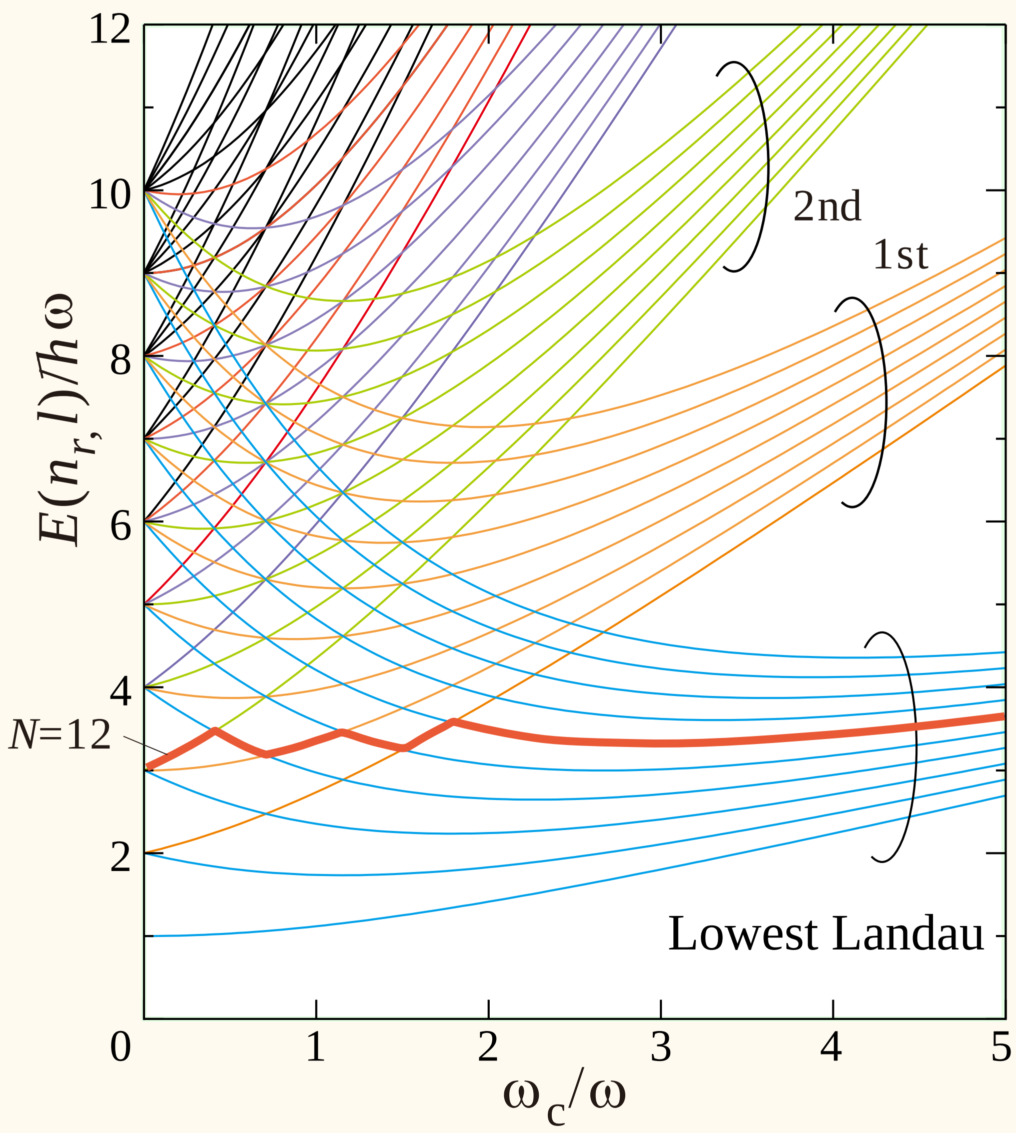
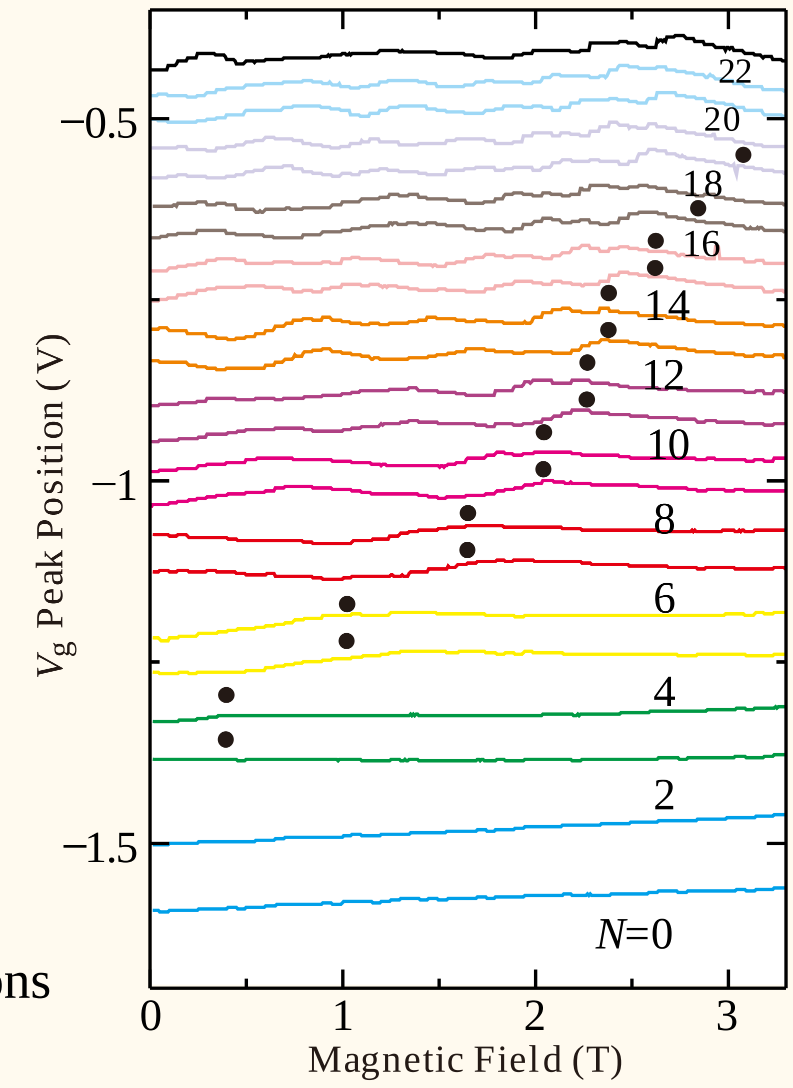
Fock-Darwin states



Level crossing points

$$\left(\frac{\omega_c}{\omega}\right)^2 = n_L - 2 + \frac{1}{n_L}$$

n_L: Landau index
$= 1, 2, \ldots.$



• : Solutions

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.7.7 Lecture 13

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

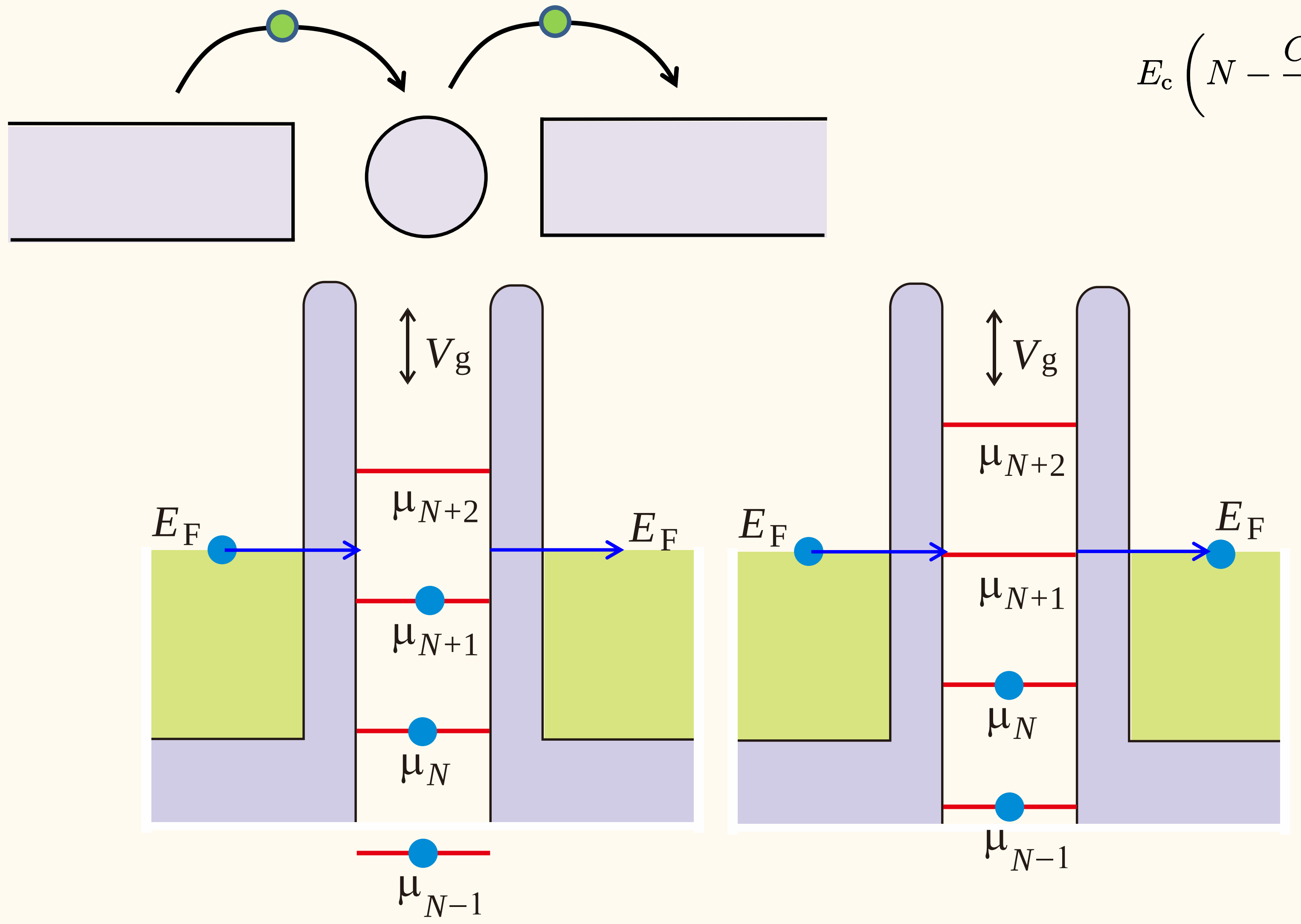
Shingo Katsumoto

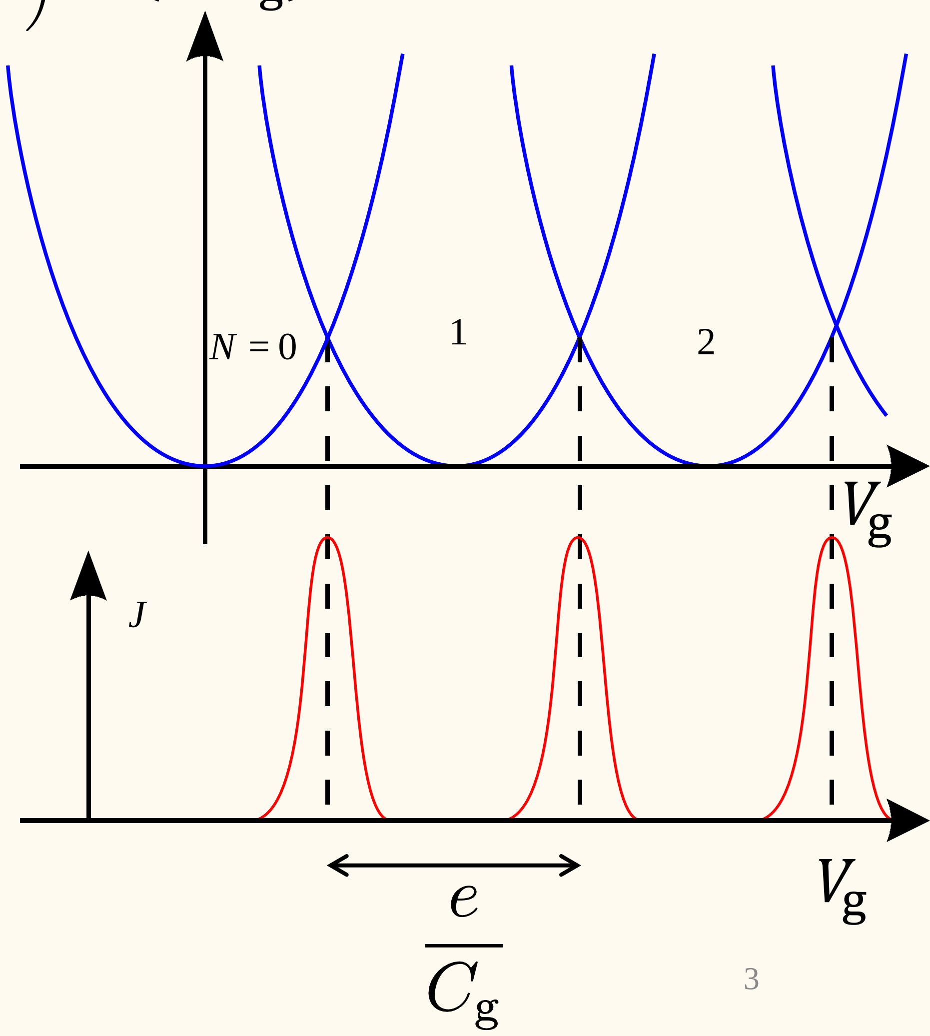
Review of the lecture in the last week

- Aharonov-Bohm effect and quantum transport
- Bunching and anti-bunching of particles (bosons and fermions)
- Waveguide propagation of exciton-polaritons
- Bose-Einstein condensation of exciton-polaritons
- Single electron effect in quantum dots

Review: Single electron effect in transport through quantum dots

Enthalpy $H(N, V_g) = \frac{(Ne - C_g V_g)^2}{2(C + C_g)} \equiv \frac{(Ne - C_g V_g)^2}{2C_s}$





Quantum confinement

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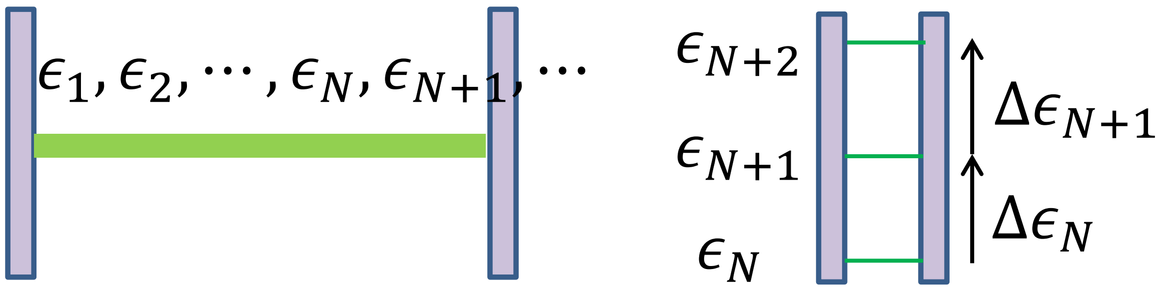

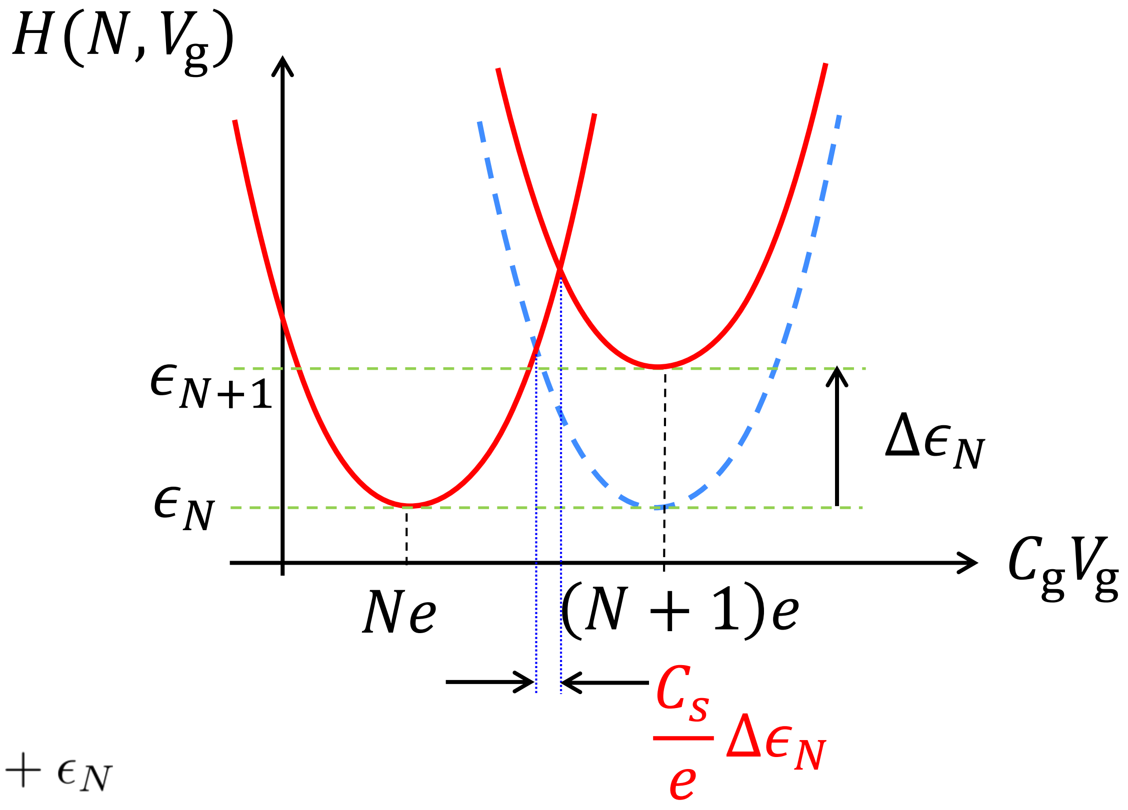

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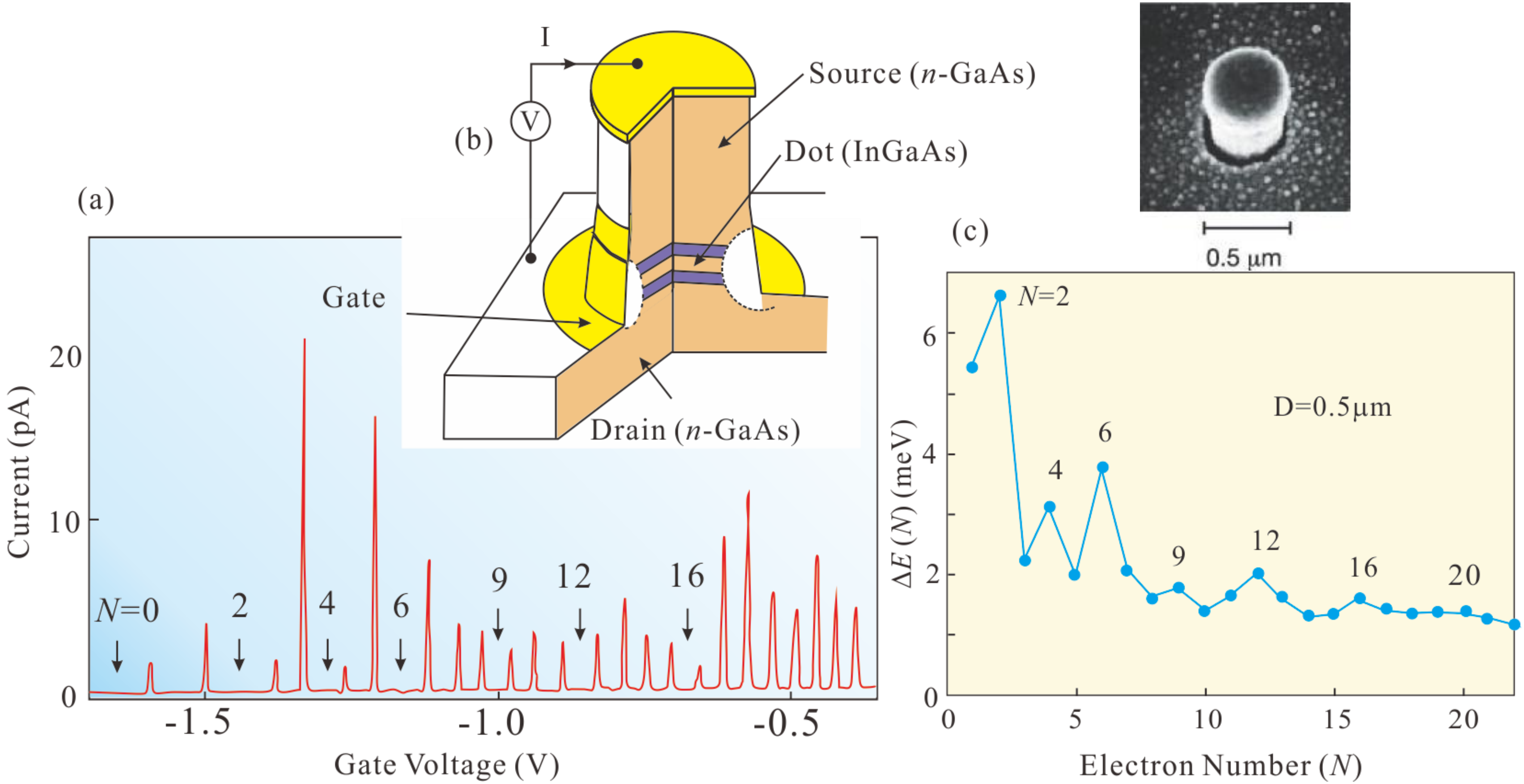
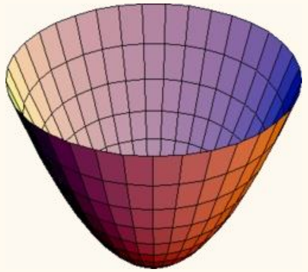


Two-dimensional harmonic potential



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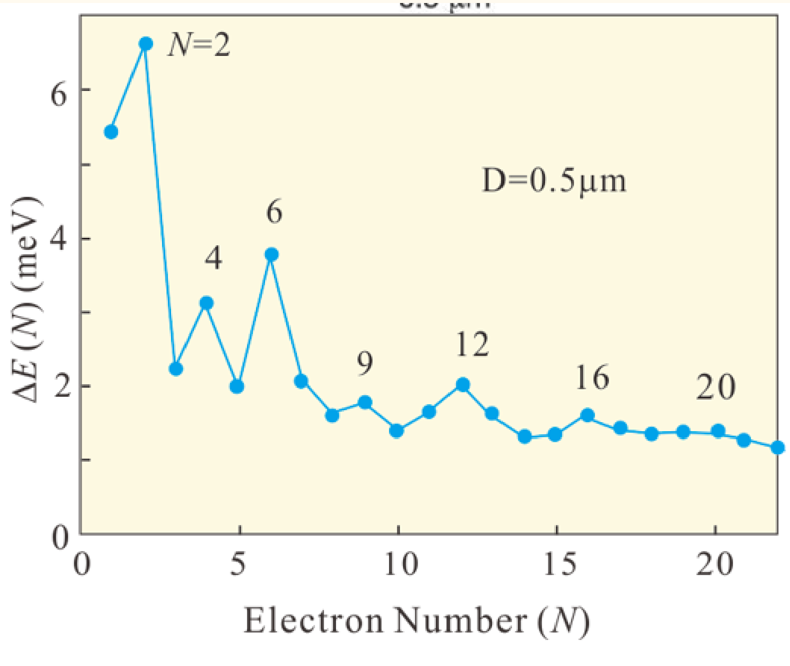

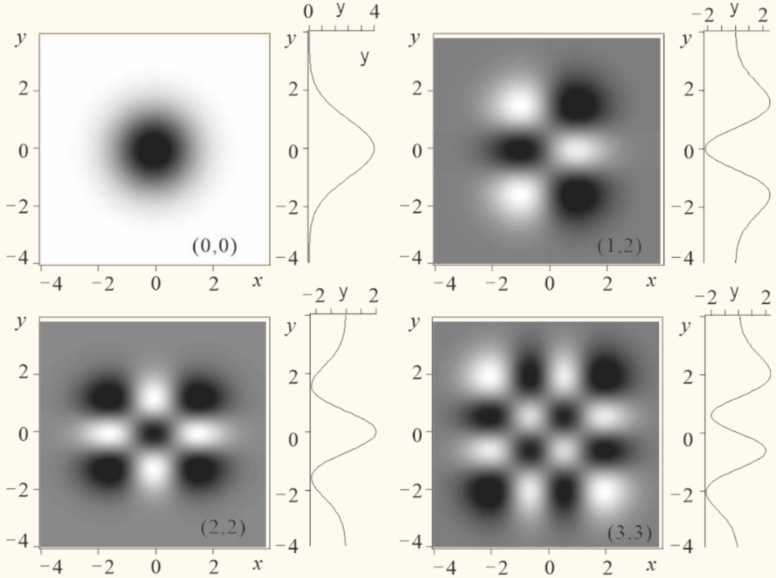

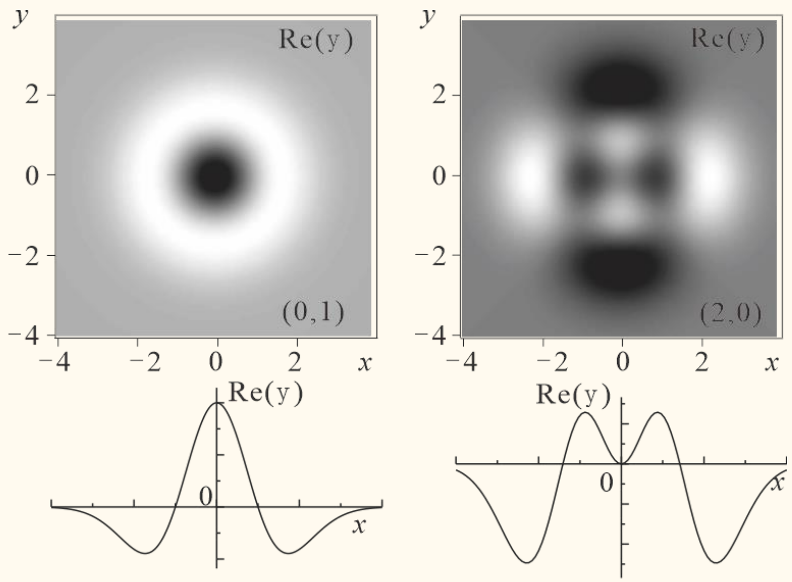

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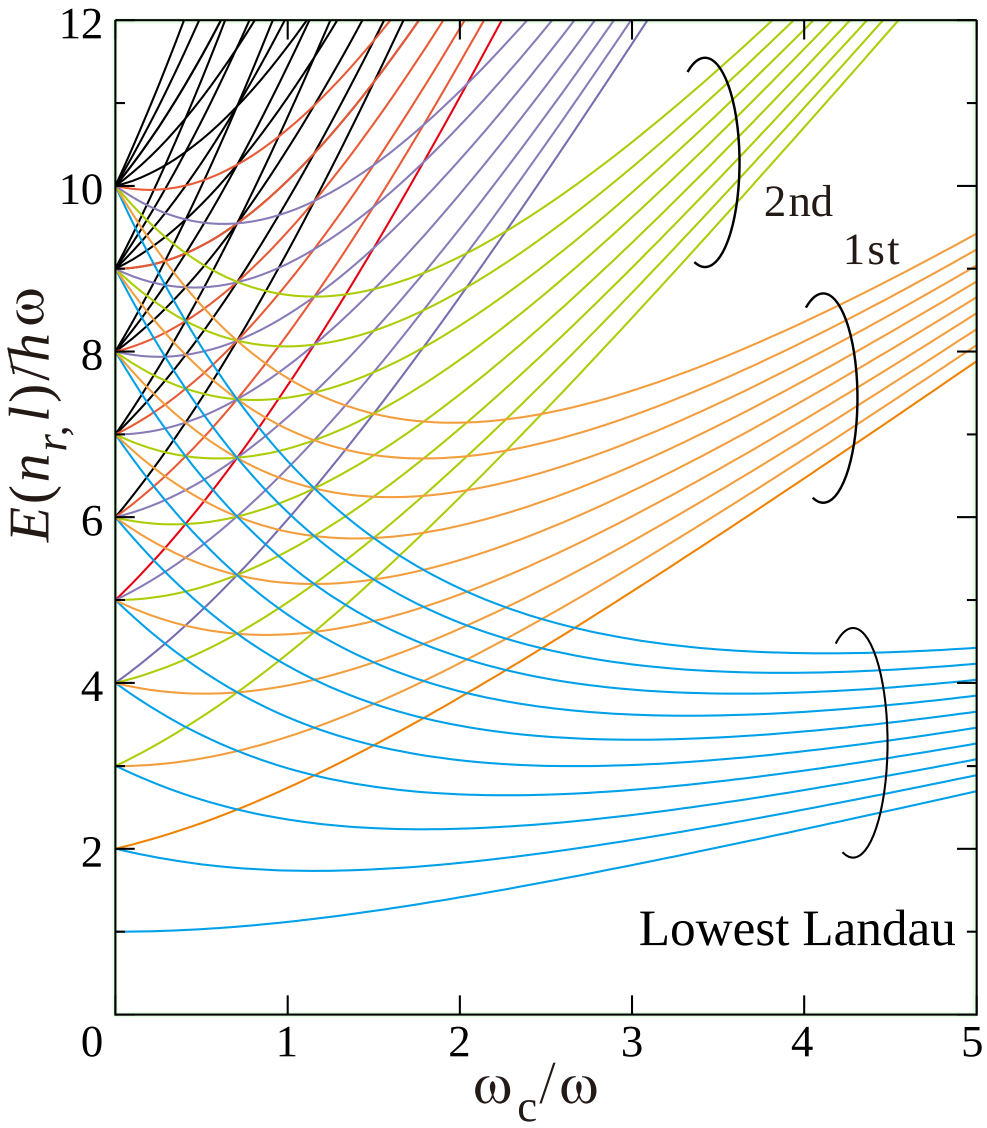
Degree of degeneracy at $B = 0$

$$2n_r + |l| + 1$$

Quantum dot in magnetic field



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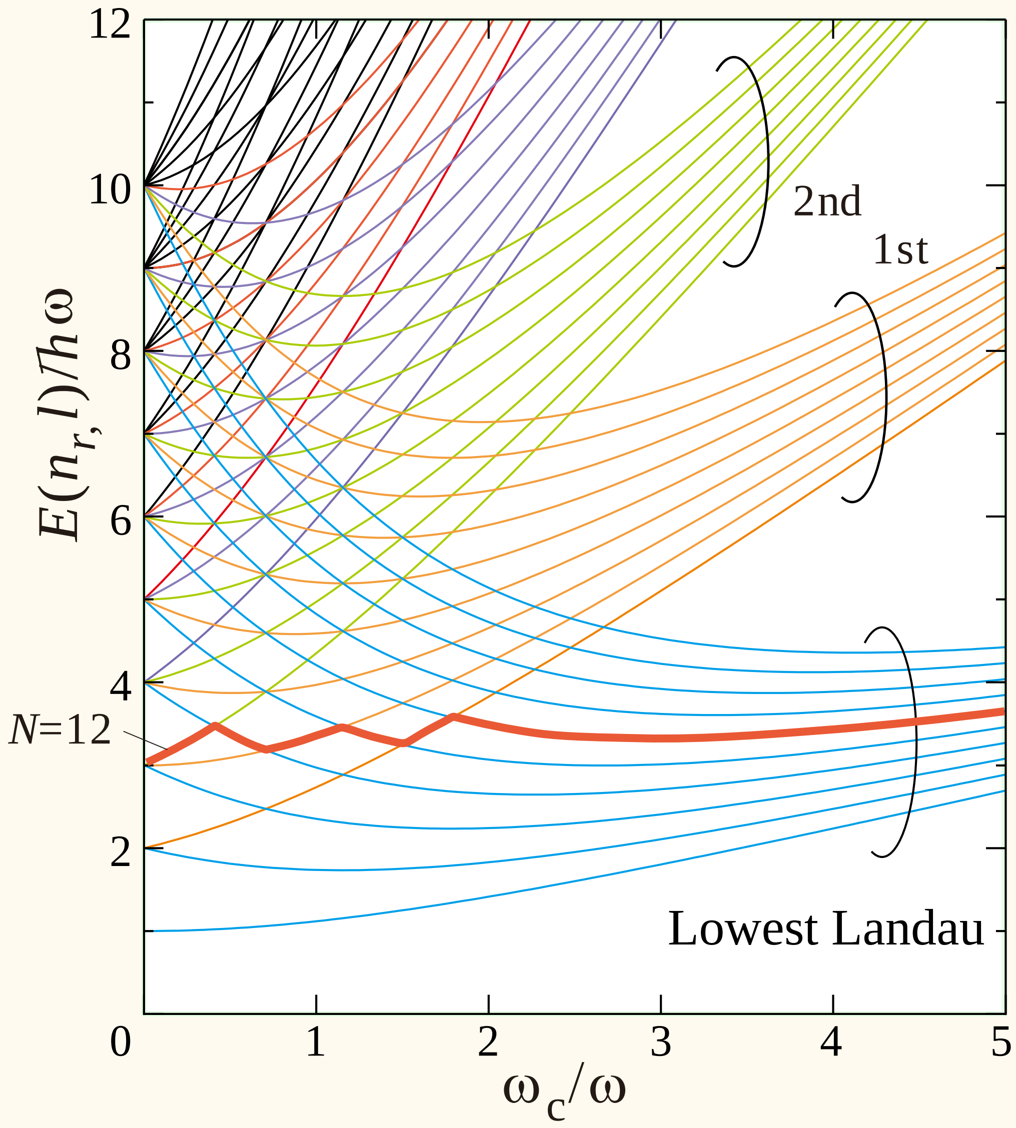
$$2n_r + |l| + 1$$

Fock-Darwin states



Level crossing points

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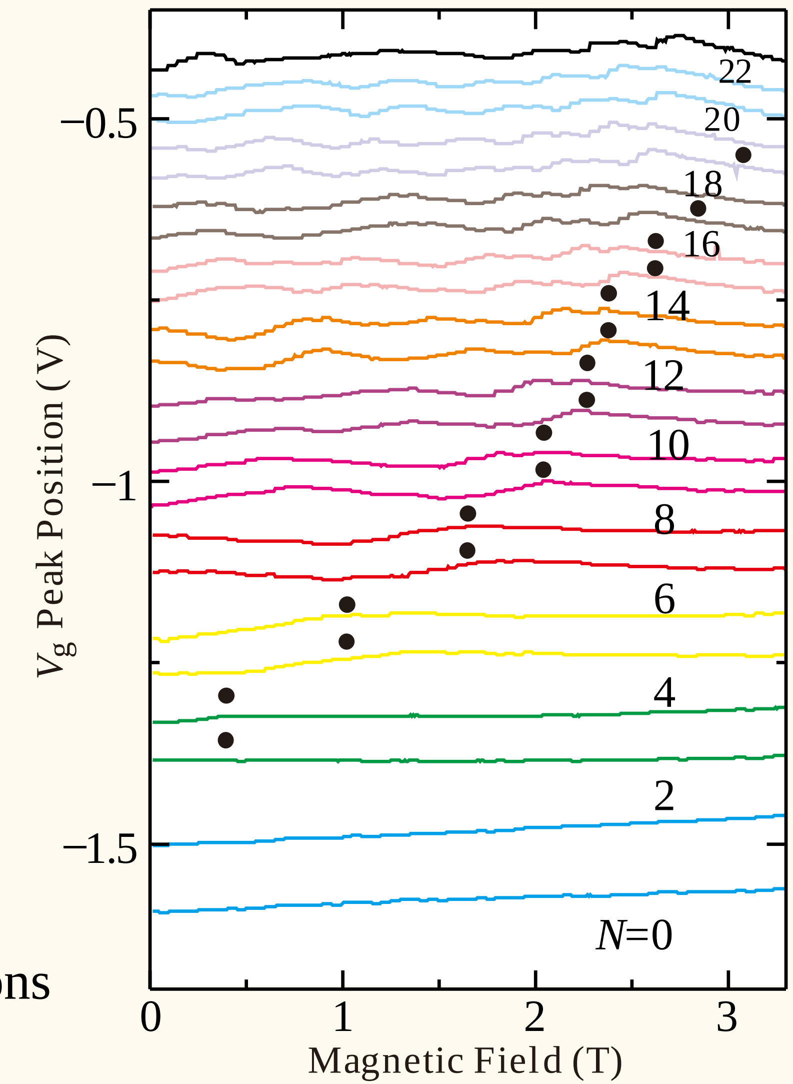
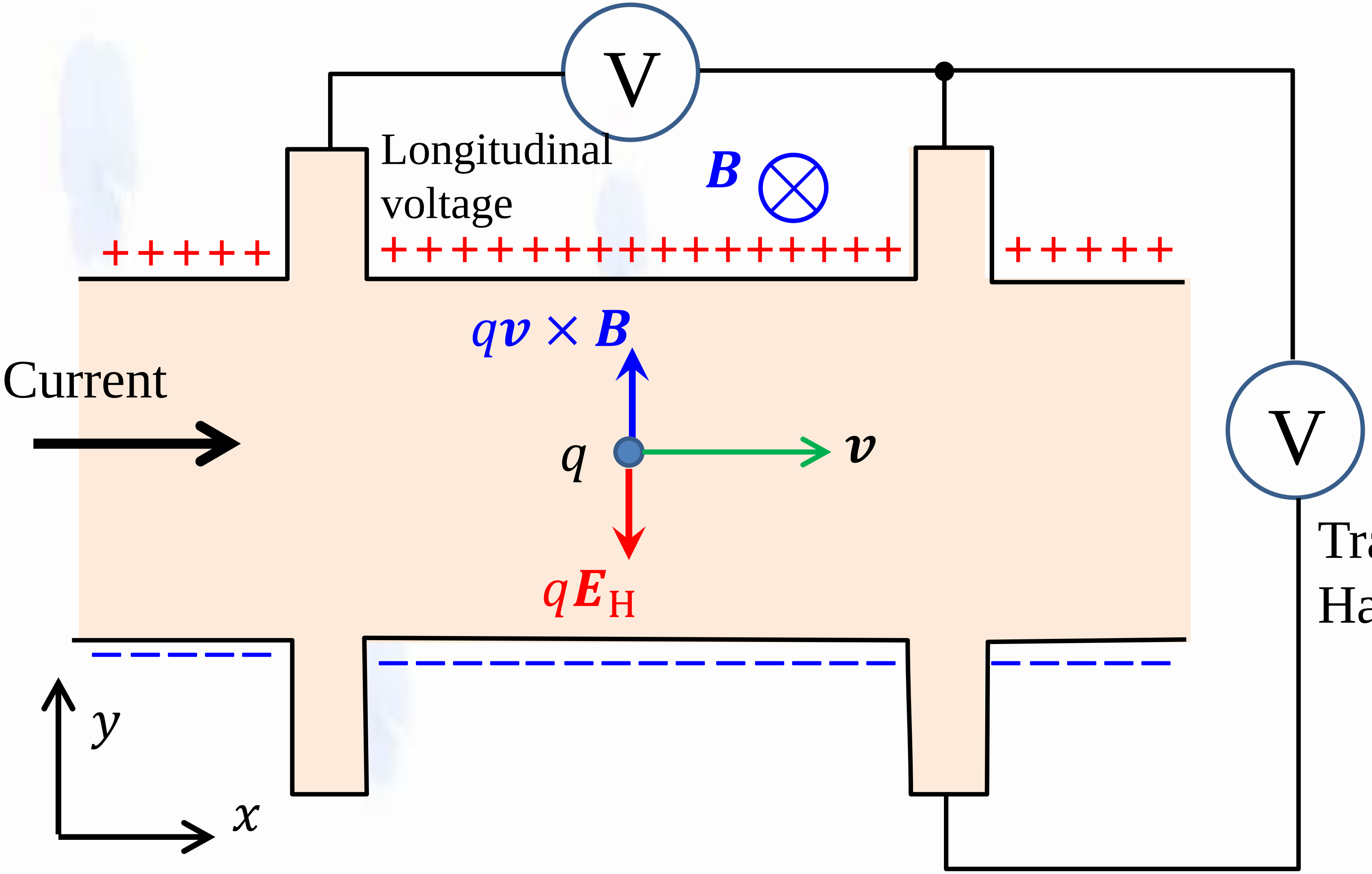
n_L: Landau index
$= 1, 2, \ldots.$
$= n_r + (|l| + l)/2$

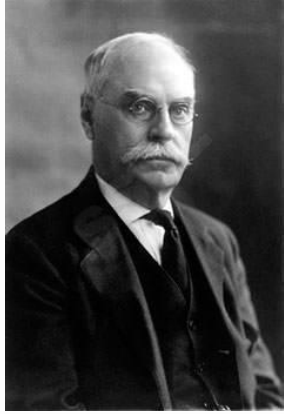


• : Solutions

Chapter 9 Quantum Hall effect

Review: the Hall effect

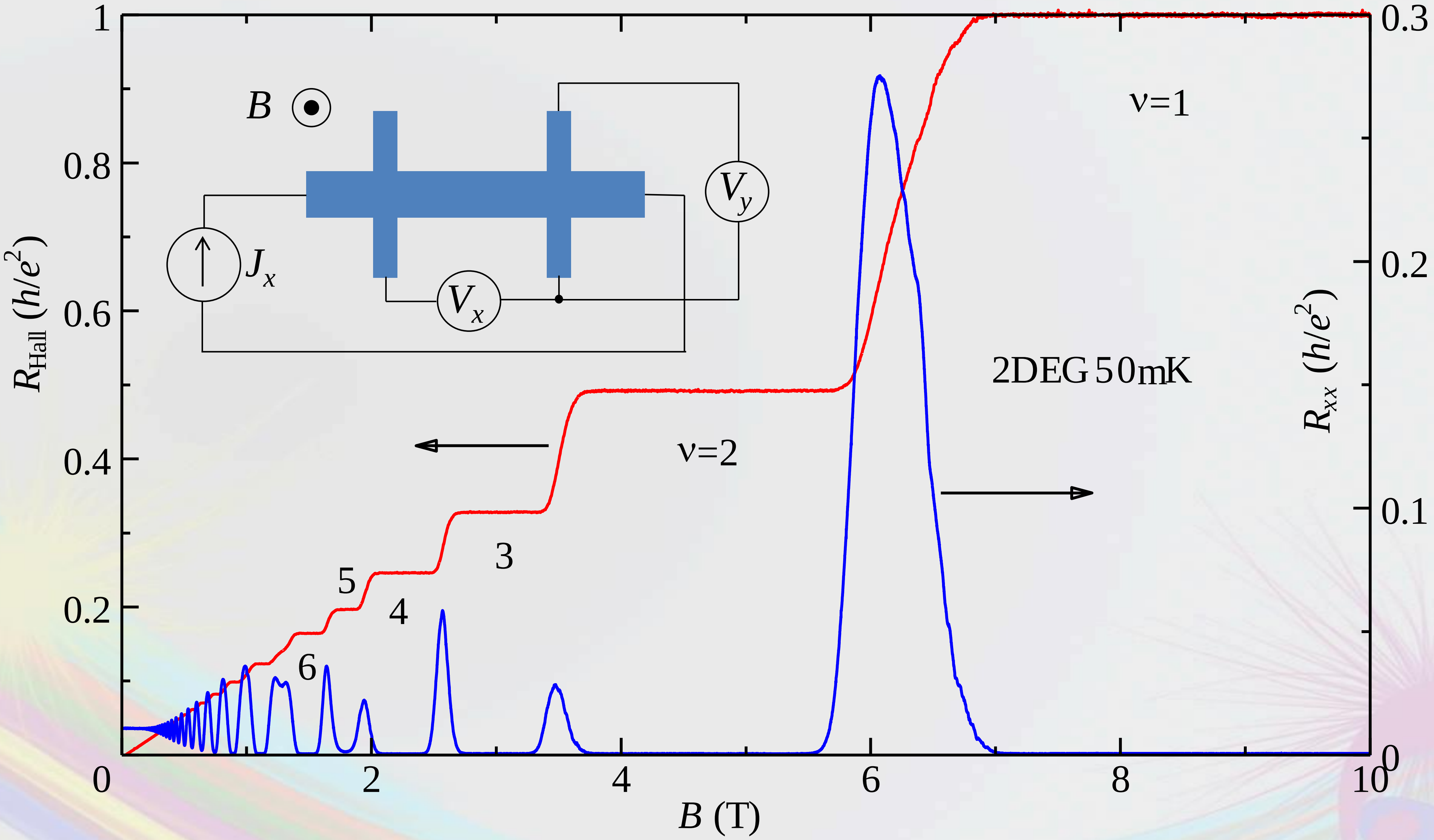



Edwin Hall
1885-1938

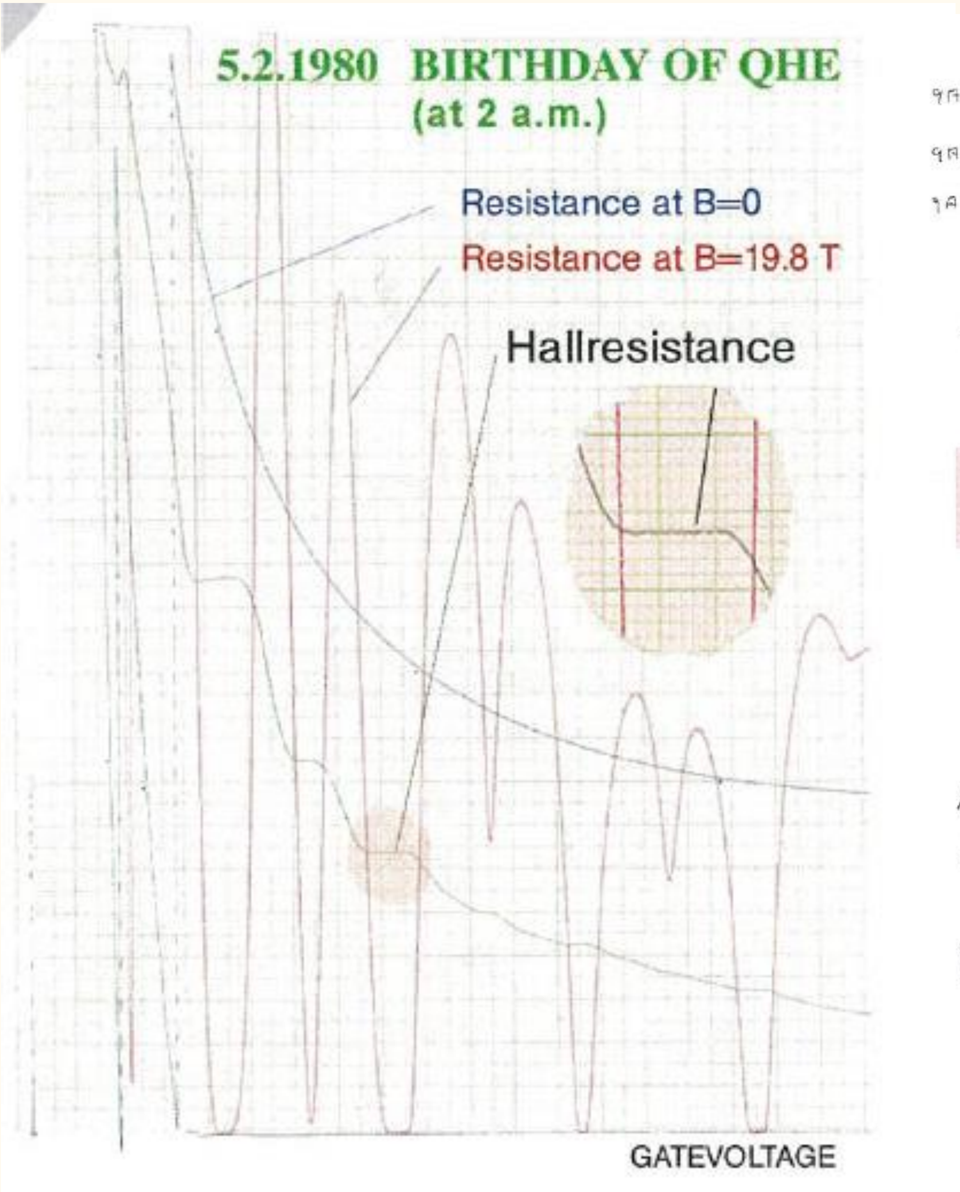
$$R_{xx} = \frac{\text{(longitudinal voltage)}}{\text{(current)}}$$ (longitudinal resistance)

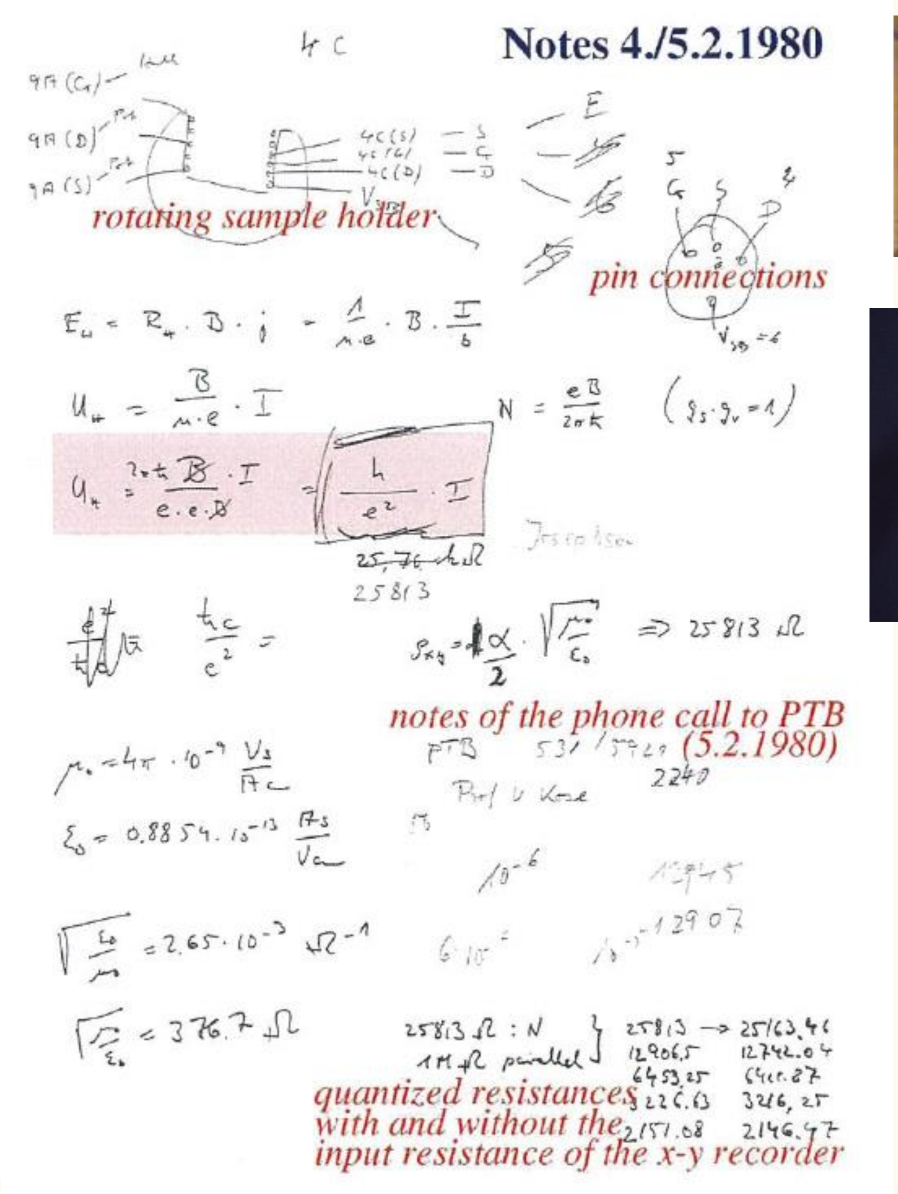
$$R_{xy} = \frac{\text{(Hall voltage)}}{\text{(current)}}$$ (Hall resistance)

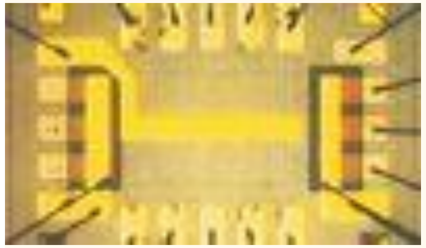
Integer Quantum Hall Effect



Birthday of quantum Hall effect

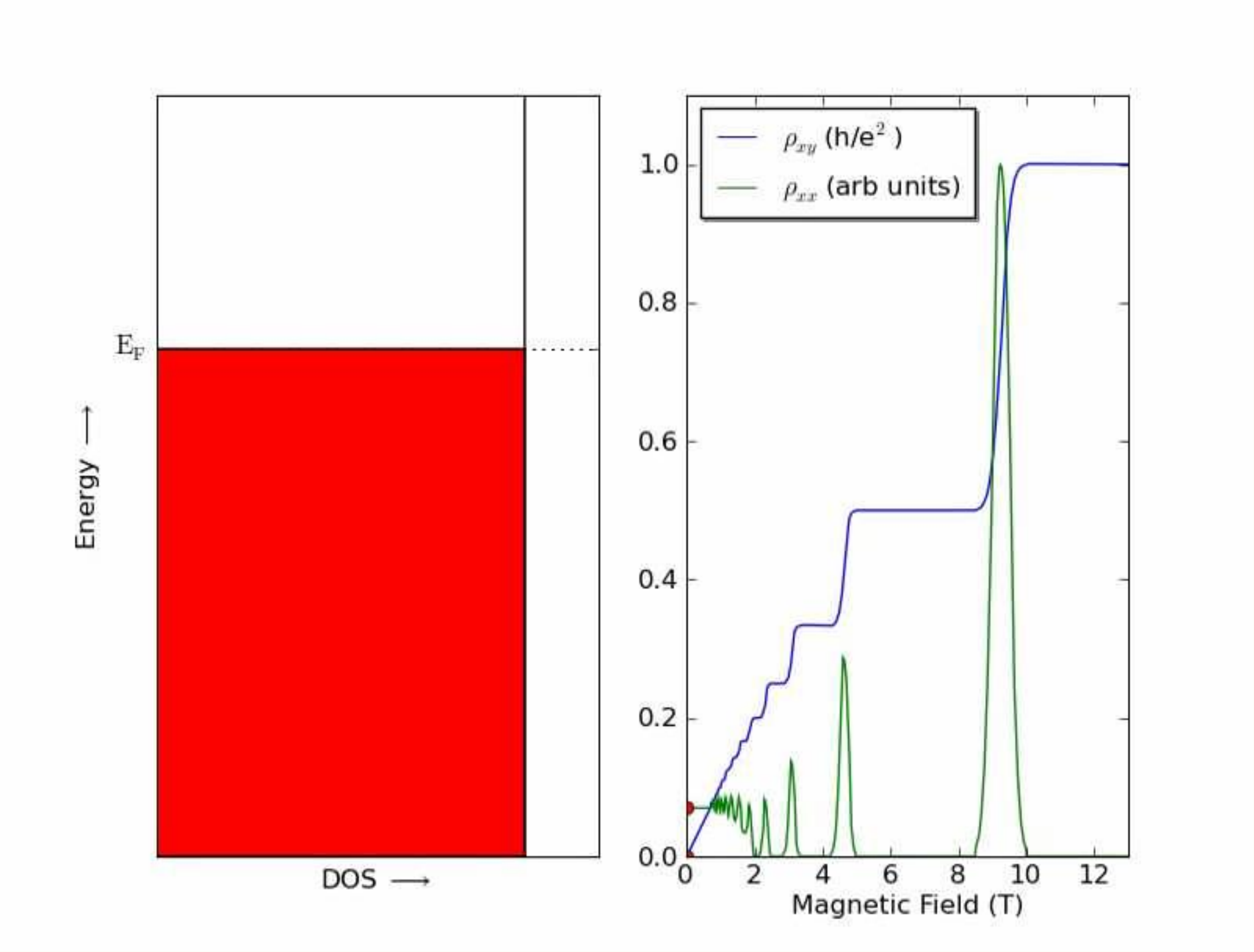






Klaus von Klitzing

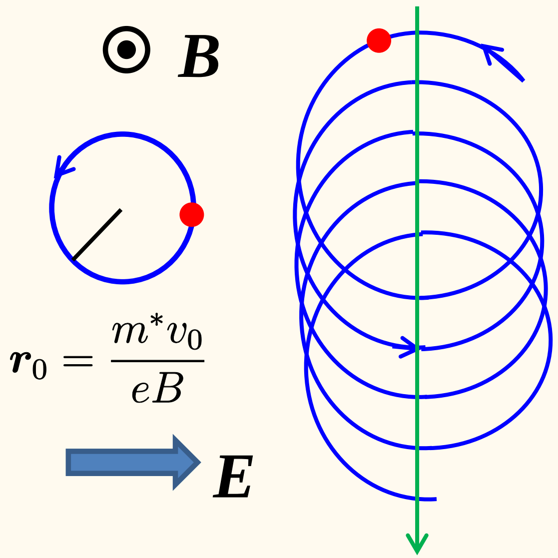
IQHE and Landau quantization



From Wikipedia

Two dimensional electrons under magnetic field

Hendrik Lorentz
1853 - 1928



Lorentz force (magnetic field only) $m\frac{d^2\boldsymbol{r}}{dt^2} = -e\boldsymbol{v}\times\boldsymbol{B}$

Cyclotron motion $\boldsymbol{r} = \boldsymbol{R} + r_0(\cos\omega_c t, \sin\omega_c t)$

$\omega_c \equiv \frac{eB}{m}$: cyclotron frequency, $r_0 \equiv \frac{v_0}{\omega_c}$: cyclotron radius,

$\boldsymbol{R}$: guiding center

This can be viewed as a motion in harmonic potential.

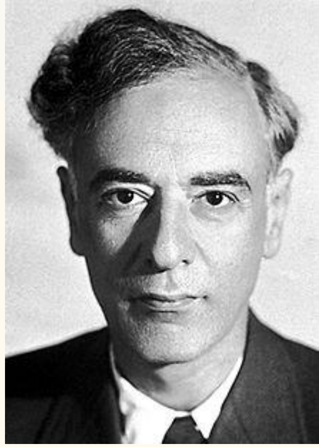
With electric field $m\frac{d^2\boldsymbol{r}}{dt^2} = -e(\boldsymbol{E} + \boldsymbol{v}\times\boldsymbol{B})$

R: Moves vertically to ***E*** with constant velocity *E*/*B*

Quantum mechanical Hamiltonian (no external electric field)

$$\mathscr{H} = \frac{m}{2}\boldsymbol{v}^2 = \frac{(\boldsymbol{p}+e\boldsymbol{A})^2}{2m} \equiv \frac{\boldsymbol{\pi}^2}{2m} = \frac{\pi_x^2+\pi_y^2}{2m} \qquad \boldsymbol{\pi} \equiv \boldsymbol{p} + e\boldsymbol{A}$$

Landau quantization (two-dimensional)



Lev Landau
1908 - 1968

Commutation relation $[\pi_\alpha, \beta] = -i\hbar\delta_{\alpha\beta}\ (\alpha, \beta = x, y), \quad [\pi_x, \pi_y] = -i\dfrac{\hbar^2}{l^2}$

Magnetic length $l \equiv \sqrt{\dfrac{\hbar}{eB}} = \sqrt{\dfrac{1}{2}}\sqrt{\dfrac{\phi_0}{\pi B}} \qquad (2\pi l^2)B = \phi_0 = \dfrac{h}{e}$

Space coordinate operator $\hat{\boldsymbol{r}} = \hat{\boldsymbol{R}} + \dfrac{l^2}{\hbar}(\pi_y, -\pi_x)$

Guiding center operator $\hat{\boldsymbol{R}} = (\hat{X}, \hat{Y}), \quad [\hat{X}, \hat{Y}] = il^2$

down/up operator $a = \dfrac{l}{\sqrt{2}\hbar}(\pi_x - i\pi_y), \quad a^\dagger = \dfrac{l}{\sqrt{2}\hbar}(\pi_x + i\pi_y)$

Remember:

1-d harmonic oscillator $\dfrac{\hbar\omega}{2}\left(-\dfrac{d^2}{dq^2} + q^2\right)\phi = E\phi$ down/up operators $a, a^\dagger = \dfrac{1}{\sqrt{2}}\left(\pm\dfrac{d}{dq} + q\right), \quad [a, a^\dagger] = 1$

$$[a, a^\dagger] = 1, \quad \mathscr{H} = \hbar\omega_c\left(a^\dagger a + \frac{1}{2}\right) \quad E_n = \hbar\omega_c\left(n + \frac{1}{2}\right)\ (n = 0, 1, 2, \cdots)$$

Landau quantization: Landau gauge

Diagonalize X : Landau gauge $\boldsymbol{A} = (0, Bx)$

Schrödinger equation $$\mathscr{H}\psi = \frac{(\boldsymbol{p}+e\boldsymbol{A})^2}{2m}\psi = -\frac{1}{2m}\left[\frac{\hbar^2\partial^2}{\partial x^2} - \left(-i\hbar\frac{\partial}{\partial y} + eBx\right)^2\right]\psi(\boldsymbol{r})$$

$$= \frac{1}{2m}\left[-\hbar^2\nabla^2 - 2i\hbar eBx\frac{\partial}{\partial y} + e^2B^2x^2\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

Plane wave solution along *y* $\psi(\boldsymbol{r}) = u(x)\exp(iky)$

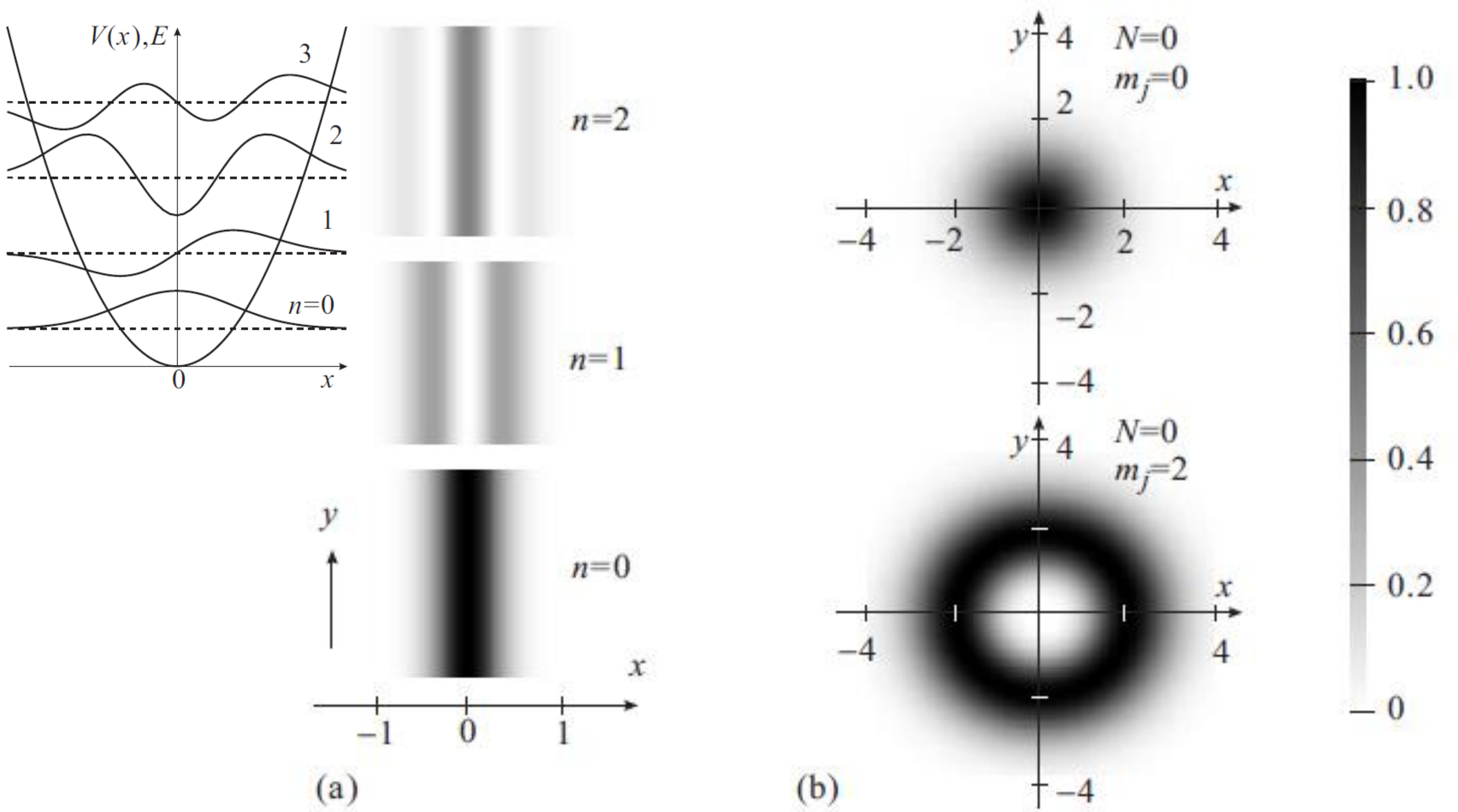
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{(eB)^2}{2m}\left(x + \frac{\hbar}{eB}k\right)^2\right]u(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_c^2}{2}(x+l^2k)^2\right]u(x) = Eu(x)$$

Harmonic oscillator solution $$\psi_{nk}(\boldsymbol{r}) \propto H_n\left(\frac{x-x_k}{l}\right)\exp\left(-\frac{(x-x_k)^2}{2l^2}\right)\exp(iky) \quad (x_k \equiv -l^2k)$$

x-direction Gaussian center $X = x_k = -l^2k = -l^2p_y/\hbar$

y-direction group velocity = 0 $$\frac{dE}{dk} = 0$$

Landau quantization: forms of wavefunctions



Diagonalize X

Diagonalize $X^2 + Y^2$ ← Symmetric gauge $\boldsymbol{A} = \boldsymbol{B} \times \boldsymbol{r}/2$

Shubnikov-de Haas oscillation

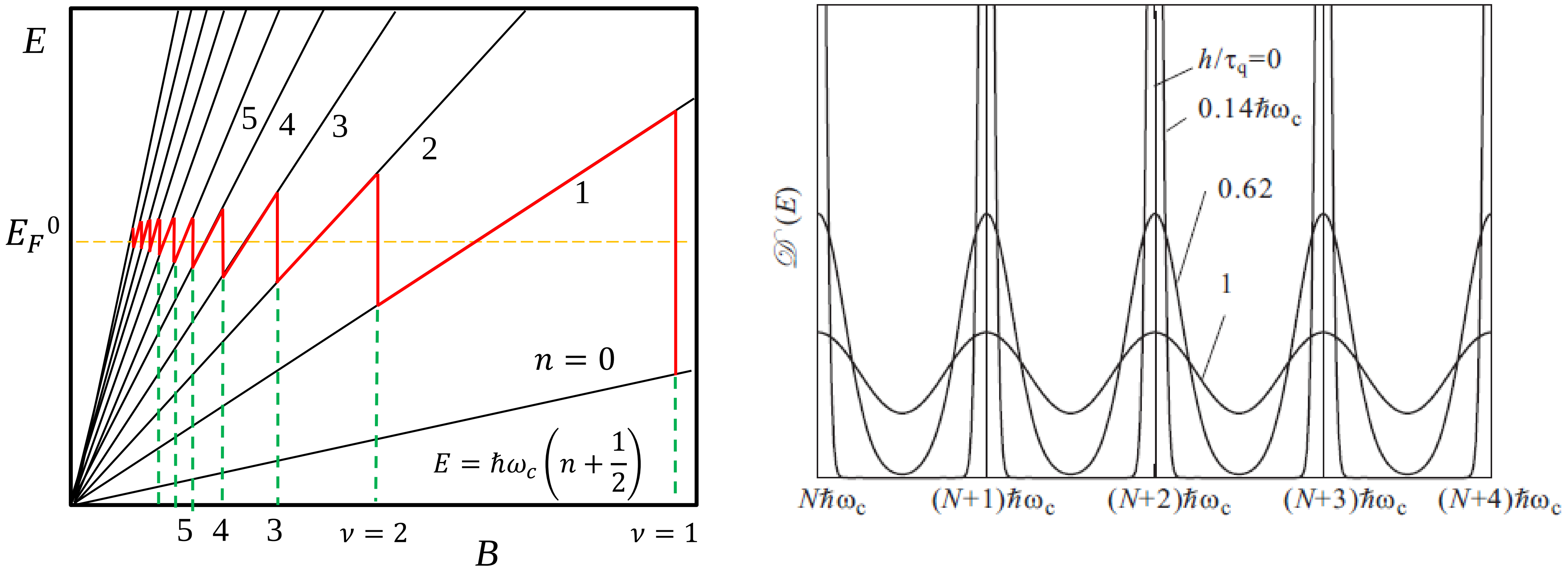
Number of states in $S = W_x \times W_y$

$$0 \le X \le W_x \to -W_x l^2 \le k \le 0$$

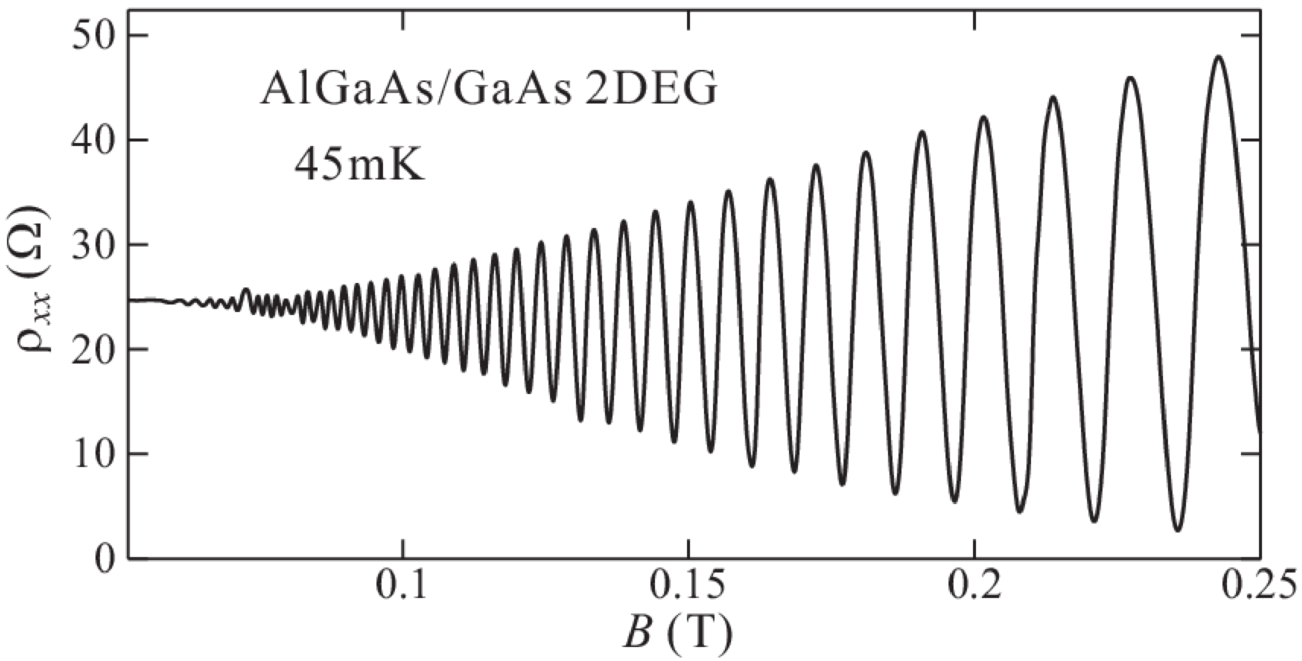
"Distance" of k-values in y-direction: $2\pi / W_y$

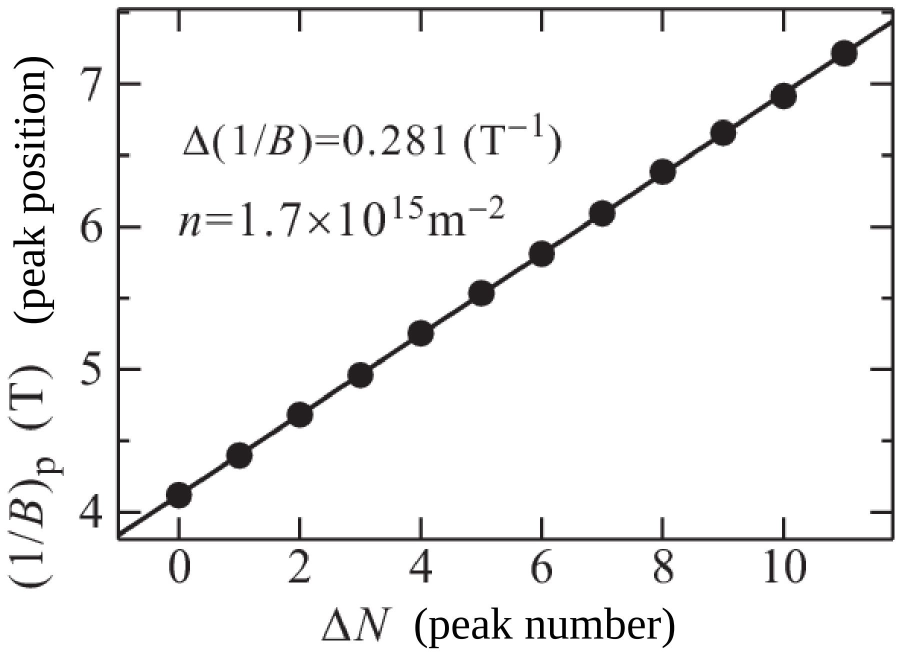
$$\frac{W_x/l^2}{2\pi/W_y} = \frac{S}{2\pi l^2} \quad \rho_{\mathrm{L}} = \frac{1}{2\pi l^2} = \frac{eB}{h} = \frac{B}{\phi_0}$$

$\nu = \dfrac{\phi_0 n_s}{B}$: Filling factor (number of Landau levels filled with electrons)



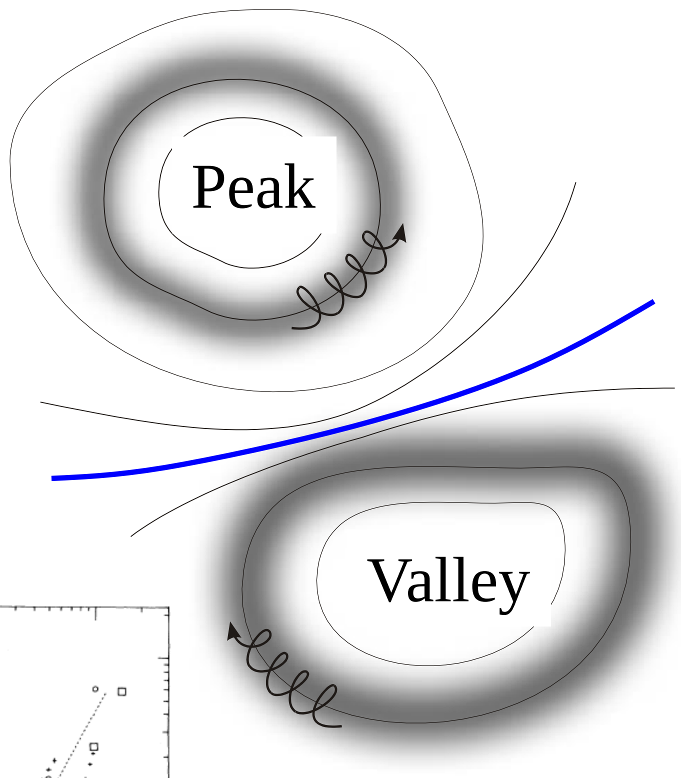
SdH oscillation (example)

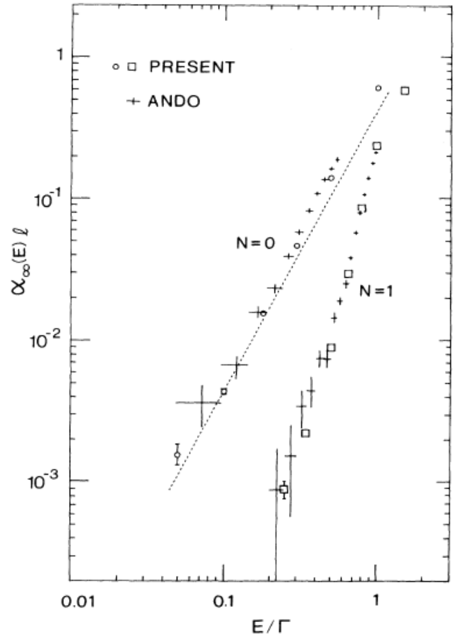


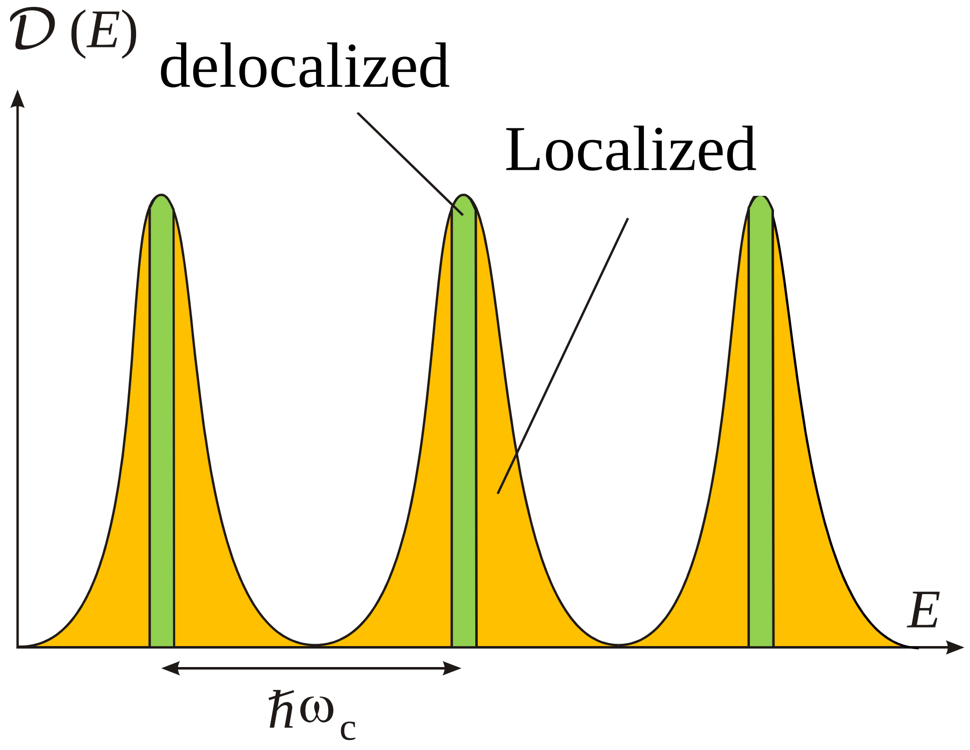


$$n = \frac{2}{\phi_0 \Delta(1/B)} = \frac{4.83 \times 10^{14}}{\Delta(1/B)} \quad (\mathrm{m}^{-2})$$

Localization/delocalization of wavefunctions





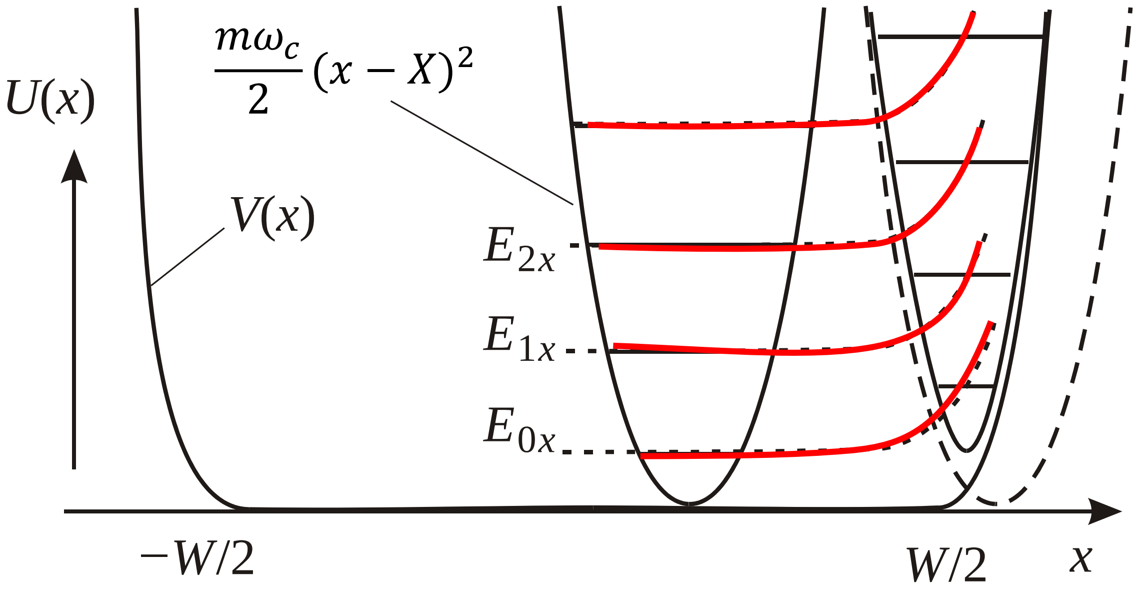


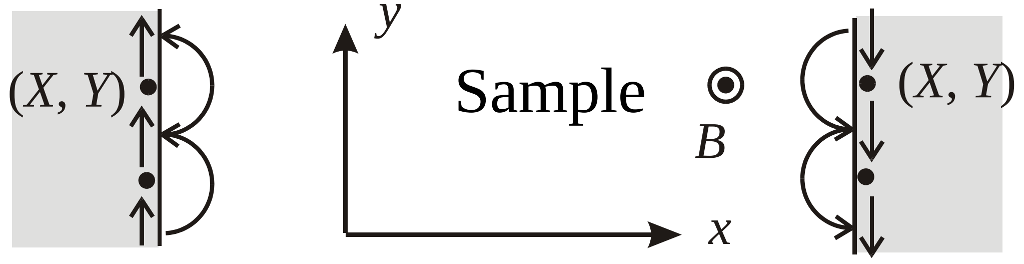
$$\xi(E)^{-1} = \alpha(E) \propto |E - E_N|^s$$

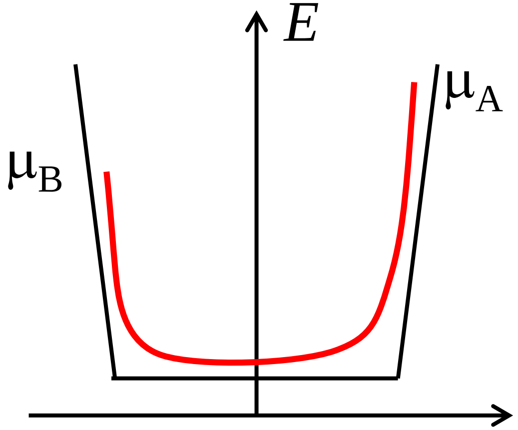
Numerical simulation $s = 2$ for $N = 0$

Aoki & Ando, PRL **54**, 831 (1985).

Edge mode explanation of IQHE







In an edge mode, the group velocity appears because the energy levels varies with *x*.

$$\langle v_y \rangle = \frac{dE}{\hbar dk} = -\frac{l_B^2}{\hbar}\frac{dE}{dX}$$

Current brought by a Landau edge mode

$$J = \int_{X_0}^{X_\mu} \frac{L_y dX}{2\pi l_B^2} \frac{e}{L_y} \langle v_y \rangle = \frac{e}{h} \int \mathrm{d}X \frac{\mathrm{d}E}{\mathrm{d}X} = \frac{e}{h}(\mu - E_0)$$

One dimensional system:

Landauer formula is applicable

$$\sigma_{xy} = \frac{J_y}{V_x} = \frac{e(J_\mathrm{A} - J_\mathrm{B})}{\mu_\mathrm{A} - \mu_\mathrm{B}} = \frac{e^2}{h}$$

Chiral edge mode: No backscattering!

Explanation from topological aspect

Bloch electrons under magnetic field: tight binding model

Translational operator: $T_{\boldsymbol{R}} f(\boldsymbol{r}) = f(\boldsymbol{r}+\boldsymbol{R}), \quad T_{\boldsymbol{R}} = \exp\left(\frac{i}{\hbar}\boldsymbol{R}\cdot\boldsymbol{p}\right)$

Hamiltonian: $\mathscr{H}_0 = -\frac{\hbar^2\nabla^2}{2m} + V(\boldsymbol{r})$

→ simultaneous diagonalization → Bloch states

$$\mathscr{H} = \frac{1}{2m}(\boldsymbol{p}+e\boldsymbol{A})^2 + V(\boldsymbol{r})$$

$\boldsymbol{A}(\boldsymbol{r}) = \boldsymbol{A}(\boldsymbol{r}+\boldsymbol{R}) + \boldsymbol{\nabla} g(\boldsymbol{r})$ does not have translational symmetry

Magnetic translation operator $\boldsymbol{p} \to \boldsymbol{p} + e\boldsymbol{A}$

Symmetric gauge $\boldsymbol{A} = \boldsymbol{B}\times\boldsymbol{r}/2$

$$T_{B\boldsymbol{R}} \equiv \exp\left\{\frac{i}{\hbar}\boldsymbol{R}\cdot\left[\boldsymbol{p}+\frac{e}{2}(\boldsymbol{r}\times\boldsymbol{B})\right]\right\} = T_{\boldsymbol{R}}\exp\left[\frac{ie}{\hbar}(\boldsymbol{B}\times\boldsymbol{R})\cdot\frac{\boldsymbol{r}}{2}\right]$$

$$[\mathscr{H}, T_{B\boldsymbol{R}}] = 0$$

Magnetic Brillouin zone

However $$T_{B\boldsymbol{R}a}T_{B\boldsymbol{R}b} = \exp(2\pi i\phi)T_{B\boldsymbol{R}b}T_{B\boldsymbol{R}a}, \quad \phi = \frac{eB}{h}ab$$

$$\phi = p/q \quad : \quad \text{rational number}$$

Magnetic unit cell: unit vectors $(\boldsymbol{a}, \boldsymbol{b}) \to$ magnetic unit vectors $(q\boldsymbol{a}, \boldsymbol{b})$

Lattice vector : $R' = n(q\boldsymbol{a}) + m\boldsymbol{b}$ $T_{B\boldsymbol{R}'}$: elements commute

ψ: simultaneously diagonalizes $\mathcal{H}$ and $T_{B\boldsymbol{R}'}$

Magnetic Brillouin zone: $0 \le k_1 < 2\pi/qa,\ 0 \le k_2 < 2\pi/b$

$$T_{q\boldsymbol{a}+\boldsymbol{b}}\psi = \exp[i(k_x qa + k_y b)]\psi$$

Magnetic Bloch function: $\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\boldsymbol{r}}u_{n\boldsymbol{k}}(\boldsymbol{r})$

Magnetic Bloch function

$$u_{n\boldsymbol{k}}(x+qa,y)=\exp\left(i\frac{\pi py}{b}\right)u_{n\boldsymbol{k}}(x,y),$$
$$u_{n\boldsymbol{k}}(x,y+b)=\exp\left(-i\frac{\pi px}{qa}\right)u_{n\boldsymbol{k}}(x,y).$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r})=\left|u_{n\boldsymbol{k}(\boldsymbol{r})}\right|\exp[i\theta_{\boldsymbol{k}}(\boldsymbol{r})] \quad p=-\frac{1}{2\pi}\oint d\boldsymbol{l}\cdot\frac{\partial\theta_{\boldsymbol{k}}(\boldsymbol{r})}{\partial\boldsymbol{l}}$$

Remember k·p approximation $\boldsymbol{p}e^{i\boldsymbol{kr}}=e^{i\boldsymbol{kr}}(\hbar\boldsymbol{k}+\boldsymbol{p})$

$$(\boldsymbol{p}+e\boldsymbol{A})^2e^{i\boldsymbol{kr}}u_{n\boldsymbol{k}}(\boldsymbol{r})=e^{i\boldsymbol{kr}}(\hbar\boldsymbol{k}+\boldsymbol{p}+e\boldsymbol{A})^2u_{n\boldsymbol{k}}(\boldsymbol{r})$$

Schrodinger-like equation for $u_{n\boldsymbol{k}}(\boldsymbol{r})$

$$\mathscr{H}_{\boldsymbol{k}}u_{n\boldsymbol{k}}(\boldsymbol{r})=E_{n\boldsymbol{k}}u_{n\boldsymbol{k}}(\boldsymbol{r}), \quad \mathscr{H}_{\boldsymbol{k}}=\frac{1}{2m}(-i\hbar\boldsymbol{\nabla}+\hbar\boldsymbol{k}+e\boldsymbol{A})^2+V(\boldsymbol{r})$$

k- dependent Hamiltonian

Kubo formula for σ_{xy}

Ryogo Kubo
1920 - 1995

Electric field along *y*-axis: E

$$|\alpha'\rangle = |\alpha\rangle + \sum_{\beta\neq\alpha} \frac{\langle\beta|eEy|\alpha\rangle}{E_\alpha - E_\beta}|\beta\rangle$$

Unperturbed state

$$j_x = \frac{1}{L^2}\sum_\alpha f(E_{\alpha'})\langle\alpha'|\hat{j}_x|\alpha'\rangle = \frac{1}{L^2}\sum_\alpha f(E_\alpha)\sum_{\beta\neq\alpha}\frac{\langle\alpha|(-ev_x)|\beta\rangle\langle\beta|eEy|\alpha\rangle}{E_\alpha - E_\beta} + \text{c.c.}$$

$$\langle\beta|v_y|\alpha\rangle = \langle\beta|\dot{y}|\alpha\rangle = -\frac{i}{\hbar}\langle\beta|[y,\mathscr{H}]|\alpha\rangle = -\frac{i}{\hbar}(E_\alpha - E_\beta)\langle\beta|y|\alpha\rangle$$

$$\sigma_{xy} = \frac{j_x}{E} = \frac{e^2\hbar}{iL^2}\sum_\alpha f(E_\alpha)\sum_\beta \frac{\langle\alpha|v_x|\beta\rangle\langle\beta|v_y|\alpha\rangle}{(E_\alpha - E_\beta)^2} + \text{c.c.}$$

Magnetic Bloch function (II)

Velocity operator: $\boldsymbol{v} = (-i\hbar\boldsymbol{\nabla} + e\boldsymbol{A})/m$

$$u_{n\boldsymbol{k}}(\boldsymbol{r}) \to |n, \boldsymbol{k}\rangle$$

$$\langle n, \boldsymbol{k}|\boldsymbol{v}|m, \boldsymbol{k}'\rangle = \delta_{\boldsymbol{k}\boldsymbol{k}'} \int_0^{qa} dx \int_0^{b} dy u^*_{n\boldsymbol{k}} \boldsymbol{v} u_{m\boldsymbol{k}'} \equiv \delta_{\boldsymbol{k}\boldsymbol{k}'} \langle n|\boldsymbol{v}|m\rangle$$

Normalization: $\displaystyle\int_0^{qa} dx \int_0^{b} dy |u_{n\boldsymbol{k}}(\boldsymbol{r})|^2 = 1$

$$\langle n|v_x|m\rangle = \frac{1}{\hbar}\left\langle n\left|\frac{\partial \mathscr{H}_{\boldsymbol{k}}}{\partial k_x}\right|m\right\rangle, \quad \langle n|v_y|m\rangle = \frac{1}{\hbar}\left\langle n\left|\frac{\partial \mathscr{H}_{\boldsymbol{k}}}{\partial k_y}\right|m\right\rangle.$$

$$\left\langle n\left|\frac{\partial \mathscr{H}_{\boldsymbol{k}}}{\partial k_j}\right|m\right\rangle = (E_m - E_n)\left\langle n\left|\frac{\partial u_m}{\partial k_j}\right.\right\rangle = -(E_m - E_n)\left\langle \frac{\partial u_n}{\partial k_j}\right|m\right\rangle,$$

$j = x.y$

Kubo conductivity calculated with magnetic Bloch functions

$$\sigma_{xy} = -i\frac{e^2}{\hbar}\sum_{\boldsymbol{k}}\sum_{n} f(E_{n\boldsymbol{k}}) \sum_{m(\neq n)} \left[\frac{\langle n\boldsymbol{k}|\partial \mathscr{H}_{\boldsymbol{k}}/\partial k_x|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|\partial \mathscr{H}_{\boldsymbol{k}}/\partial k_y|n\boldsymbol{k}\rangle}{(E_{n\boldsymbol{k}}-E_{m\boldsymbol{k}})^2} - \text{c.c.}\right]$$

$$= -i\frac{e^2}{\hbar}\sum_{\boldsymbol{k}}\sum_{n} f(E_{n\boldsymbol{k}}) \sum_{m(\neq n)} \left[\left\langle \frac{\partial u_n}{\partial k_x}\middle| m\right\rangle\left\langle m\middle|\frac{\partial u_n}{\partial k_y}\right\rangle - \left\langle \frac{\partial u_n}{\partial k_y}\middle| m\right\rangle\left\langle m\middle|\frac{\partial u_n}{\partial k_x}\right\rangle\right]$$

$$= \frac{e^2}{h}\frac{2\pi}{i}\sum_{\boldsymbol{k}}\sum_{n} f(E_{n\boldsymbol{k}}) \left[\left\langle \frac{\partial u_n}{\partial k_x}\middle|\frac{\partial u_n}{\partial k_y}\right\rangle - \left\langle \frac{\partial u_n}{\partial k_y}\middle|\frac{\partial u_n}{\partial k_x}\right\rangle\right].$$

Vector field: $\boldsymbol{A}_{n\boldsymbol{k}} = \int d^2\boldsymbol{r}\, u^*_{n\boldsymbol{k}} \boldsymbol{\nabla}_{\boldsymbol{k}} u_{n\boldsymbol{k}} = \langle u_{n\boldsymbol{k}}|\boldsymbol{\nabla}_{\boldsymbol{k}}|u_{n\boldsymbol{k}}\rangle$ Berry connection

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\sum_{E_n<E_{\rm F}}\int_{\rm MBZ} d^2k[\boldsymbol{\nabla}_{\boldsymbol{k}}\times \boldsymbol{A}_{n\boldsymbol{k}}]_{k_z} = \frac{e^2}{h}\frac{1}{2\pi i}\sum_{E_n<E_{\rm F}}\int_{\rm MBZ} d^2k[\text{rot}_{\boldsymbol{k}}\boldsymbol{A}_{n\boldsymbol{k}}]_{k_z}$$

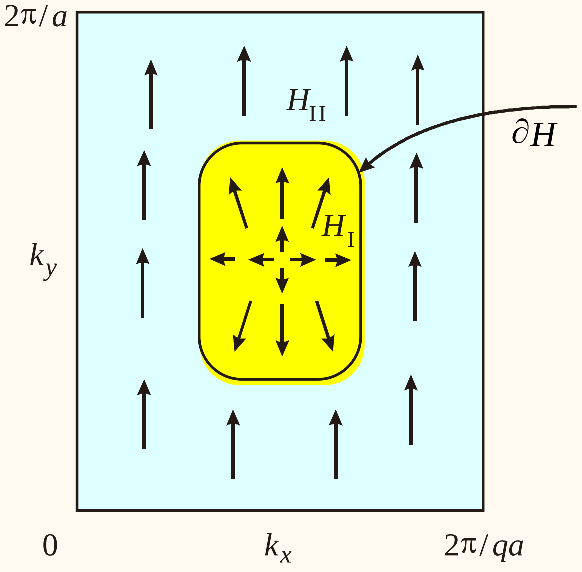
Berry curvature

TKNN Formula

Existence of zero or anomaly

Magnetic Brillouin zone

$$I = \frac{1}{2\pi i}\left[\int_{\mathrm{I}} d^2k[\mathrm{rot}\boldsymbol{A}]_{k_z} + \int_{\mathrm{II}} d^2k[\mathrm{rot}\boldsymbol{A}]_{k_z}\right] = \oint_{\partial H}(\boldsymbol{A}^{\mathrm{II}} - \boldsymbol{A}^{\mathrm{I}})\cdot\frac{d\boldsymbol{k}}{2\pi i}$$



On the boundary ∂H $\quad u_{\boldsymbol{k}}^{\mathrm{I}} = u_{\boldsymbol{k}}^{\mathrm{II}} e^{i\theta(\boldsymbol{k})}$

$$I = \oint_{\partial H}\left[\langle u_{\boldsymbol{k}}^{\mathrm{II}}|\boldsymbol{\nabla}_{\boldsymbol{k}}|u_{\boldsymbol{k}}^{\mathrm{II}}\rangle + (i\boldsymbol{\nabla}_{\boldsymbol{k}}\theta)\langle u_{\boldsymbol{k}}^{\mathrm{II}}|u_{\boldsymbol{k}}^{\mathrm{II}}\rangle - \langle u_{\boldsymbol{k}}^{\mathrm{II}}|\boldsymbol{\nabla}_{\boldsymbol{k}}|u_{\boldsymbol{k}}^{\mathrm{II}}\rangle\right]\cdot\frac{d\boldsymbol{k}}{2\pi i}$$

$$= \frac{\Delta_{\partial H}\theta}{2\pi} = \nu_{\mathrm{C}}$$

: Chern number (integer)

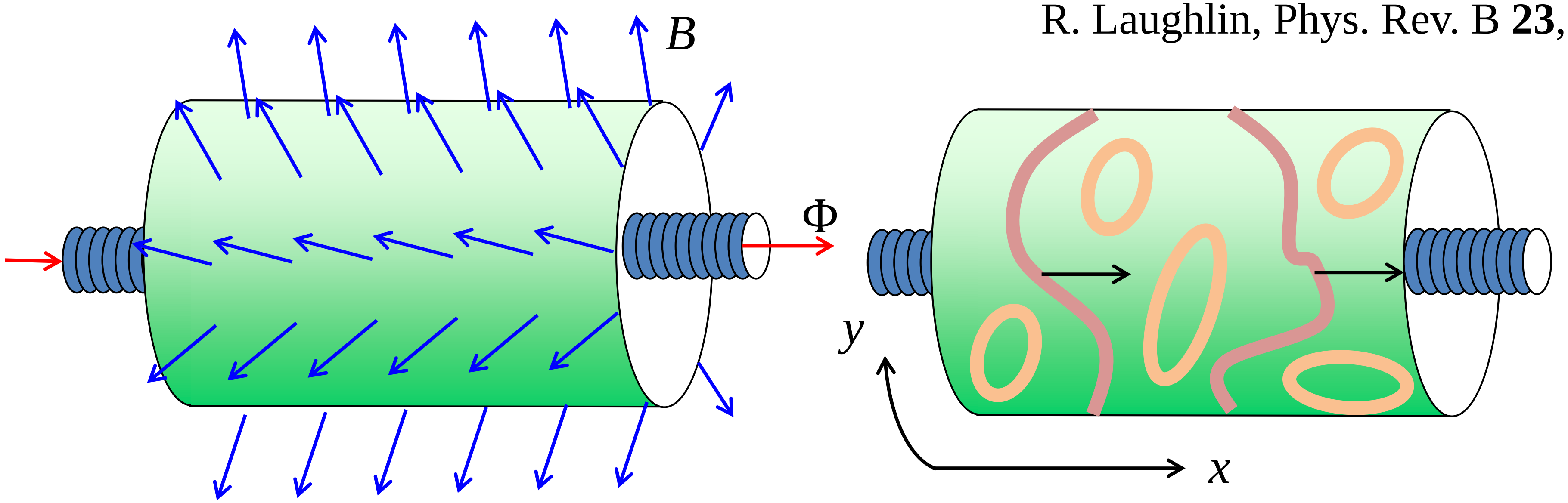
Topological invariant

$$\sigma_{xy} = \nu_{\mathrm{C}}\frac{e^2}{h}$$

Thouless-Kohmoto-Nightingale-den Nijs (TKNN) Formula

Laughlin's discussion

R. Laughlin, Phys. Rev. B **23**, 5632 (1981).



Robert Laughlin

Landau gauge $\boldsymbol{A} = (0, Bx - \Phi/L_y) = (0, B(x - \Phi/L_yB))$

Magnetic flux Φ : *X* shift $X \to X + \dfrac{\Phi}{L_yB} \;:\; \dfrac{\Phi}{\phi_0}\dfrac{L_x}{N_\mathrm{L}} \quad (N_\mathrm{L} \equiv n_\mathrm{L} L_x L_y)$

$$j_y = \frac{J_y}{L_x} = \frac{1}{L_x}\frac{\partial E_{L_x}}{\partial \Phi} \quad \left(cf.\ E = \frac{L}{2}J^2,\ \Phi = LJ\right)$$

$$= \frac{1}{L_x}\frac{\Delta E_{L_x}}{\Delta \Phi} = \frac{1}{L_x}\left(-e\mathcal{E}_x \frac{L_x}{N_\mathrm{L}}\right)\frac{N_e}{\phi_0} = \nu\frac{e^2}{h}\mathcal{E}_x$$

Chern number =1

Summary of “topological aspect”

(a) In 2D system under magnetic field: magnetic Bloch functions, magnetic Brillouin zone

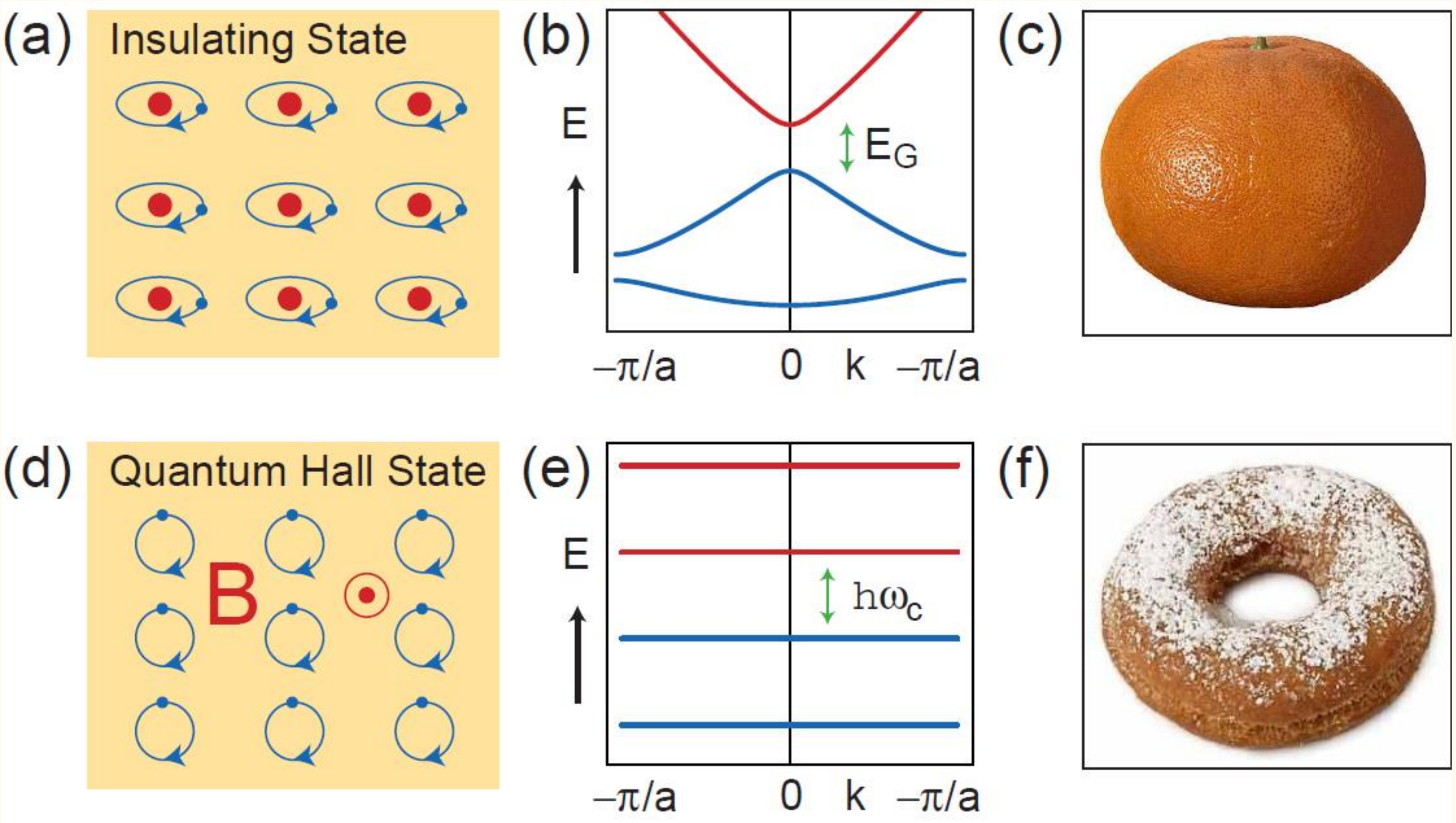
(b) Kubo formula for Hall conductivity: matrix elements of velocity operator

(c) From (a) and (b) Hall conductivity is obtained as the integration of Berry curvature over magnetic Brillouin zone

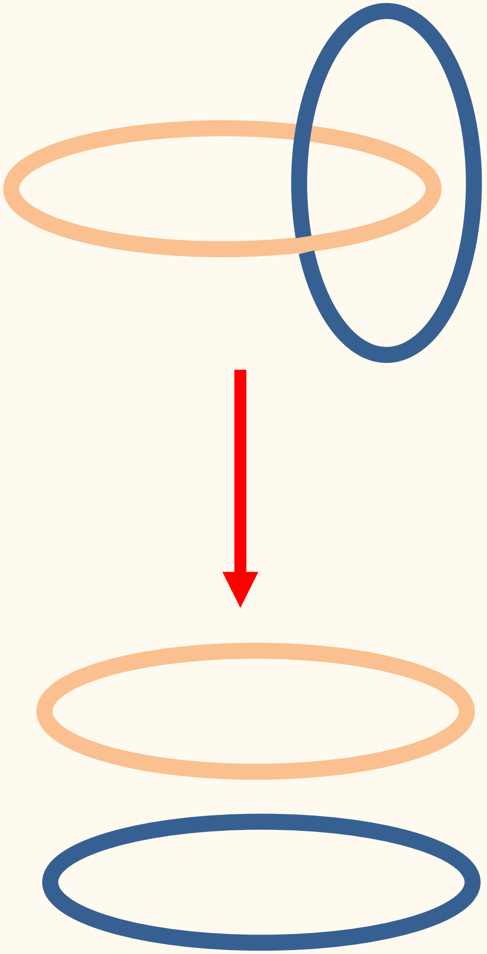
(d) TKNN formula: Chern number (topological invariant) times quantum conductance

(e) Chern number is integer (due to single-valuedness of atomic part) and non-zero in quantum Hall system (Laughlin’s discussion)

Bulk-Edge correspondence

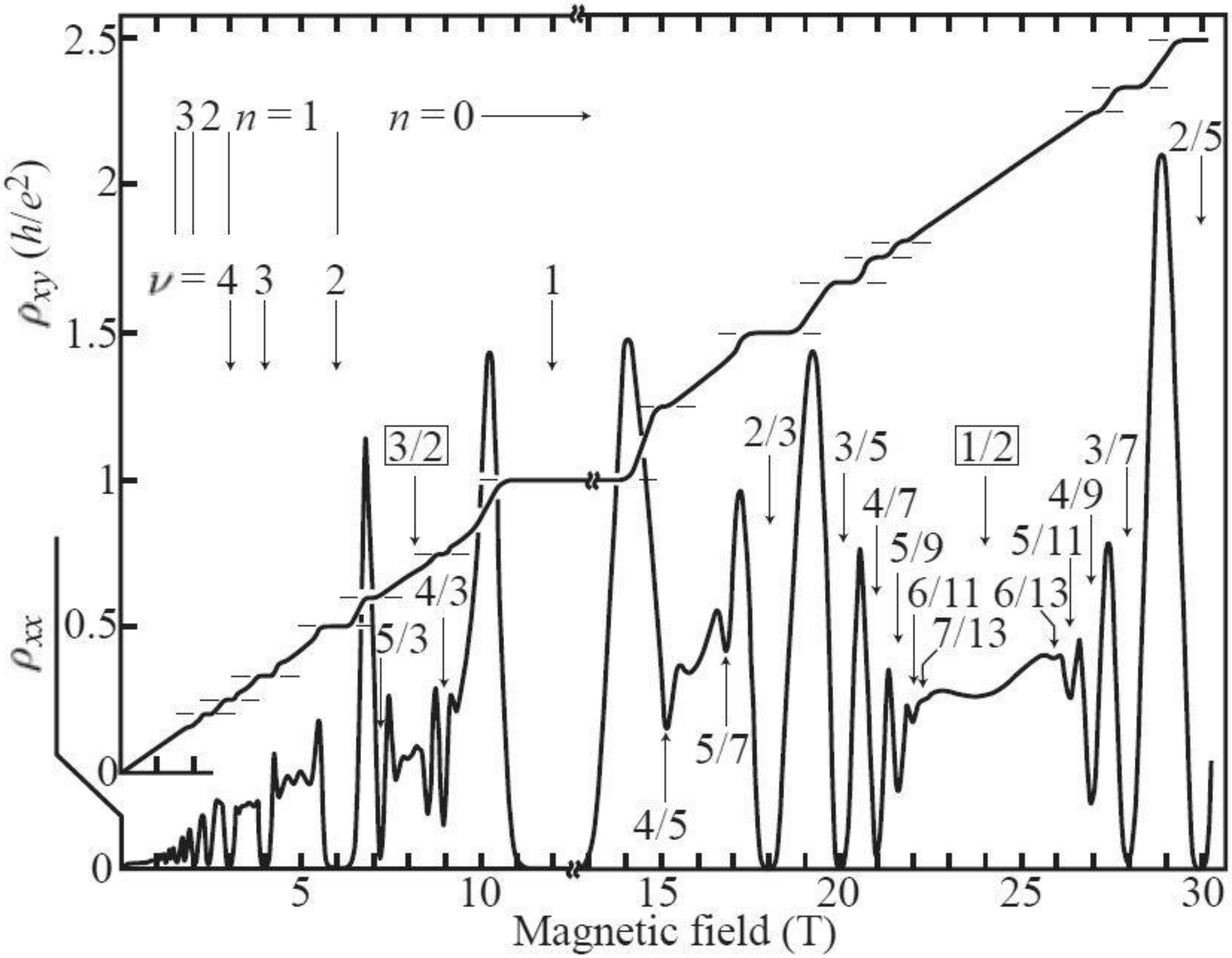


Hasan & Kane, Rev. Mod. Phys. **82**, 3045 (2010).



Transition between bands with different Chern number only can attained through energy gap collapse.

Fractional quantum Hall effect



Laughlin state

$$\psi_q(z_1, \cdots, z_{N_e})$$
$$= \prod_{i>j} (z_i - z_j)^q \exp\left(-\sum_i \frac{|z_i|^2}{4}\right)$$

Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.7.14 Lecture 14

10:25 – 11:55

Institute for Solid State Physics, University of Tokyo

Shingo Katsumoto

What we have seen

Semiconductor basics

- Band structure
- Effective mass approximation
- Carrier statistics
- Electron-photon couplings
- Thermodynamics
- Semi-classical transport (Boltzmann equation)

Spatial modulation basics

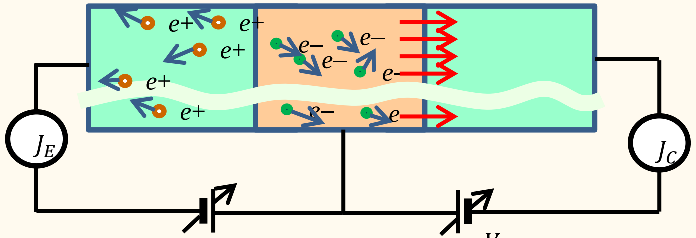
- Modulation doping: pn-junctions
- Schottky junctions, MOS junctions
- Hetero-junctions
- Quantum confinement
- Quantum wells, wires and dots
- Minority carrier confinement

Quantum physics in semiconductors

- Fermion transport: Landauer (-Büttiker) formalism
- T-matrix, S-matrix
- Boson transport, Bose-Einstein condensation
- Quantum dots: Single electron effect, quantum confinement
- Quantum Hall: Edge mode, topological number

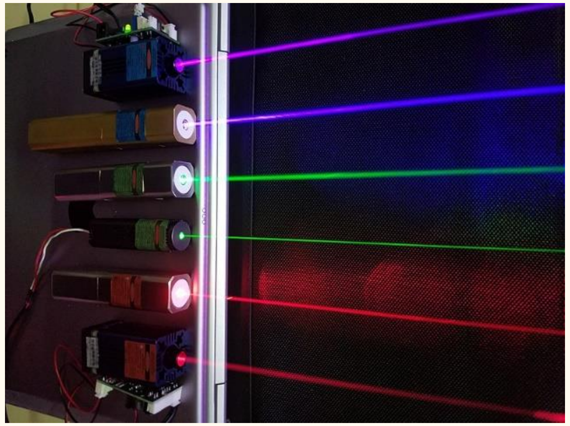
Part of topics

Charge (kinetic) freedom

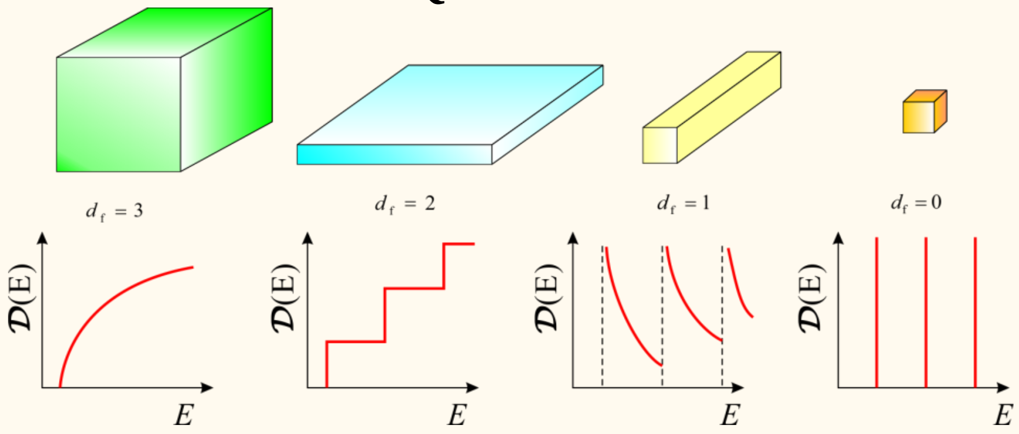


Semiclassical transport

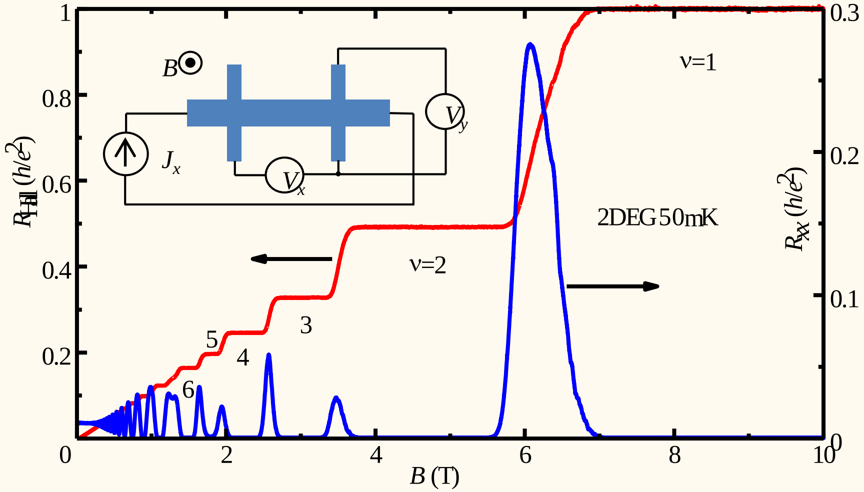
Laser diode



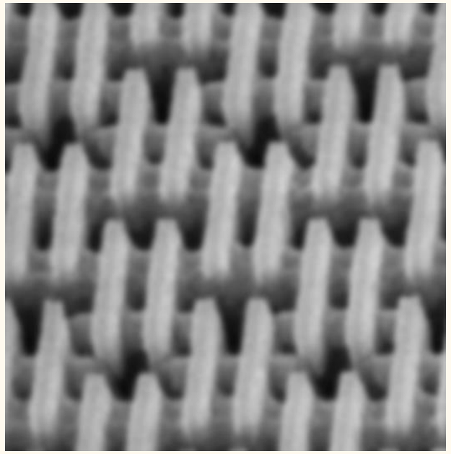
Quantum confinement



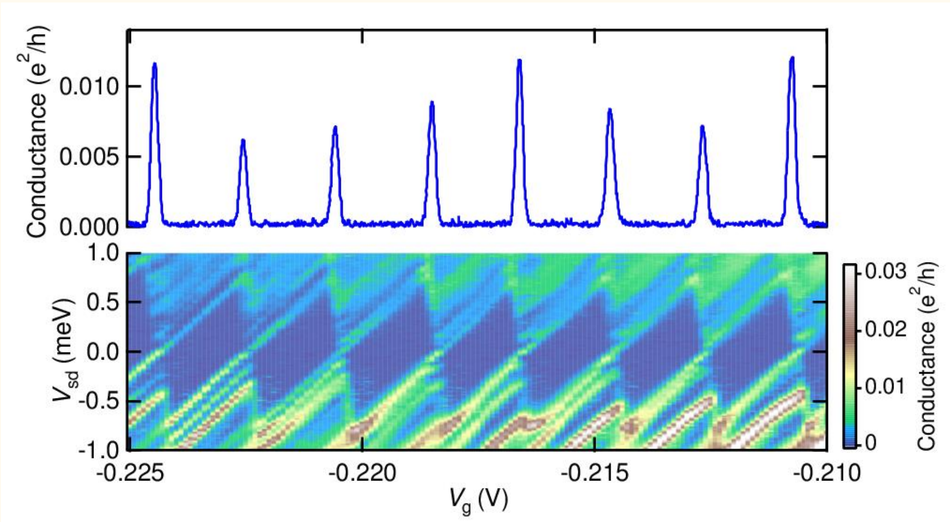
Quantum wells, wires, dots



Quantum Hall and topology
in solid state physics



Si technology: FinFET



Quantum dot: single electron, quantum confinement

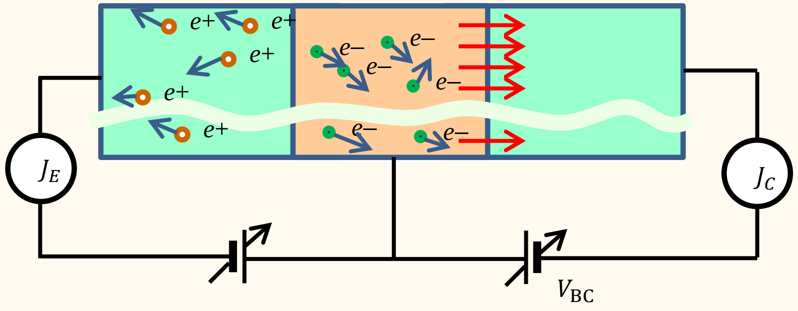
Chapter 10a Spintronics I

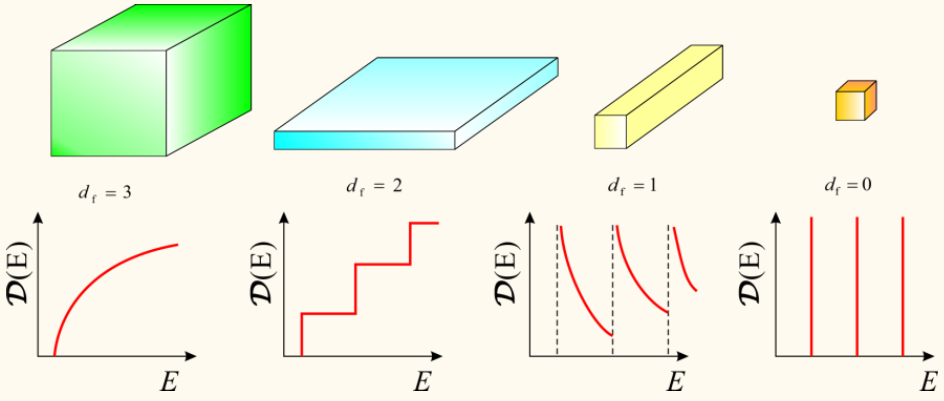
Two current model

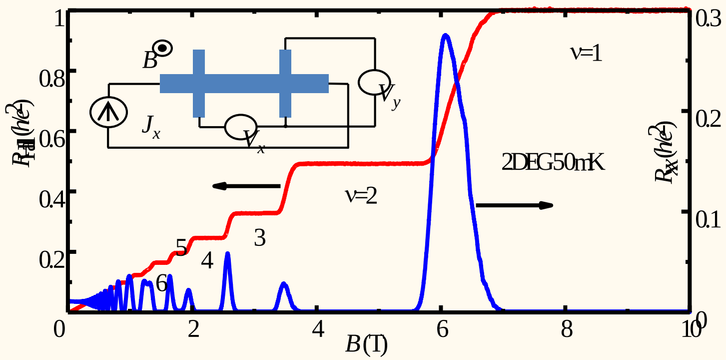
Spin injection

Spin degree of freedom: A new paradigm

Charge (kinetic) freedom







Spin degree of freedom

Giant magnetoresistance
spin valve

Spin injection

Spin-manipulation of
quantum information

Topological insulators

Nobel laureates


Photo from the Nobel Foundation archive.
William Bradford Shockley


John Bardeen
Prize share: 1/3


Photo from the Nobel Foundation archive.
Walter Houser Brattain

1956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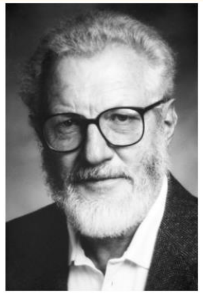
Zhores I. Alferov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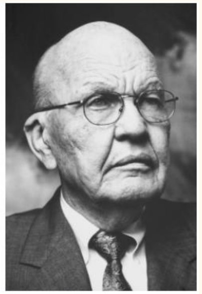
Herbert Kroemer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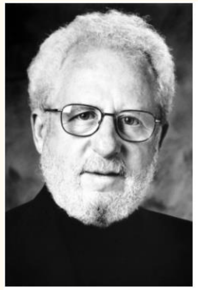
Jack S. Kilby

2000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Alan J. Heeger


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Alan G. MacDiarmid


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Hideki Shirakawa

2000 (Chemistry)


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Leo Esaki

1973


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Klaus von Klitzing

1985


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Andre Geim
Prize share: 1/2


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Konstantin Novoselov

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2016

Charge (kinetic) freedom

Spin degree of freedom


Photo from the Nobel Foundation archive.
Robert B. Laughlin


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Horst L. Störmer


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1998


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2014


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Albert Fert


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Peter Grünberg

2007

The two current model

Nevill Mott
1905-1996

Divide a current to the one with ↑ spin and the one with ↓ spin.

$$\sigma = \sigma_\uparrow + \sigma_\downarrow, \quad \frac{1}{\rho} = \frac{1}{\rho_\uparrow} + \frac{1}{\rho_\downarrow}$$

Drude: $\sigma_s = \dfrac{e^2 n_s \tau_s}{m_s^*} \quad (s = \uparrow, \downarrow)$

Condition: spin diffusion length $\lambda_s \gg l$ mean free path (or other lengths)

Spin polarized current: $\boldsymbol{j}_{\mathrm{p}\uparrow} = \boldsymbol{j}_\uparrow - \boldsymbol{j}_\downarrow$

$$P_{\mathrm{c}} = \frac{|\boldsymbol{j}_\uparrow - \boldsymbol{j}_\downarrow|}{|\boldsymbol{j}_\uparrow + \boldsymbol{j}_\downarrow|} = \frac{j_{\mathrm{p}\uparrow(\downarrow)}}{j_{\mathrm{c}}}$$

$$\boldsymbol{j}_{\mathrm{ps}} = \boldsymbol{\sigma}_s \boldsymbol{E} - eD_s(-\nabla \delta n_s)$$

drift — diffusion

Einstein relation for metals: $\sigma_s = e^2 N_s(E_{\mathrm{F}}) D_s \quad (cf.\ \sigma = e^2 (n/k_{\mathrm{B}} T) D)$

ϵ_s: local Fermi energy, $\delta\epsilon_s$: Shift from thermal equilibrium

$$\boldsymbol{j}_s = -\frac{\sigma_s}{e}\left[e\nabla\phi - \frac{D_s \nabla \delta n_s}{\sigma_s}\right] = \frac{\sigma_s}{e}[-e\nabla\phi + \nabla\delta\epsilon_s]$$

$\mu_s \equiv -e\phi + \epsilon_s$ Spin-dependent chemical potential $\boldsymbol{j}_s = -\dfrac{\sigma_s}{-e}\nabla\mu_s$

Spin current

Remember Boltzmann equation $$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m^*} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = -\left(\frac{\partial f}{\partial t}\right)_c$$

Because spin carriers are dipoles it is difficult to apply forces (needs magnetic field gradient)→Diffusion current only

Spin current (simplest) definition $$\boldsymbol{j}^s(\boldsymbol{r}, t) = \frac{\hbar}{2(-e)}(\boldsymbol{j}_\uparrow - \boldsymbol{j}_\downarrow)$$

Angular momentum conservation $$\frac{\partial s_z}{\partial t} + \mathrm{div}\, \boldsymbol{j}^s = 0$$

With spin relaxation $$\frac{\partial s_z}{\partial t} + \mathrm{div}\, \boldsymbol{j}^s = \frac{\partial s_z}{\partial t} + \frac{\hbar}{2(-e)} \nabla \cdot (\boldsymbol{j}_\uparrow - \boldsymbol{j}_\downarrow) = \frac{\hbar}{2}\left(\frac{\delta n_\uparrow}{\tau_\uparrow} - \frac{\delta n_\downarrow}{\tau_\downarrow}\right)$$

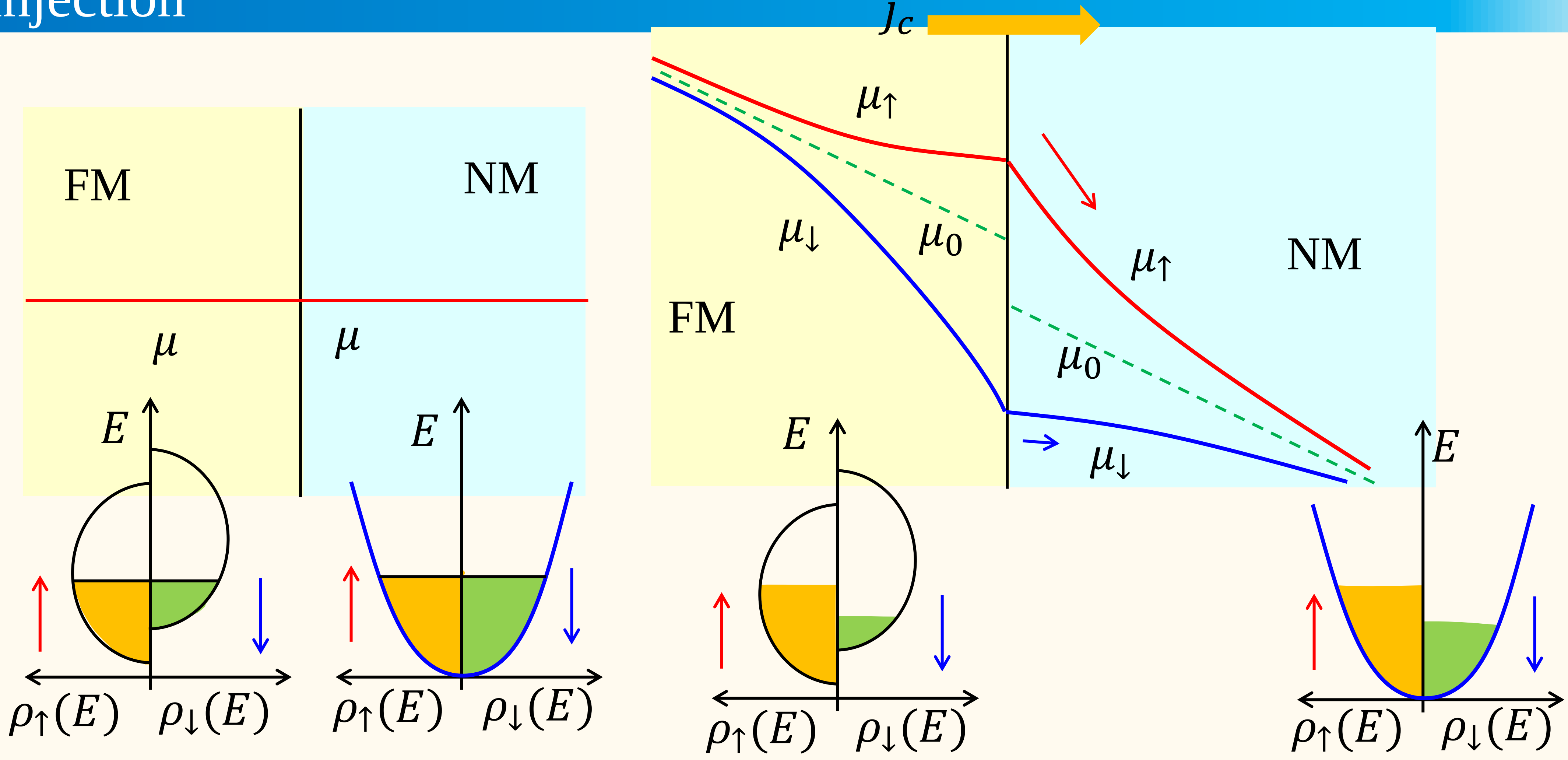
cf. Charge conservation $$\frac{\partial \rho}{\partial t} + \mathrm{div} \boldsymbol{j} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\boldsymbol{j}_\uparrow + \boldsymbol{j}_\downarrow) = 0$$

Steady state $$N_\uparrow \tau_\downarrow = N_\downarrow \tau_\uparrow$$

spin diffusion equation $$\nabla^2(\sigma_\uparrow \mu_\uparrow + \sigma_\downarrow \mu_\downarrow) = 0,\ \nabla^2(\mu_\uparrow - \mu_\downarrow) = \frac{1}{(\lambda_{\mathrm{sf}}^{\mathrm{F}})^2}(\mu_\uparrow - \mu_\downarrow)$$

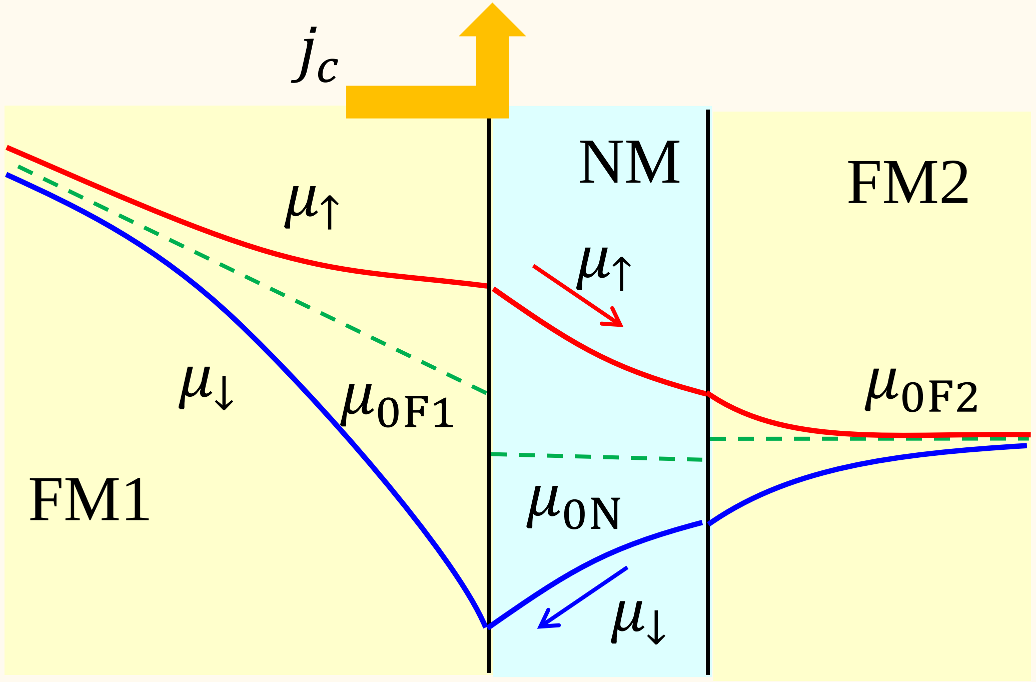
spin diffusion length $$\left(\frac{1}{(\lambda_{\mathrm{sf}}^{\mathrm{F}})^2} = \frac{1}{(\lambda_\uparrow^{\mathrm{F}})^2} + \frac{1}{(\lambda_\downarrow^{\mathrm{F}})^2}\right)$$

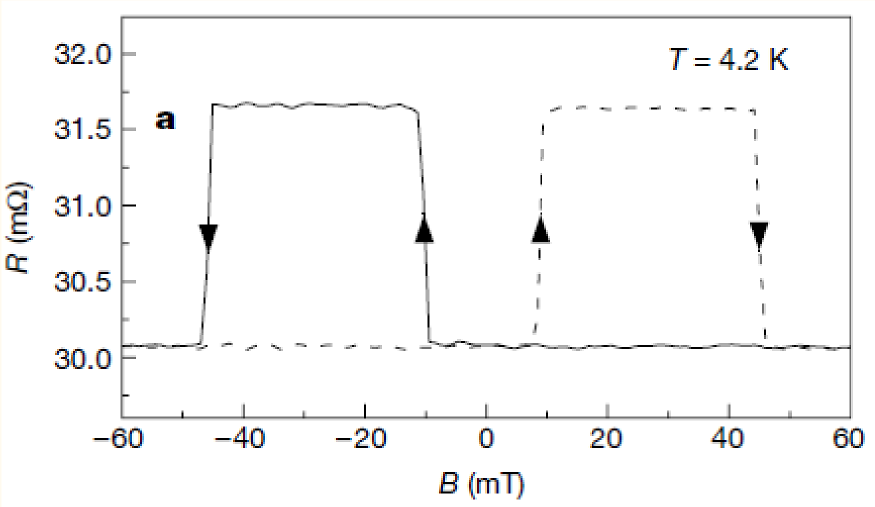
Spin injection

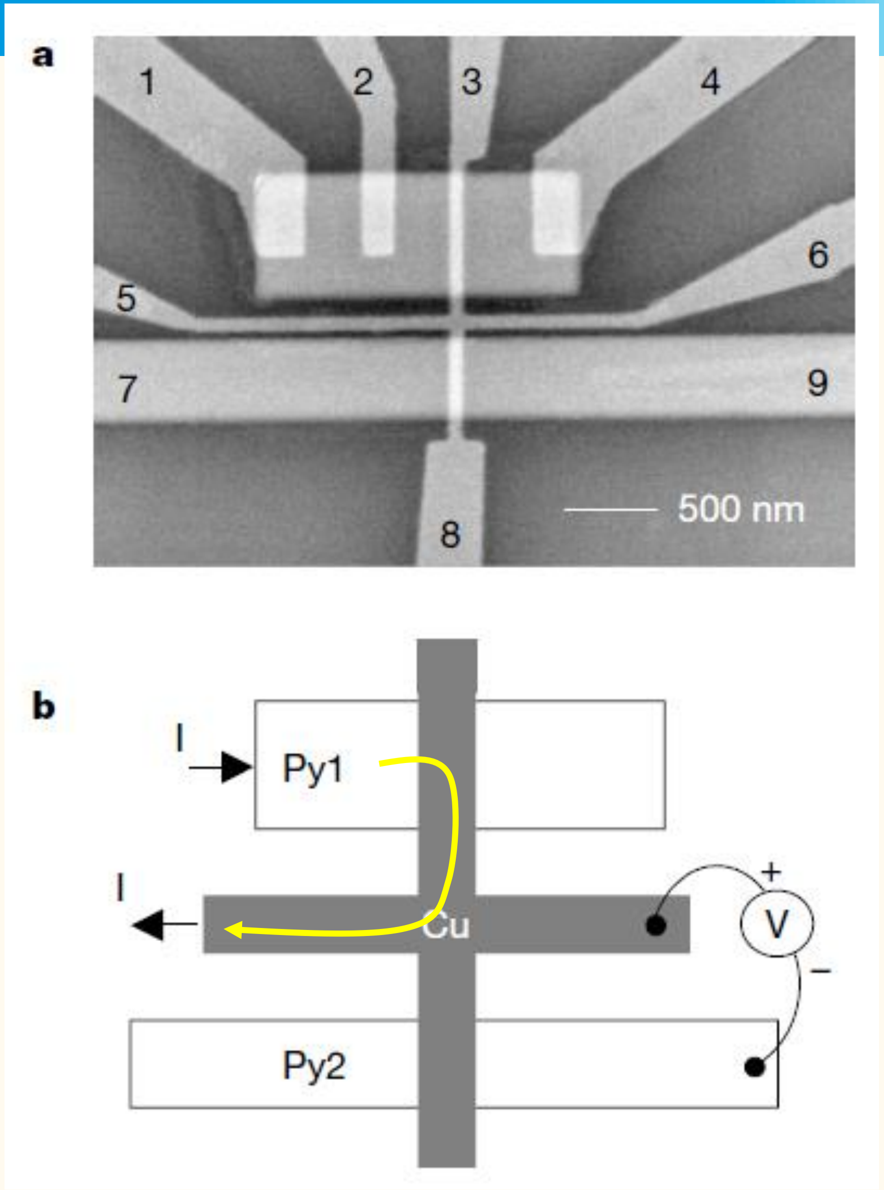


$$\mu_s^{\mathrm{M}} = a^{\mathrm{M}} + b^{\mathrm{M}} x \pm \frac{c^{\mathrm{M}}}{\sigma_s^{\mathrm{M}}} \exp\left(\frac{x}{\lambda_{\mathrm{sf}}^{\mathrm{M}}}\right) \pm \frac{d^{\mathrm{M}}}{\sigma_s^{\mathrm{M}}} \exp\left(-\frac{x}{\lambda_{\mathrm{sf}}^{\mathrm{M}}}\right) \qquad \mathrm{M} = \mathrm{F, N}$$

Spin injection and detection







Jedema et al. Nature **410**, 345 (2001).

Spin precession

Zeeman Hamiltonian $\mathscr{H} = \frac{e\hbar}{2m_0} g B_0 \hat{s}_z = g\mu_{\rm B} B_0 \hat{s}_z \qquad [\hat{s}_j, \hat{s}_k] = i\hat{s}_l/2$

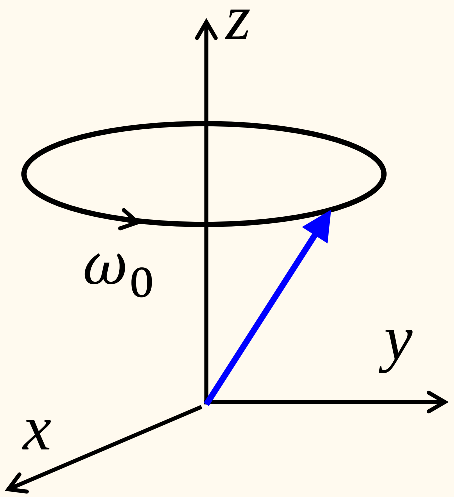
$$[\mathscr{H}, \hat{s}_x] = ig\mu_{\rm B} B_0 \hat{s}_y, \quad [\mathscr{H}, \hat{s}_y] = -ig\mu_{\rm B} B_0 \hat{s}_x, \quad [\mathscr{H}, \hat{s}_z] = 0$$

From Heisenberg equation: $\frac{\partial \langle s_x \rangle}{\partial t} = -\frac{g\mu_{\rm B}}{\hbar} B_0 \langle s_y \rangle, \quad \frac{\partial \langle s_y \rangle}{\partial t} = \frac{g\mu_{\rm B}}{\hbar} B_0 \langle s_x \rangle, \quad \frac{\partial \langle s_z \rangle}{\partial t} = 0$

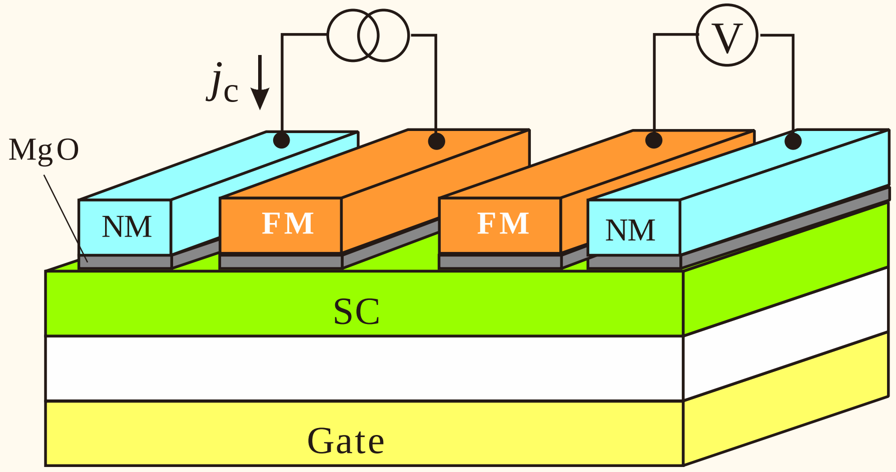
Solution $\langle s_x \rangle = A \cos \omega_0 t, \quad \langle s_y \rangle = A \sin \omega_0 t, \quad \langle s_z \rangle = C$

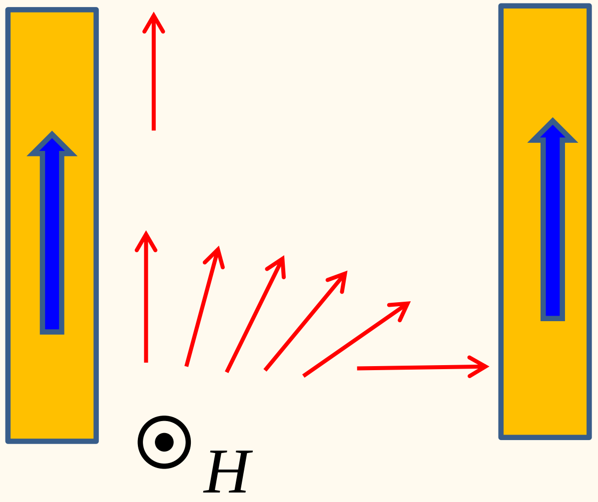
$$A^2 + C^2 = s^2, \quad \omega_0 = \frac{eg}{2m_0} B_0$$

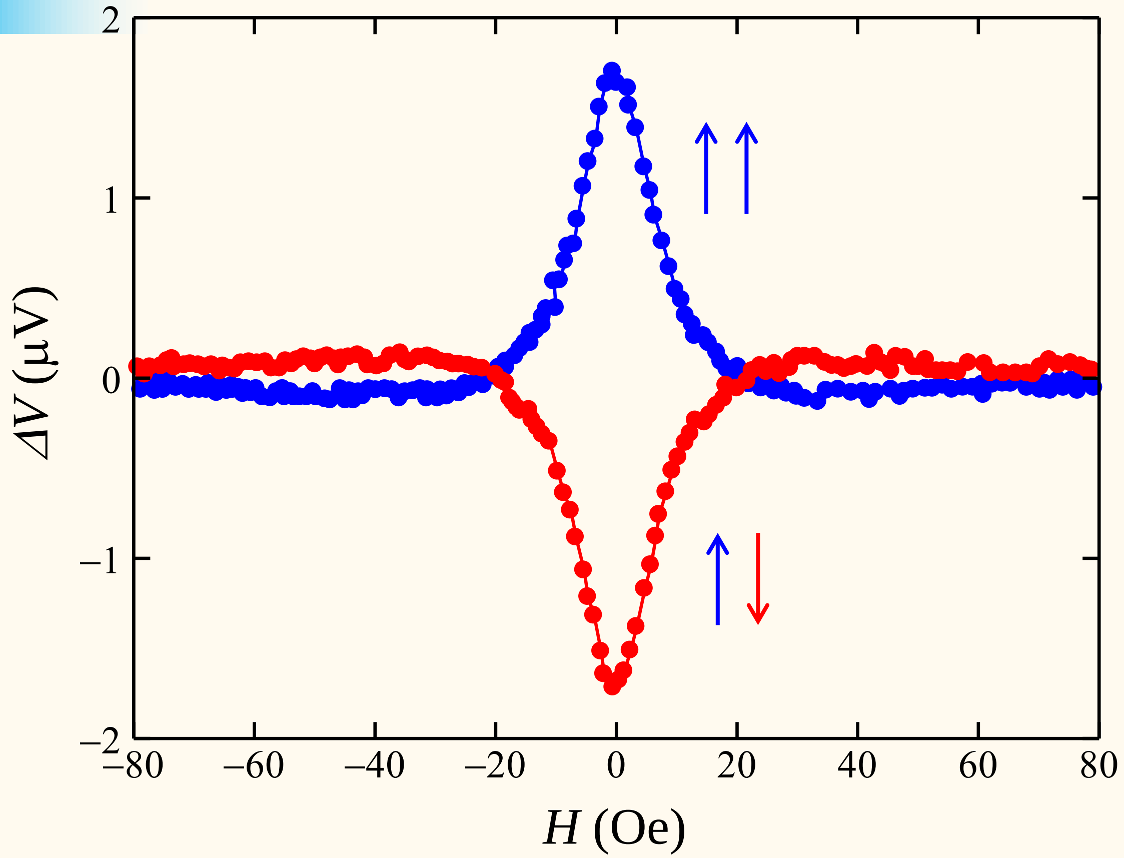
Larmor frequency



Spin precession experiment







$$\Delta V = \pm \frac{j_c P_j^2}{e^2 N_{\mathrm{SC}}} \int_0^\infty dt \varphi(t) \cos \omega t,$$

$$\varphi(t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{d^2}{4Dt}\right) \exp\left(-\frac{t}{\tau_{\mathrm{sf}}}\right)$$

Chapter 10b Spintronics II

Spin-orbit interaction

Spin Hall effect

Topological insulator (quantum spin Hall effect)

Spin-orbit interaction (in electron motion)

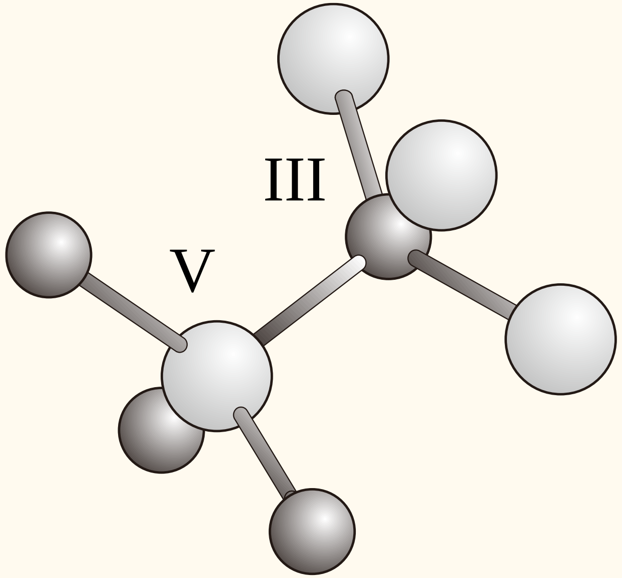
Pauli approximation of Dirac equation:

$$\frac{|P|^2}{3}\left\{\left(\frac{2}{E_{\rm g}}+\frac{1}{E_{\rm g}+\Delta}\right)k^2+V-\left(\frac{1}{E_{\rm g}}-\frac{1}{E_{\rm g}+\Delta}\right)\frac{e\boldsymbol{\sigma}\cdot\boldsymbol{B}}{\hbar}\right.$$
$$+\left[\frac{1}{E_{\rm g}^2}-\frac{1}{(E_{\rm g}+\Delta)^2}\right]e\boldsymbol{\sigma}\cdot(\boldsymbol{k}\times\boldsymbol{\mathcal{E}})$$
$$\left.-\left[\frac{2}{E_{\rm g}^2}+\frac{1}{(E_{\rm g}+\Delta)^2}\right]\frac{e\nabla\cdot\boldsymbol{\mathcal{E}}}{2}\right\}\psi_c=E'\psi_c$$

: Spin-orbit interaction

$\boldsymbol{\mathcal{E}}$: electric field

Finite $\boldsymbol{\mathcal{E}}$: requires inversion asymmetry.



BIA: Bulk inversion asymmetry

SIA: Structure inversion asymmetry

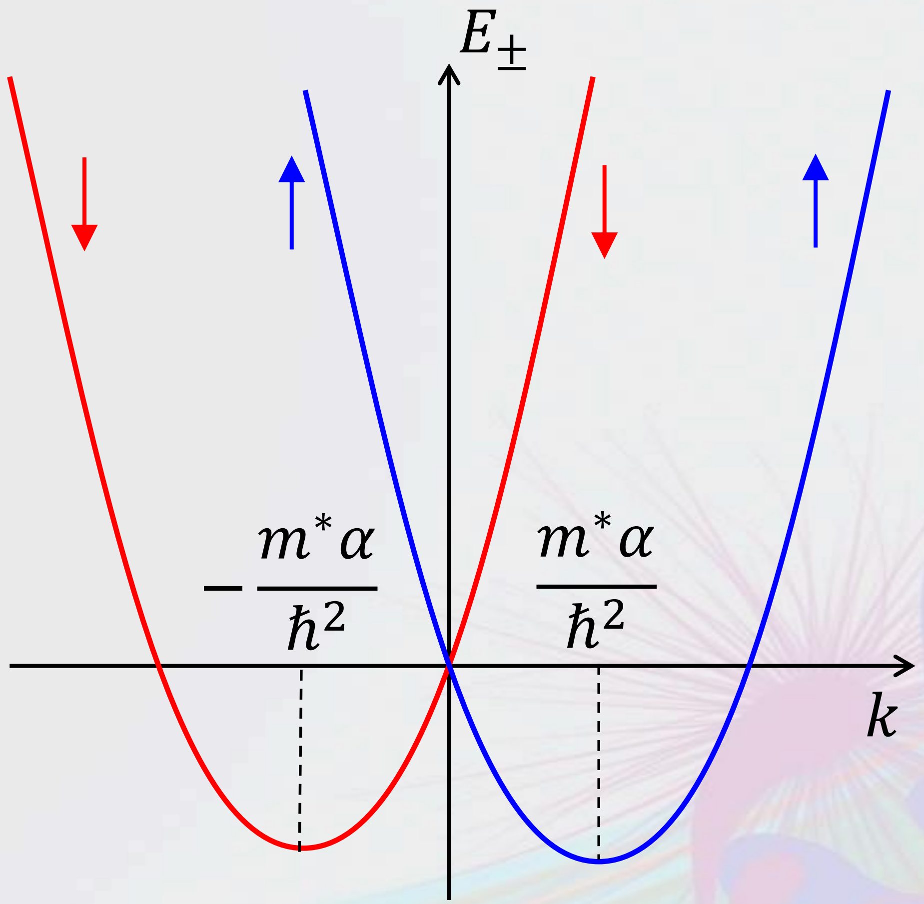
SIA-SOI Rashba-type SOI

BIA SOI $\mathscr{H}^{\text{2d}}_{\text{DSO}} = \gamma\hbar^2[k_x(k_y^2 - \langle k_z^2\rangle)\sigma_x + k_y(\langle k_z^2\rangle - k_x^2)\sigma_y] = \beta(k_y\sigma_y - k_x\sigma_x) + \gamma\hbar^2(k_x k_y^2\sigma_x - k_y k_x^2\sigma_y)$

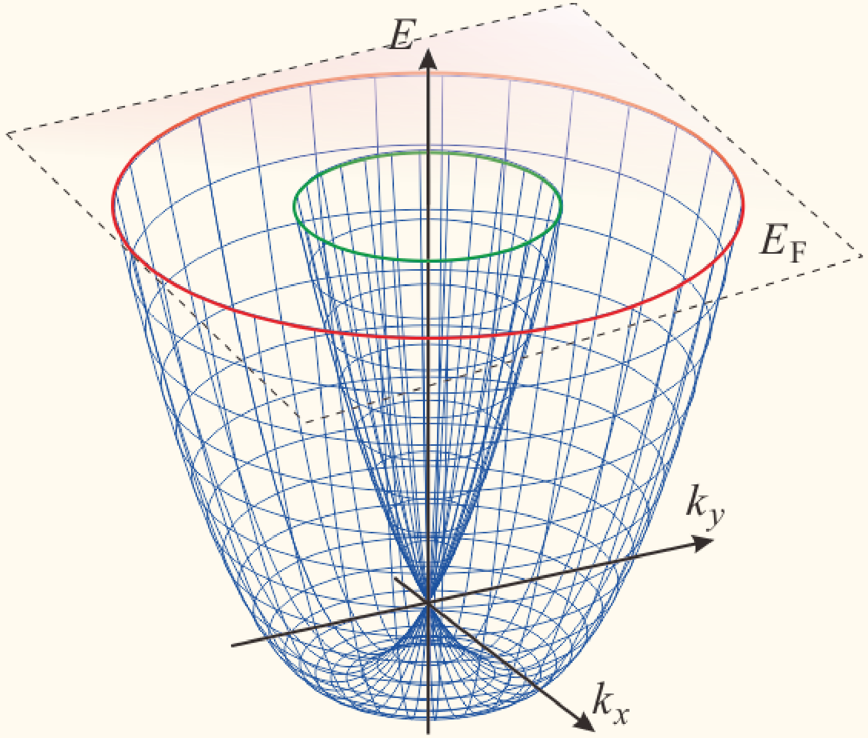
$\boldsymbol{\mathcal{E}} = (0, 0, \mathcal{E})$ on a 2DEG (x-y) (Actually through the valence band)

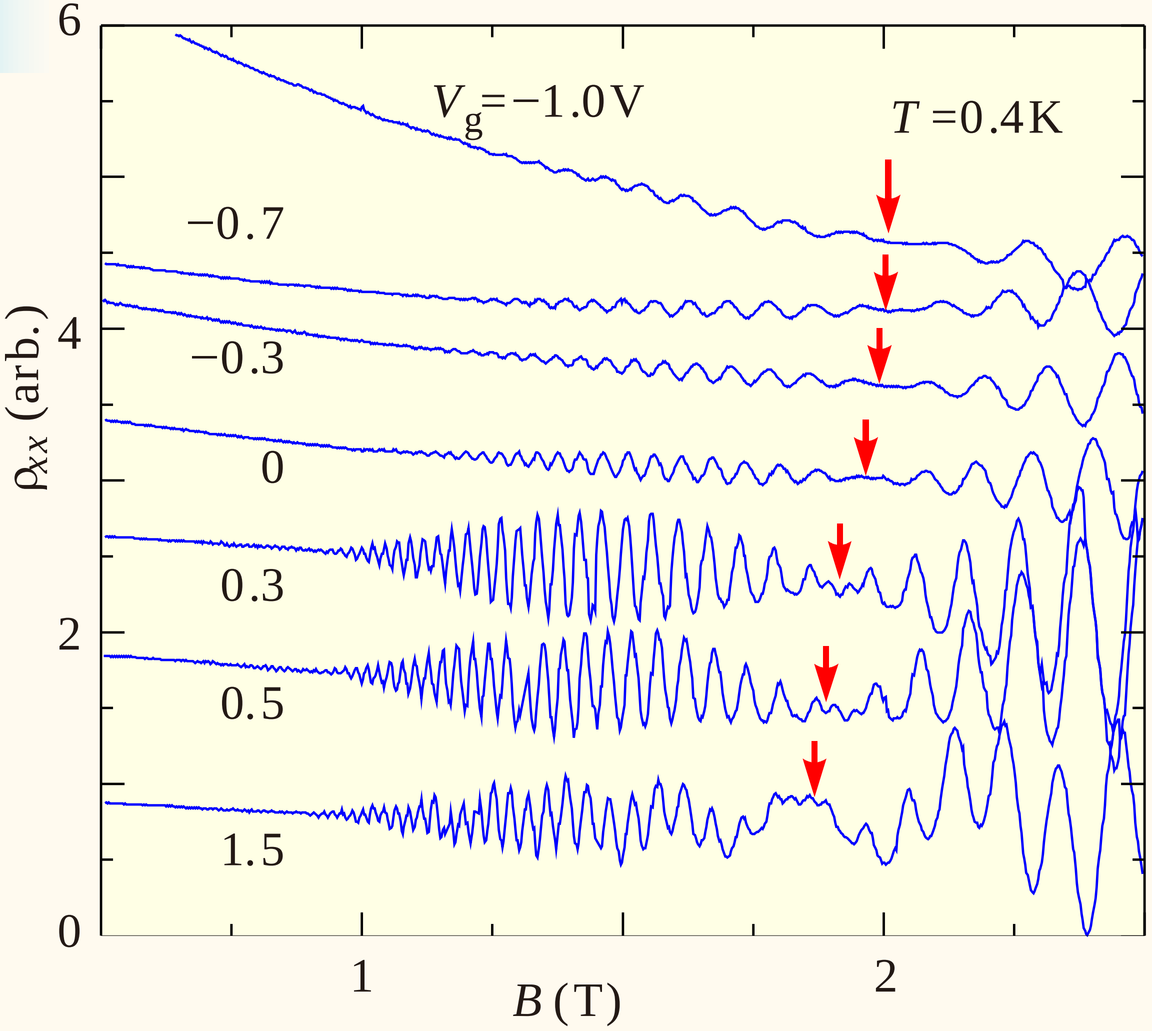
$$\mathscr{H}_{\text{RSO}} = \alpha\boldsymbol{\sigma}\cdot(\boldsymbol{k}\times\boldsymbol{e}_z) = \alpha(k_y\sigma_x - k_x\sigma_y)$$

$$E_\pm = \frac{\hbar^2 k^2}{2m^*} \mp \alpha k = \frac{\hbar^2}{2m^*}\left(k \mp \frac{m^*\alpha}{\hbar^2}\right)^2 - \frac{m^*}{2\hbar^2}\alpha^2$$



SOI and SdH oscillation



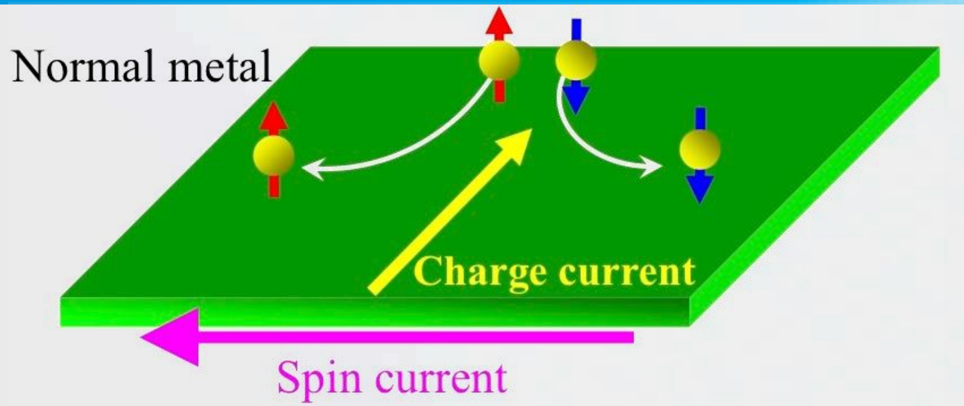


Nitta *et al.*, Phys. Rev. Lett. **78**, 1335 (1997).

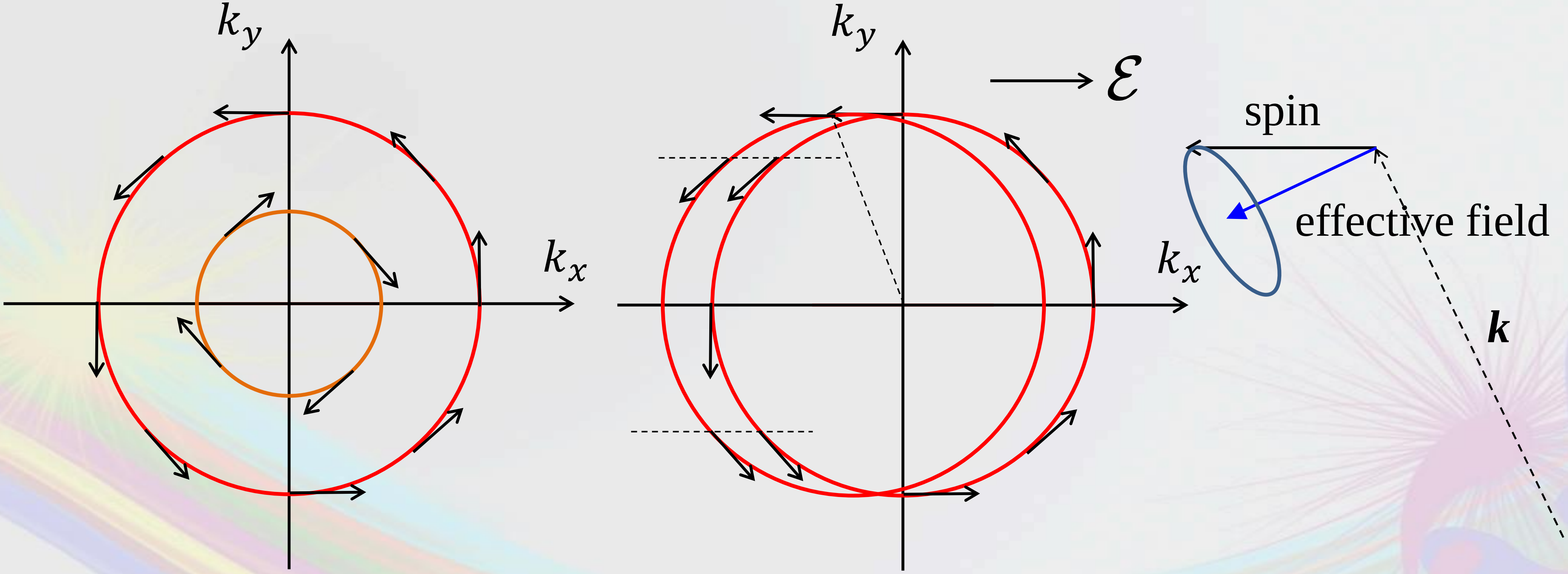
Spin Hall effect

$$J_{ij} = \sigma_s \sum_k \epsilon_{ijk} E_k$$

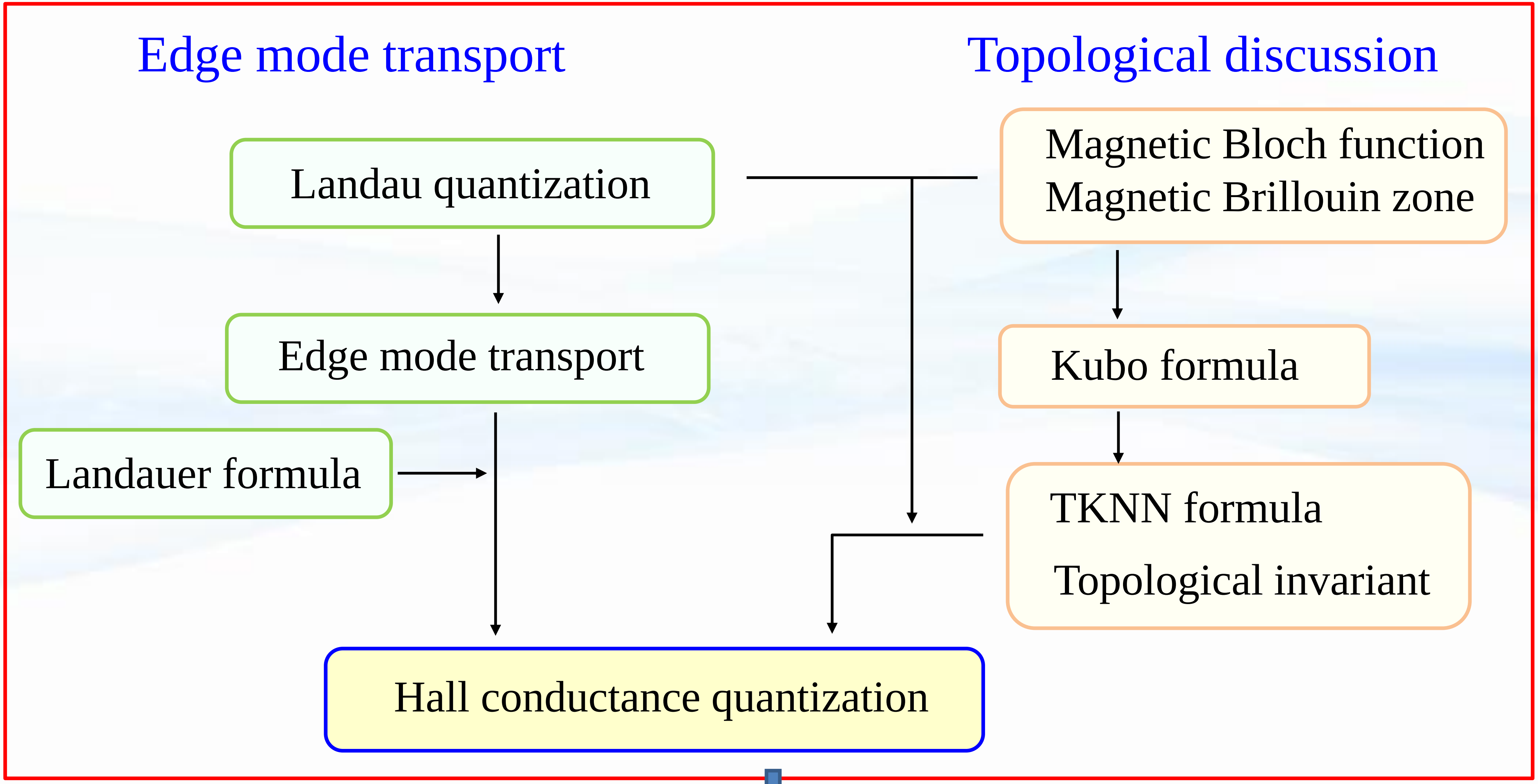
$$\mathscr{H}_{\mathrm{RSO}} = \alpha \boldsymbol{\sigma} \cdot (\boldsymbol{k} \times \boldsymbol{e}_z)$$



Effective magnetic field



How we understand the quantum Hall effect?



Bulk-edge correspondence

Spin Hall effect in an insulator

Remember k·p approximation

$$\mathscr{H}_{\boldsymbol{k}} u_{n\boldsymbol{k}}(\boldsymbol{r}) = E_{n\boldsymbol{k}} u_{n\boldsymbol{k}}(\boldsymbol{r}) \qquad |n\boldsymbol{k}\rangle$$

$$\boldsymbol{A}_n(\boldsymbol{k}) = i\left\langle n\boldsymbol{k}\left|\frac{\partial}{\partial\boldsymbol{k}}\right|n\boldsymbol{k}\right\rangle, \quad \boldsymbol{B}_n(\boldsymbol{k}) = i\left\langle\frac{\partial(n\boldsymbol{k})}{\partial\boldsymbol{k}}\right|\times\left|\frac{\partial(n\boldsymbol{k})}{\partial\boldsymbol{k}}\right\rangle$$

Consider the case these are not zero. Then the discussion is in parallel with the TKNN formula.

$$\langle\boldsymbol{k}|\hat{\boldsymbol{r}}|\boldsymbol{k}'\rangle = (i\nabla_{\boldsymbol{k}} + \boldsymbol{A})\,\delta(\boldsymbol{k}-\boldsymbol{k}')$$

$$\langle\boldsymbol{k}|[\hat{x},\hat{y}]|\boldsymbol{k}'\rangle = (i\nabla_{\boldsymbol{k}}\times\boldsymbol{A})_z\,\delta(\boldsymbol{k}-\boldsymbol{k}') = iB_z\delta(\boldsymbol{k}-\boldsymbol{k}')$$

$$\left\langle\boldsymbol{k}\left|\frac{d\hat{x}}{dt}\right|\boldsymbol{k}'\right\rangle = \left[\frac{\partial E}{\partial k_x} - (\boldsymbol{F}\times\boldsymbol{B})_x\right]\frac{\delta(\boldsymbol{k}-\boldsymbol{k}')}{\hbar},$$

$$\left\langle\boldsymbol{k}\left|\frac{d\hat{k}_x}{dt}\right|\boldsymbol{k}\right\rangle = F_x\frac{\delta(\boldsymbol{k}-\boldsymbol{k}')}{\hbar}$$

Anomalous velocity and quantum spin Hall effect

Wave packet: $f = \sum_{\boldsymbol{k}} a_{\boldsymbol{k}} |\boldsymbol{k}\rangle$ Bloch wave expansion

$$\boldsymbol{F} = -e\boldsymbol{\mathcal{E}}$$

$$\frac{d\boldsymbol{r}_0}{dt} = \boldsymbol{v} = \left\langle f \left| \frac{d\hat{\boldsymbol{r}}}{dt} \right| f \right\rangle = \sum_{\boldsymbol{k}} \frac{\langle f|\boldsymbol{k}\rangle}{\hbar} \left(\nabla_{\boldsymbol{k}} E - \boldsymbol{F} \times \boldsymbol{B}\right) \langle \boldsymbol{k}|f\rangle$$

$$\approx \frac{1}{\hbar} \left(\nabla_{\boldsymbol{k}} E - \boldsymbol{F} \times \boldsymbol{B}\right)\Big|_{\boldsymbol{k}=\boldsymbol{k}_0}$$

Anomalous velocity

$$\frac{d\boldsymbol{k}_0}{dt} = \frac{\boldsymbol{F}}{\hbar}$$

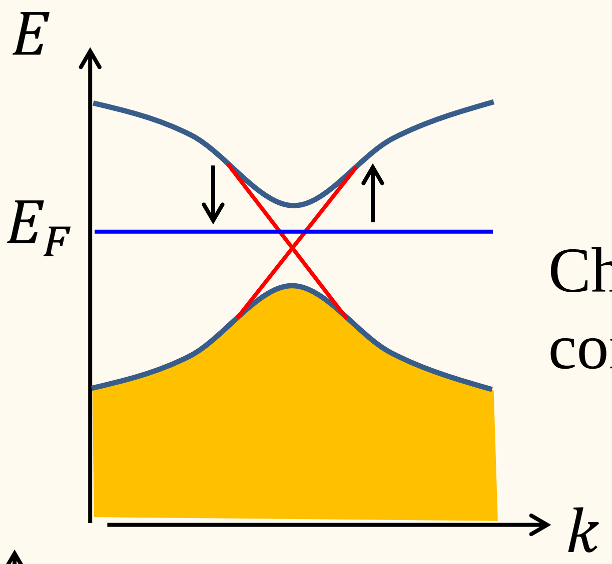
TKNN

$$\sigma_{xy}^{s} = \frac{\hbar}{-2e}\left(\sigma_{xy}^{\uparrow} - \sigma_{xy}^{\downarrow}\right) = \frac{-e}{4\pi}\left(\nu^{\uparrow} - \nu^{\downarrow}\right) = \frac{-e}{4\pi}\nu_{\mathrm{s}}$$

Spin-subband Chern number

Spin Chern number

Topological insulator: helical edge state



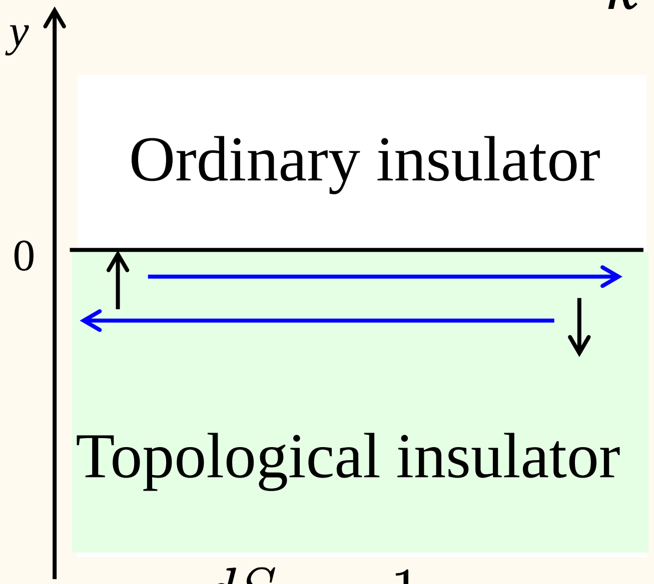
$$j_x^\chi = \Theta(y)\sigma_{xy}^\chi E_y, \quad j_y^\chi = -\Theta(y)\sigma_{xy}^\chi E_x \quad \chi = \uparrow, \downarrow$$

Charge conservation:

$$\frac{d\rho^\chi}{dt} + \nabla \cdot \boldsymbol{j}^\chi = \frac{d\rho^\chi}{dt} - \delta(y)\sigma_{xy}\chi E_x$$

$$= \frac{d\rho^\chi}{dt} - \delta(y)\nu^\chi \frac{e^2}{h} E_x = 0$$

$$\frac{d}{dt}(\rho^\uparrow - \rho^\downarrow) - \delta(y)\frac{e^2}{h}(\nu^\uparrow - \nu^\downarrow)E_x = 0$$



$$\frac{dS_z}{dt} = L\frac{-e}{2\pi}\nu_\mathrm{s} E_x \longrightarrow$$ Extra spin flow at the edge

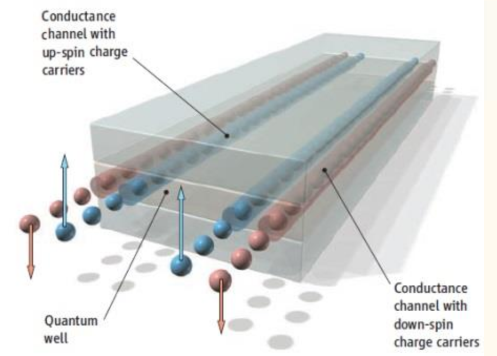
Helical edge mode:

$$E_k^{\uparrow\downarrow} = \pm v(\delta k_x - eE_x t) \quad \uparrow: +, \ \downarrow: -$$

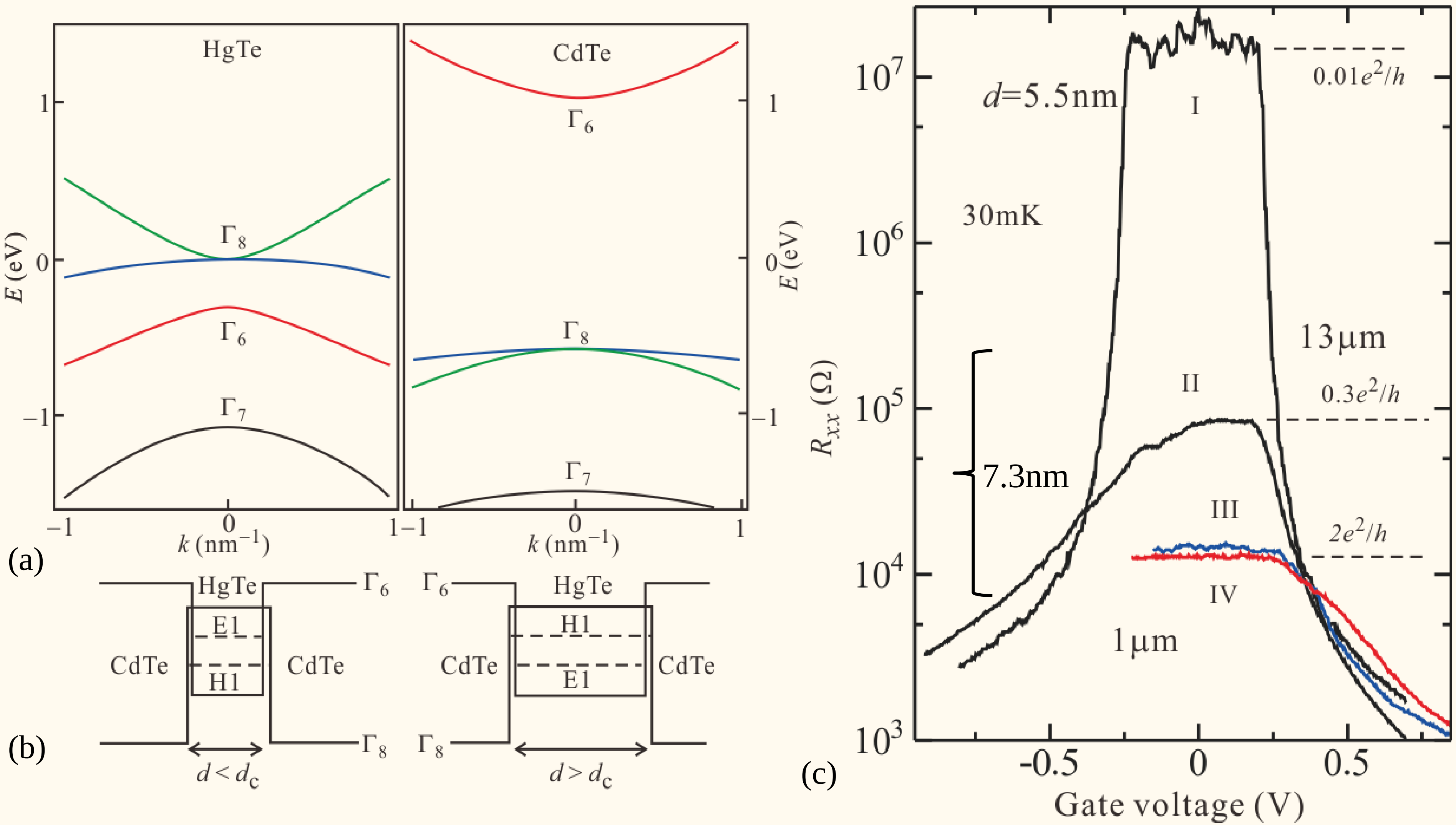
$$\frac{dS_z}{dt} = \frac{1}{2}(\delta N_\uparrow - \delta N_\downarrow) = L\frac{e}{2\pi}E_x$$

Edge mode number = Chern number

Topologically insulating quantum well

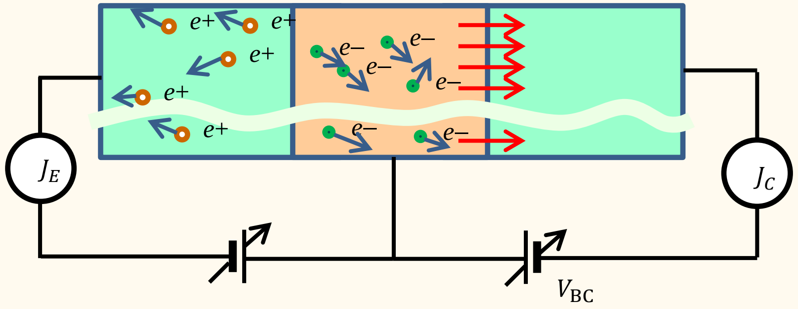


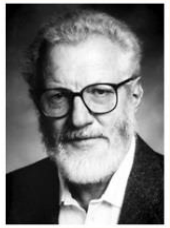
König *et al*., Science **318**, 766 (2007).

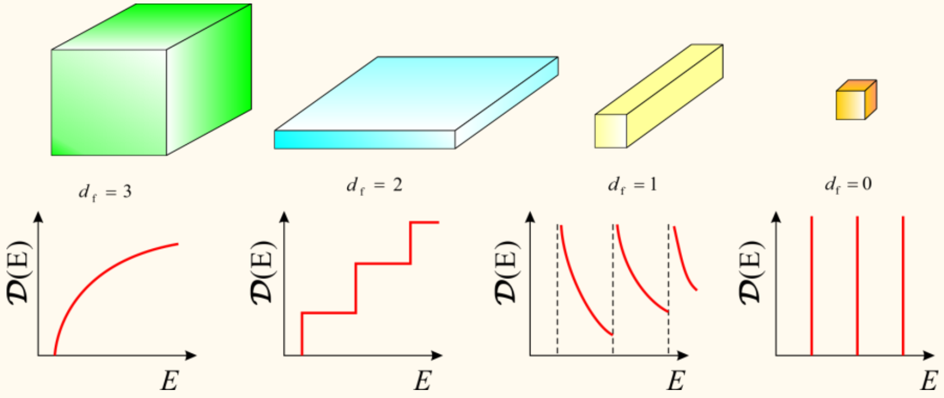


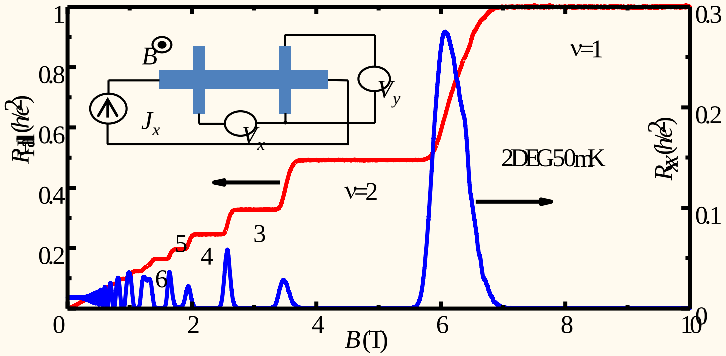
Summary

Charge (kinetic) freedom



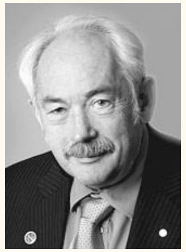




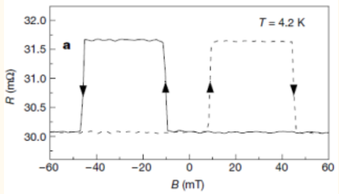


Spin degree of freedom

Giant magnetoresistance
spin valve



Spin injection



Spin-manipulation of
quantum information

Topological insulators