December, 2005
University Lecture
Science of Material

Lecture 6 What is Condensed Matter Physics?

Lecture 7 Quantum Mechanics and Artificial Materials

-- High-tech and the State-of-the-art Physics

Lecture 8 Atom Control and Quantum Control

--Nano-science and Quantum Information

Lecture 9 Diverse Matter and Physical Properties

The University of Tokyo,
The Institute For Solid State Physics

Yasuhiro Iye

Review of Lecture (1)

Atom control and quantum control:

- Observation and manipulation of atoms
  - Scanning probe microscope (STM and AFM)
  - Nanoscience
- Macroscopic quantum phenomenon
  - Quantum statistics
    - Bosons and fermions
    - ^{4}He and ^{3}He
  - Superfluidity of Liquid helium (^{4}He).
  - Bose-Einstein condensation of vapor atom.

Review of Lecture (2)

- Quantum information processing
  - Measurement in quantum mechanics
    - Stern-Gerlach experiment
    - Loss of interference by observation (decoherence)
    - EPR experiment and Bell’s inequality
  - Cryptosystems
    - Keys and encryption
    - Public key encryption and factorization in prime numbers
  - Quantum computers
    - Qubits
    - Quantum gates
  - Quantum cryptosystems (private key distribution)

Today’s Topics

- Properties of electrons in a solid state (band structure)
- Metals, insulators, and semiconductors
- Magnetism
- Superconductivity

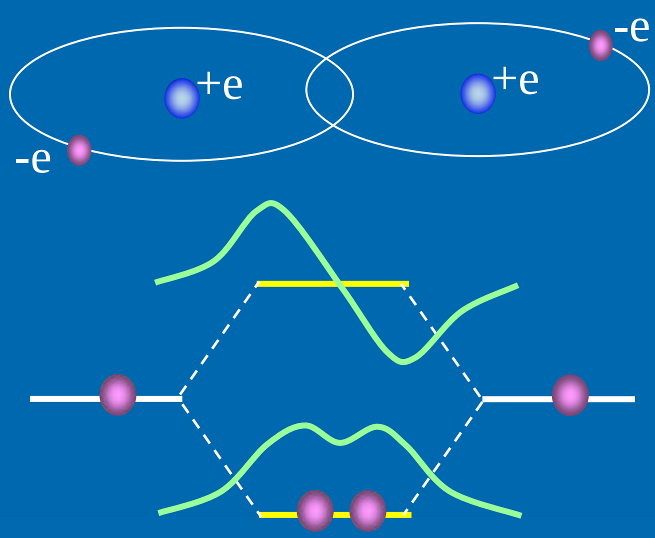
Properties of Electrons in a Solid State (Band Structure)

Properties of Electrons in a Solid State

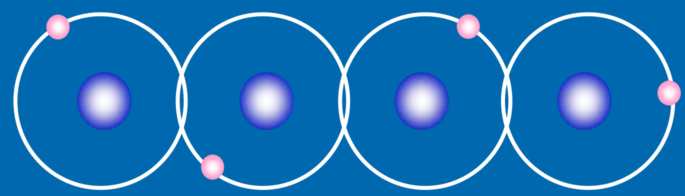
- Quantum mechanically, understand the behavior of electrons found in potential where atoms are arranged periodically.
- Two ways of understanding:
  - Place the atoms in order $\Rightarrow$ tight-binding electron model
  - Start from free space to introduce periodic potential $\Rightarrow$ nearly-free electron model

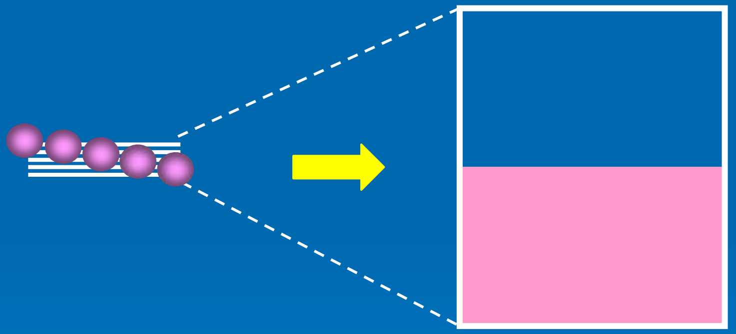
Arrangement of Atoms

Hydrogen molecule：H_2



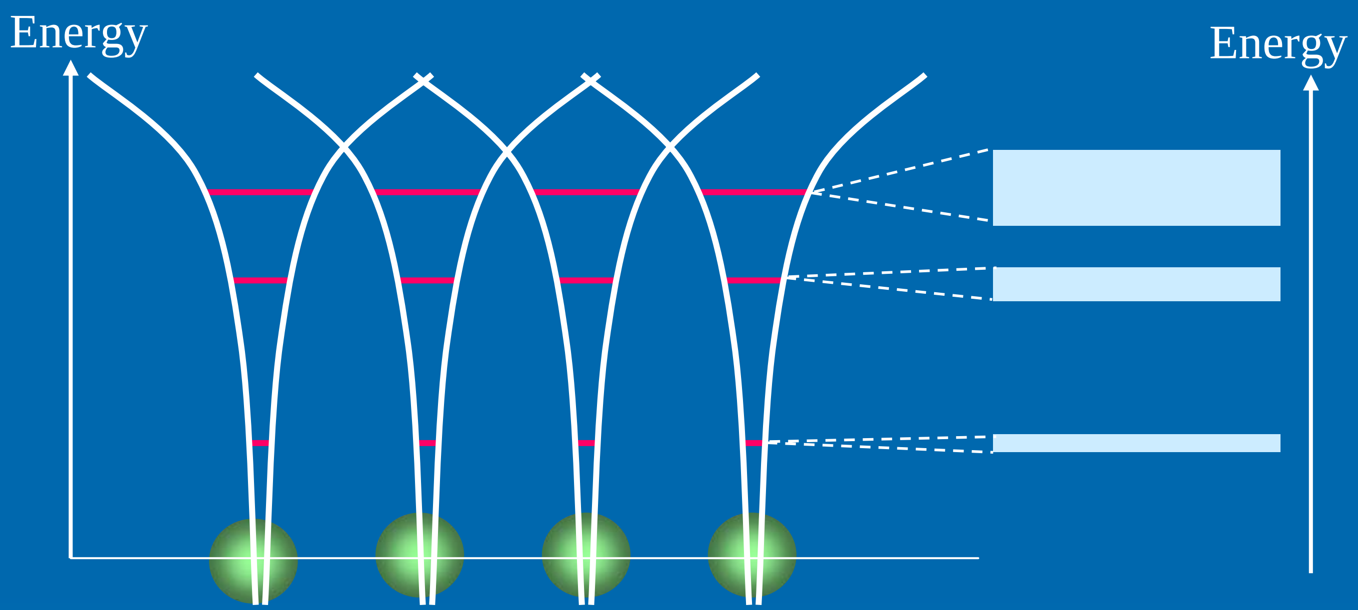
Periodic arrangement of hydrogen atoms





The superpositioning electron cloud in the adjacent atoms may cause electrons to jump between two orbitals; the electrons travel around in the whole crystal.

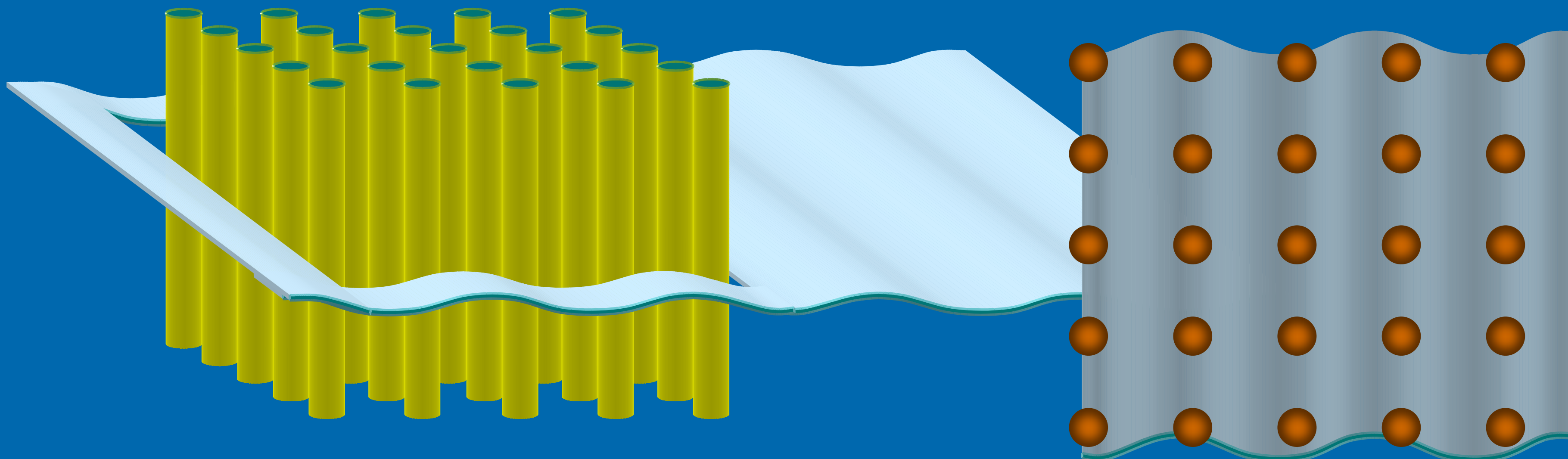
Energy Spreads by “Electron Jumping”



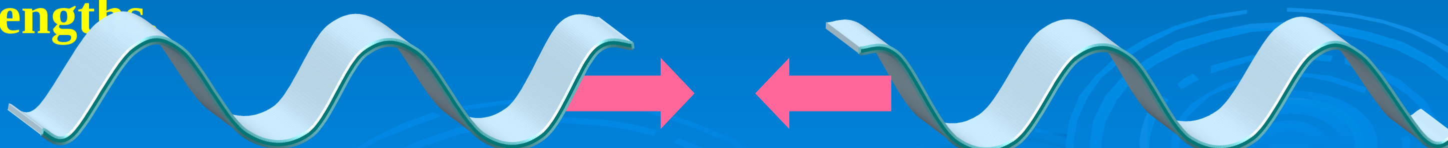
Each energy level of electrons in atoms may spread and form bands; caused by electron jumping.

Scattering of Waves Obtained by Periodic Structure

The waves are lapping against the stakes that are lined up in a pond.

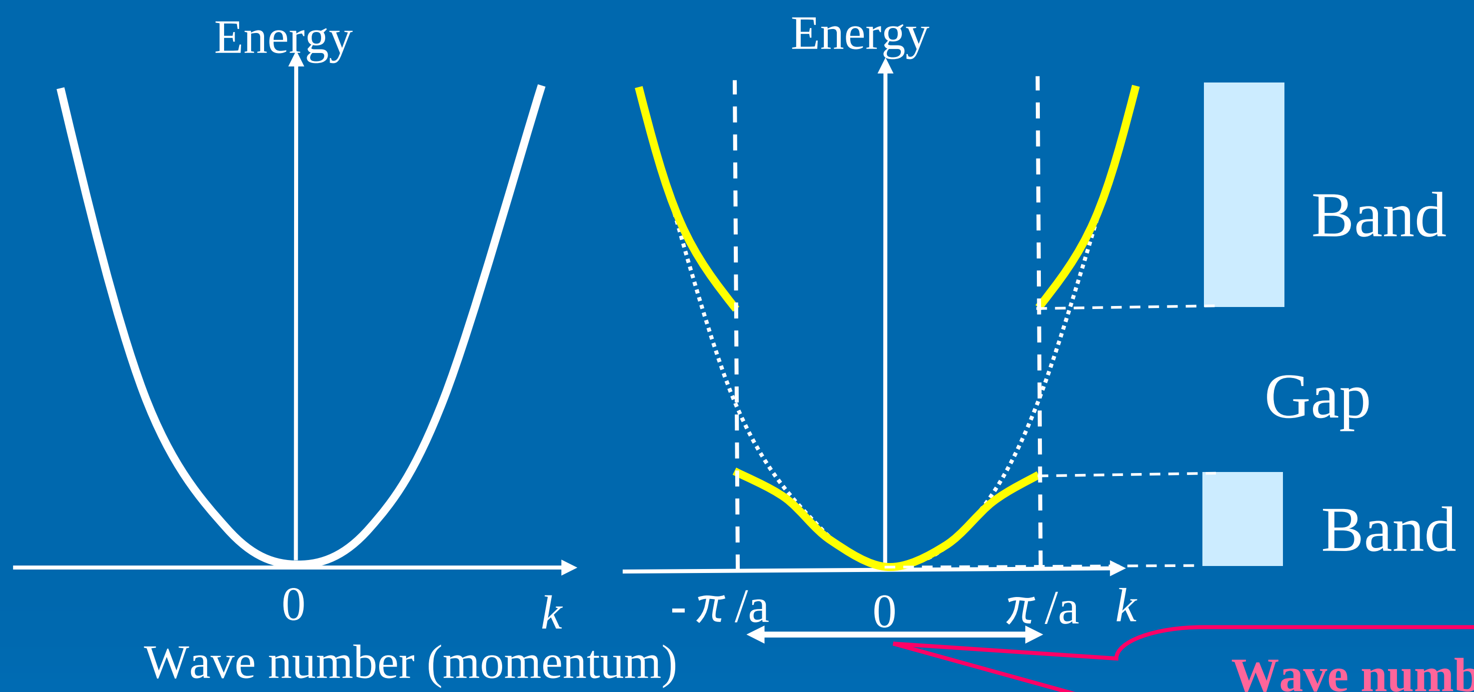


The wavelengths that are integral multiplication of periodic arrangements in the scattering body are reflected strongly (Bragg reflection); the stationary waves are formed by incident waves and reflected waves ⇒ traveling waves cannot be formed from particular wavelengths.



$$e^{i(kx-\omega t)} + e^{i(-kx-\omega t)} = 2e^{-i\omega t}\cos(kx)$$

Formation of Band and Gap via Bragg Reflection

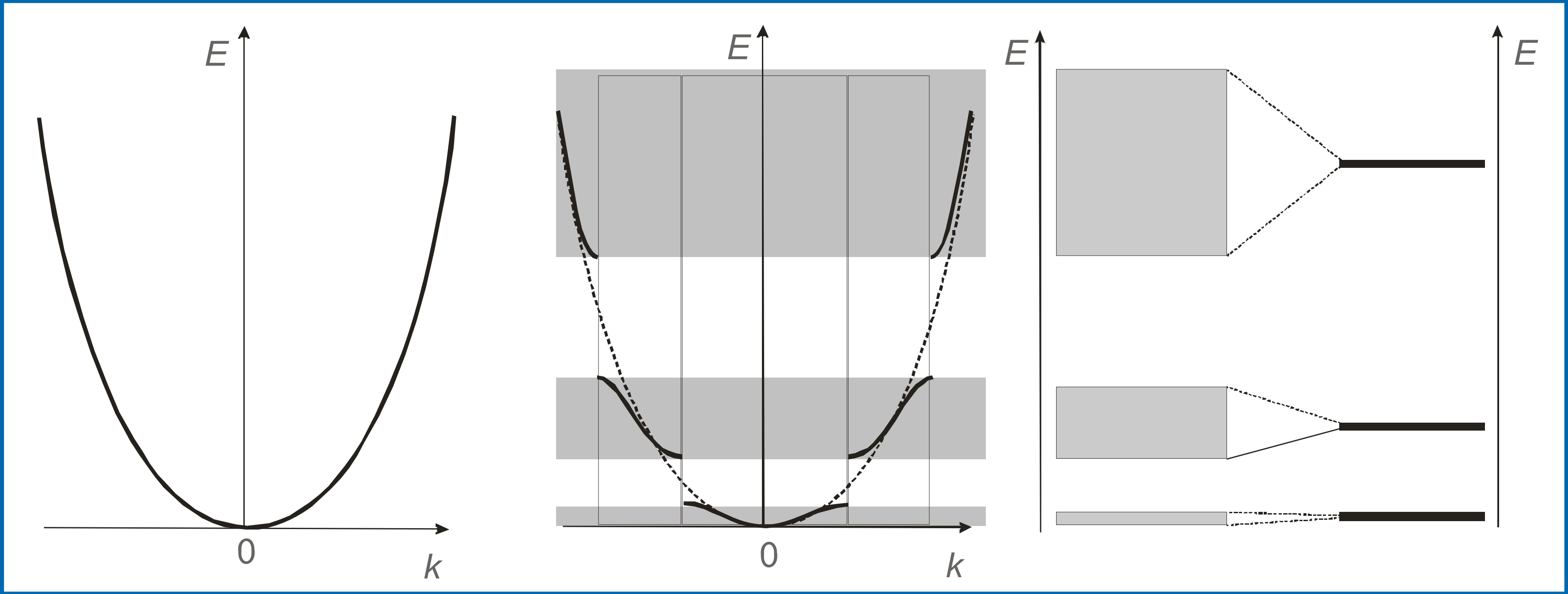


Wave number equivalent to the period.

An electron's existing energy range (band) and absence range (gap) are formed.

The role of periodic potential ⇒to change the dispersion relation between energy and momentum of the electron. (Bloch electron)

Electron Band Structure



Free electron → Electron in crystal (Bloch electron) ← Isolated atom

Near-free electron model

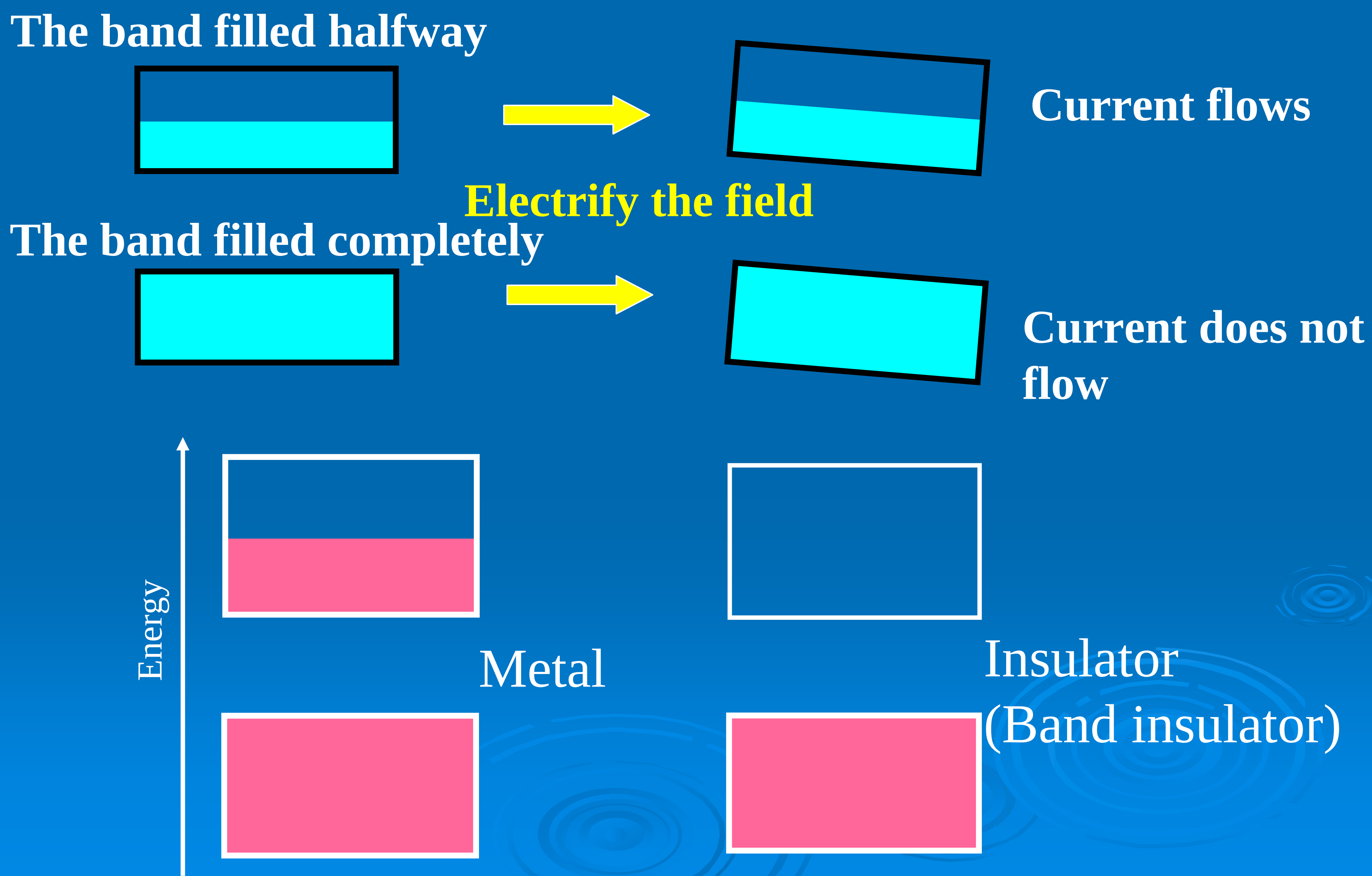
Tight-binding model

Itinerant electron

Localized electron

Metals, Insulators, and Semiconductors

Metals and Insulators

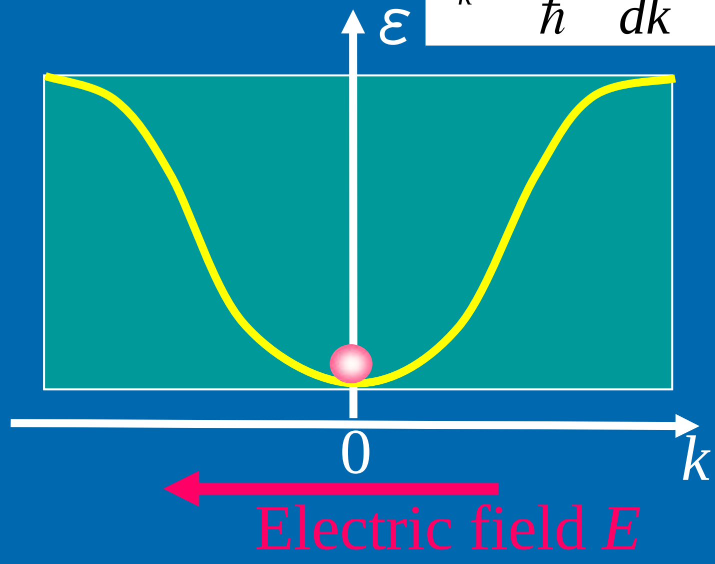


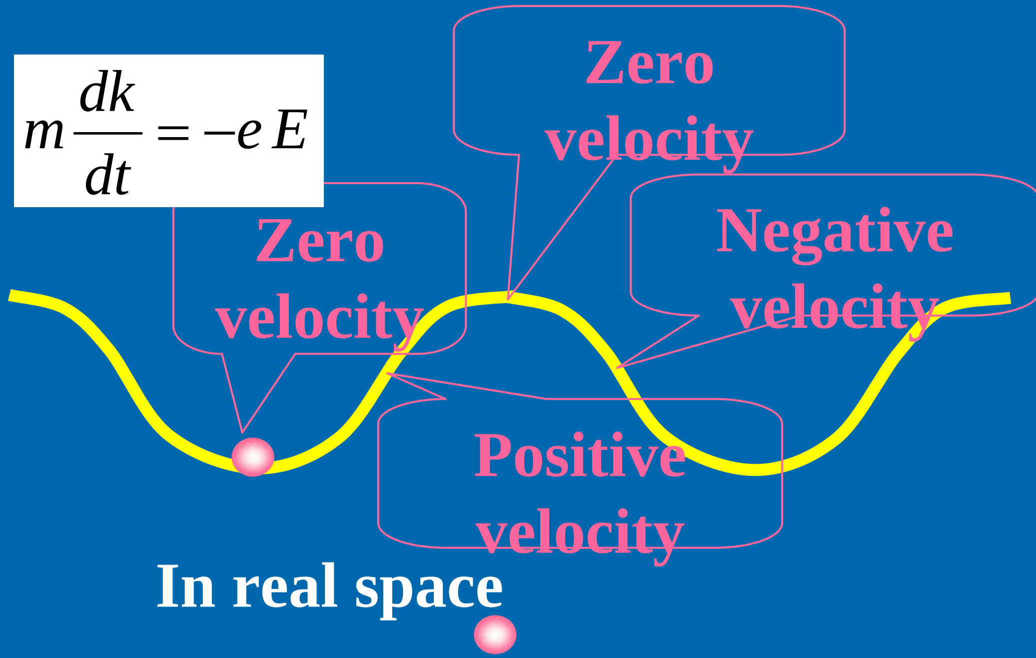
Behavior of Bloch Electrons

Momentum space

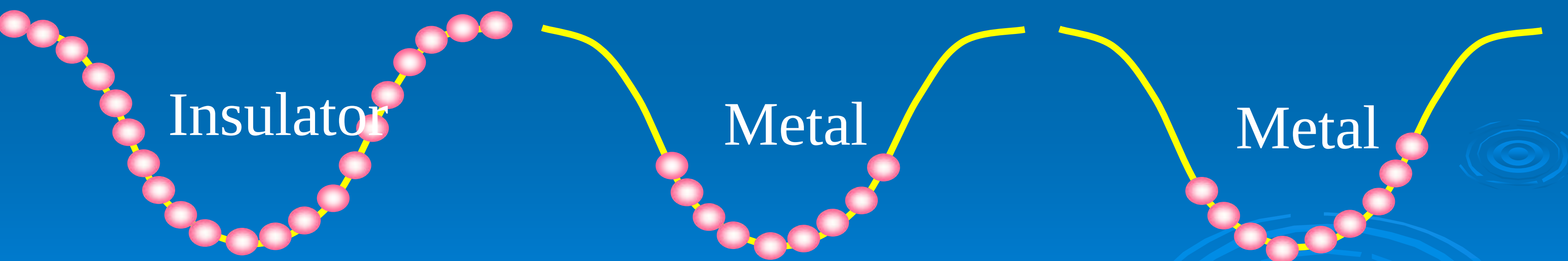
$$v_k = \frac{1}{\hbar}\frac{d\varepsilon(k)}{dk}$$

$$m\frac{dk}{dt} = -eE$$





In real space

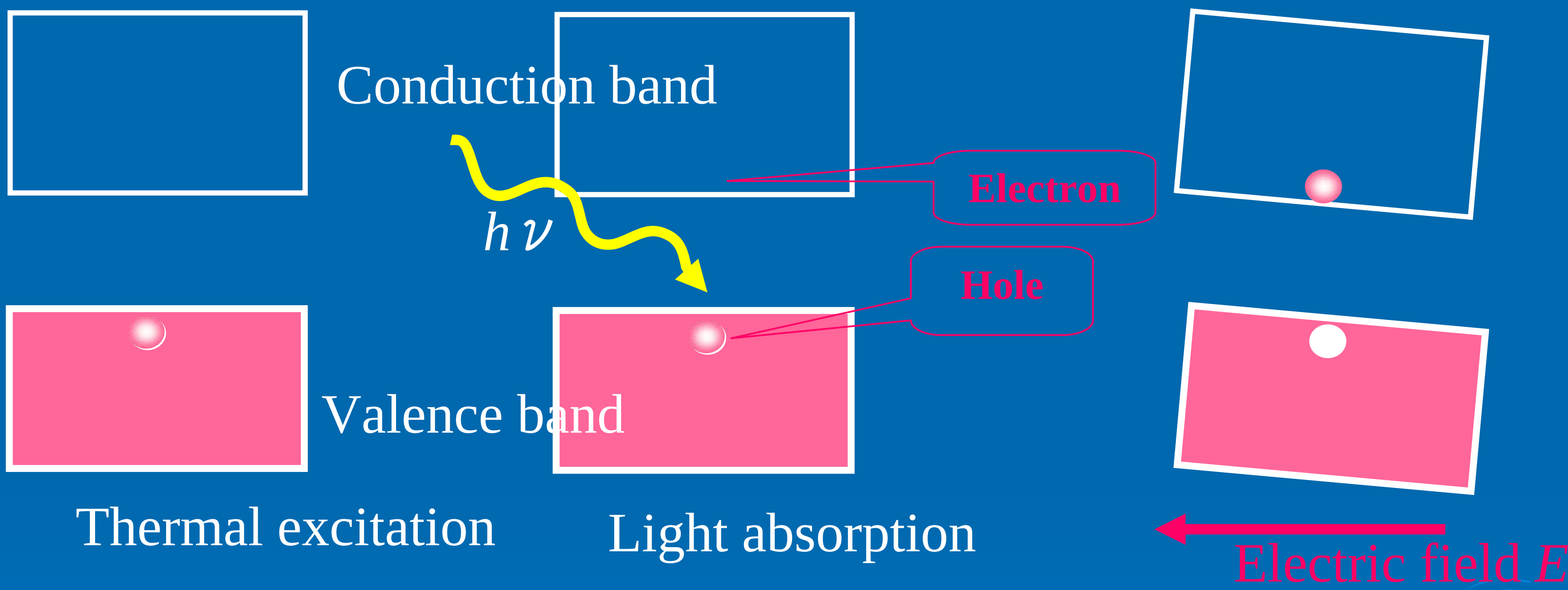


No change in occupying process of electrons in the electric field.

Will electrons simply travel back and forth after scattering disappears completely?

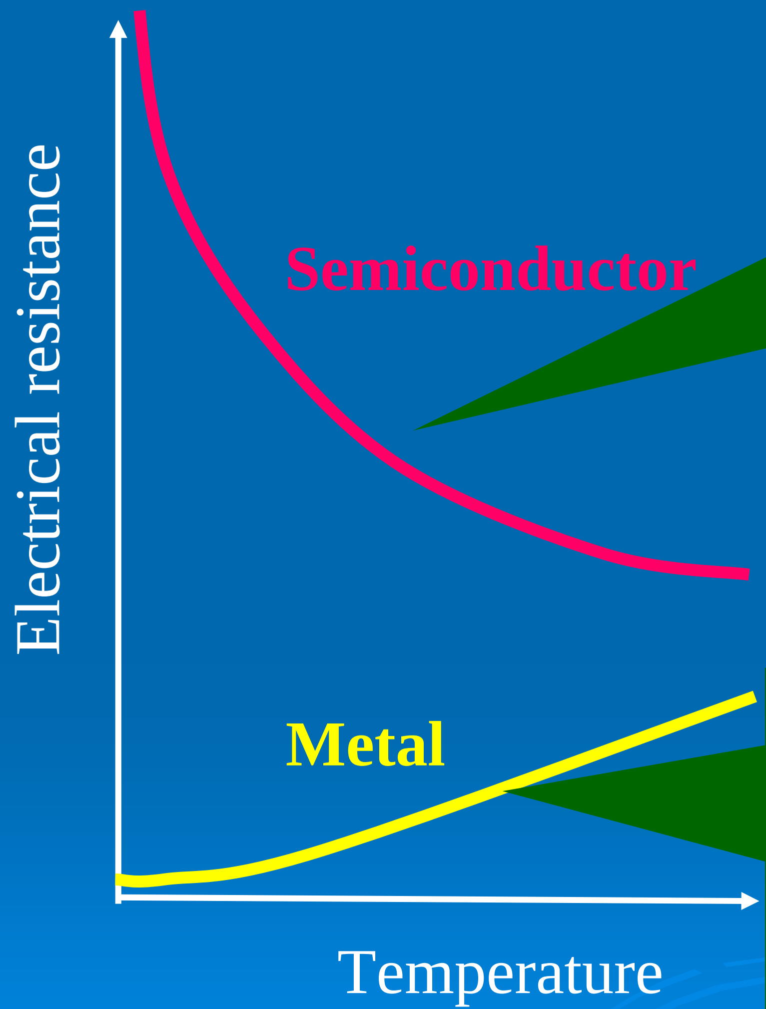
As for existing materials, the state that is slightly off the Fermi surface due to scattering becomes a regular one.

Electrons and Holes in Semiconductors



In semiconductors, a few carries (electrons in conduction bands and holes in valence electrons) generated by thermal excitation or the optical absorption are responsible for electric conduction.

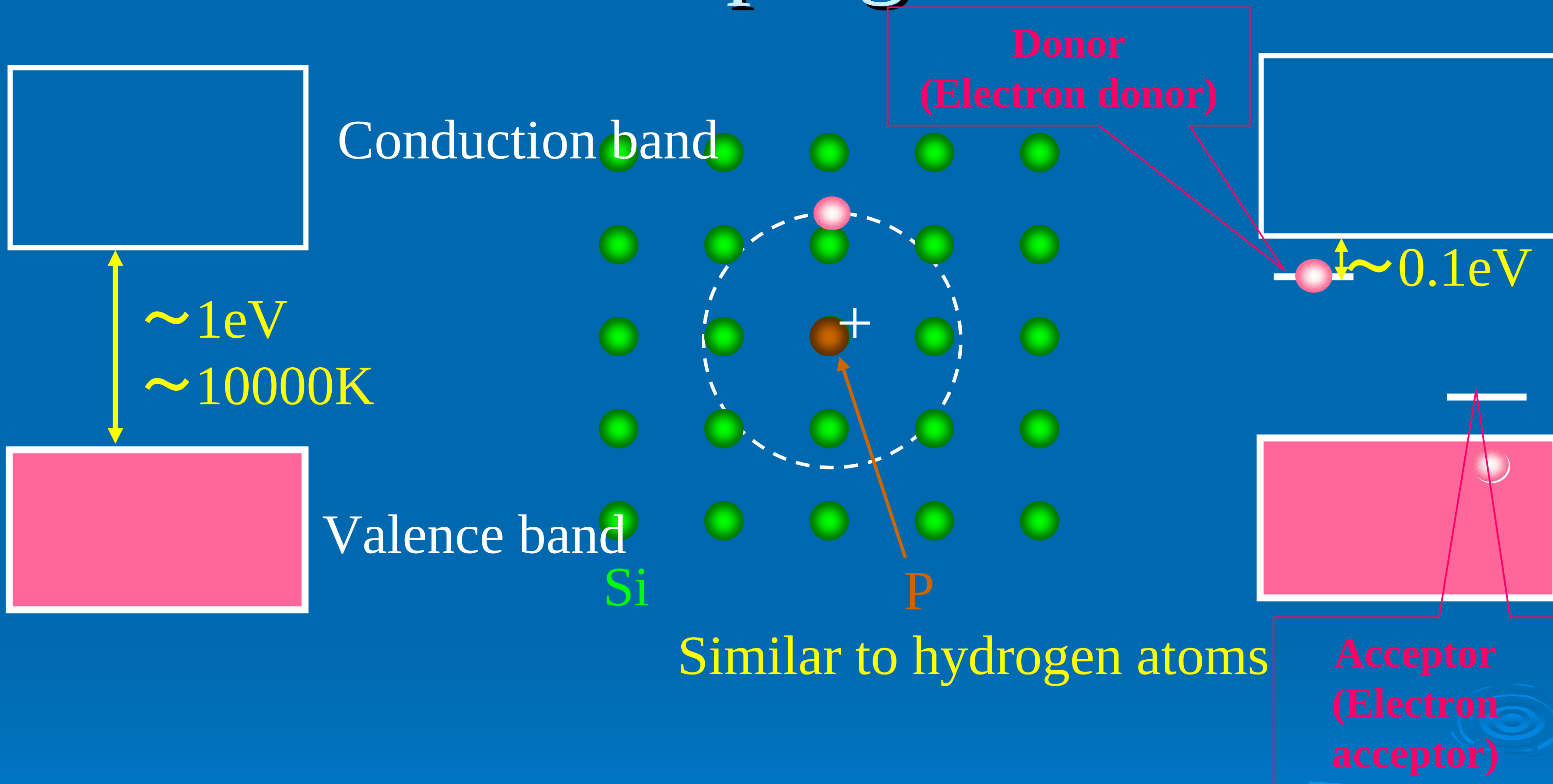
Temperature Change in Electric Resistance



Semiconductors (insulators) have low electric resistance because many carrier electrons and holes are generated by thermal excitation under higher temperatures.

In metals, the number of existing electrons will not be changed by changes in temperature. Under high temperatures, the lattice oscillation causes scattering against electrons. Under low temperature limit, electron scattering is determined by impurities and deficiencies.

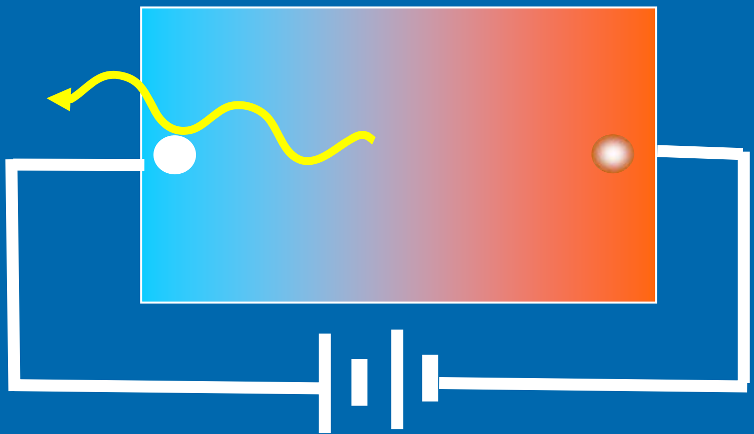
Doping

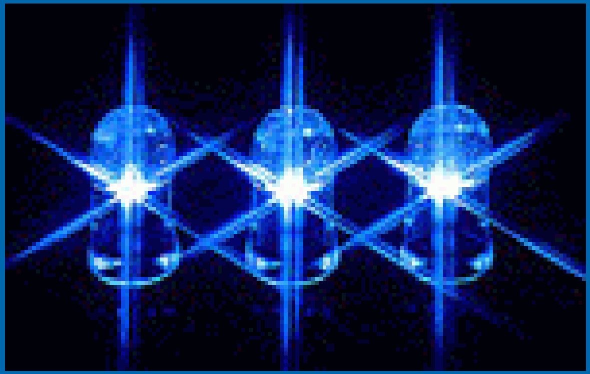


(Electron) donor impurities are added to feed the electrons in the conduction band and are called n-type semiconductors.
(Electron) acceptor impurities are added in order to form holes in the valence band and are called p-type semiconductors.

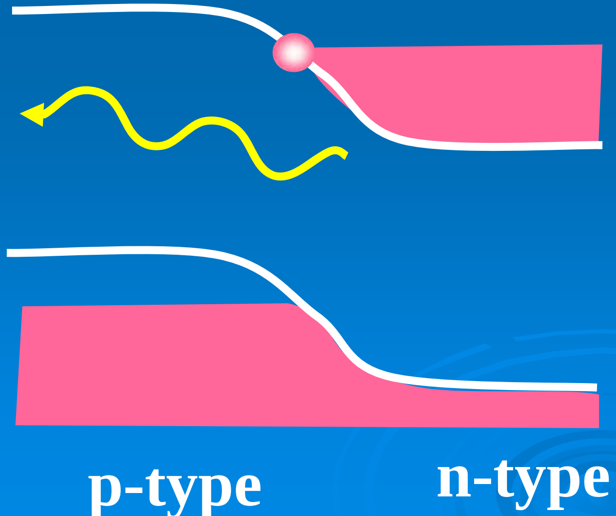
Light Emitting Diode

p-n junction





Light emitting diode

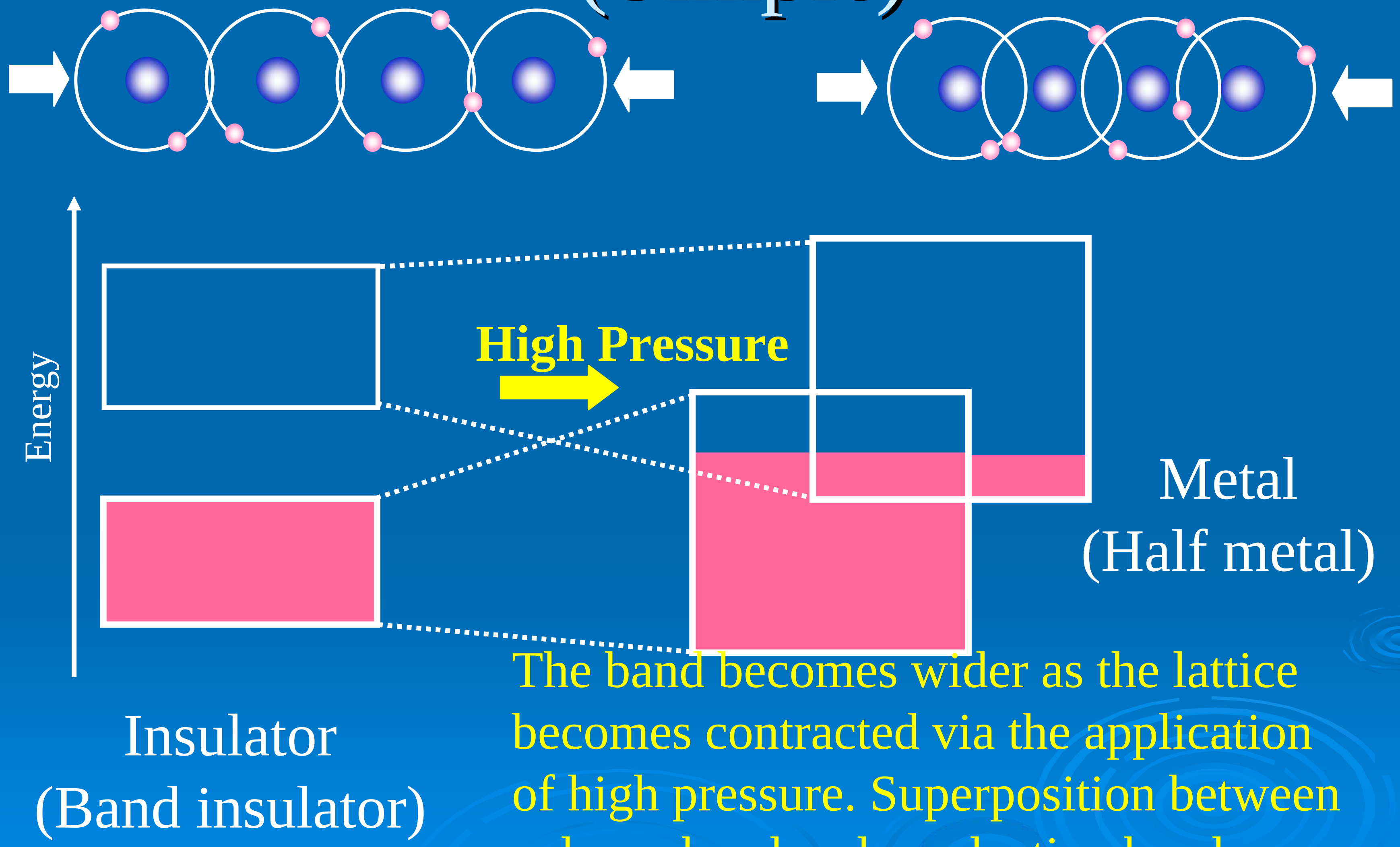


The color of the emitted light is determined by the band gap of the semiconductor.

1eV ～ 3eV

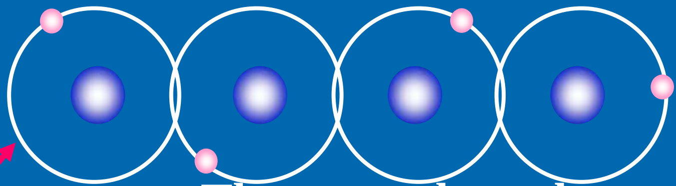
UV ～ Blue

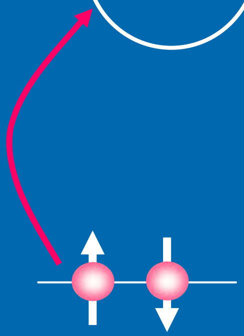
Metal-insulator Transition (Simple)



The band becomes wider as the lattice becomes contracted via the application of high pressure. Superposition between valence band and conduction band occurs. (Energy gaps are closed.)

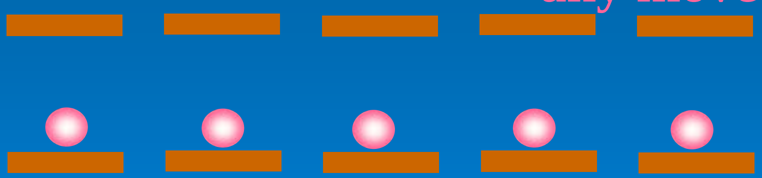
Mott Insulators





The state where there are two electrons occupying the same orbit, the energy is increased by the amount of interelectron Coulomb repulsion ***U*** **.**

When the number of children and the number of beds are equal **⇒cannot make any move**

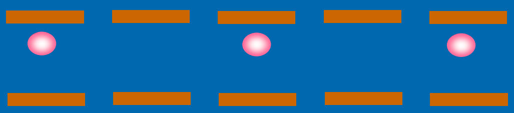


In order for there to be a movement, the electrons have to climb onto the upper bunk.

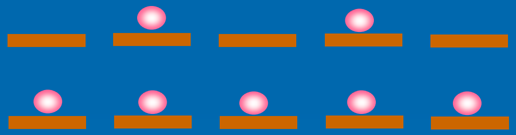
Children play on bunk beds:

The children who show up later have to go to the upper bunk to play.

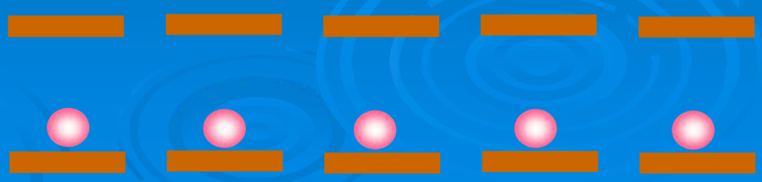
When number of children is less than the number of beds:



When number of children is greater than the number of beds:



Mott insulator



Strongly-Correlated Electron Systems

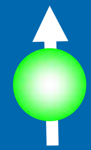
- System in which the strong Coulomb interaction of electrons governs the behavior of the electron, e.g., the Mott insulator, is called a strongly-correlated electron system.
- Many dynamic phenomena such as high-temperature superconductivity and giant magneto-resistance effects take place in strongly-correlated electron systems.
- The behavior of strongly-correlated electron systems is an intrinsically complicated many-body problem, which many physicists are currently working to understand its physical nature.

Magnetism

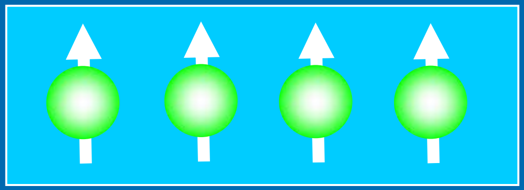
Ferromagnetism

In order for a material to hold the properties of a magnet (ferromagnet):

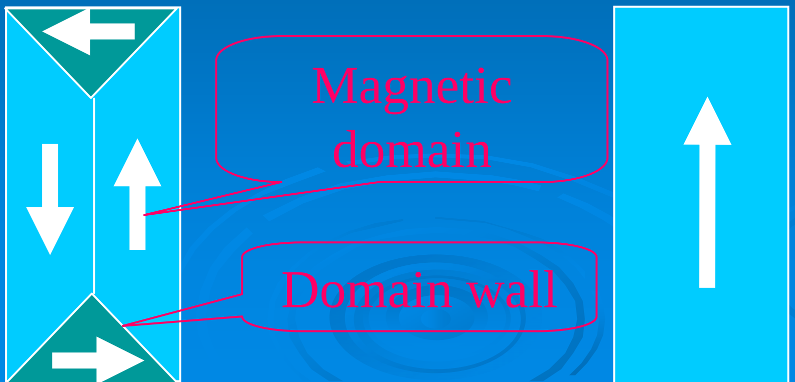
（1）Atoms or molecules must have a magnetic moment (micro-magne



（2）Those magnetic moments are aligned in the same direction.

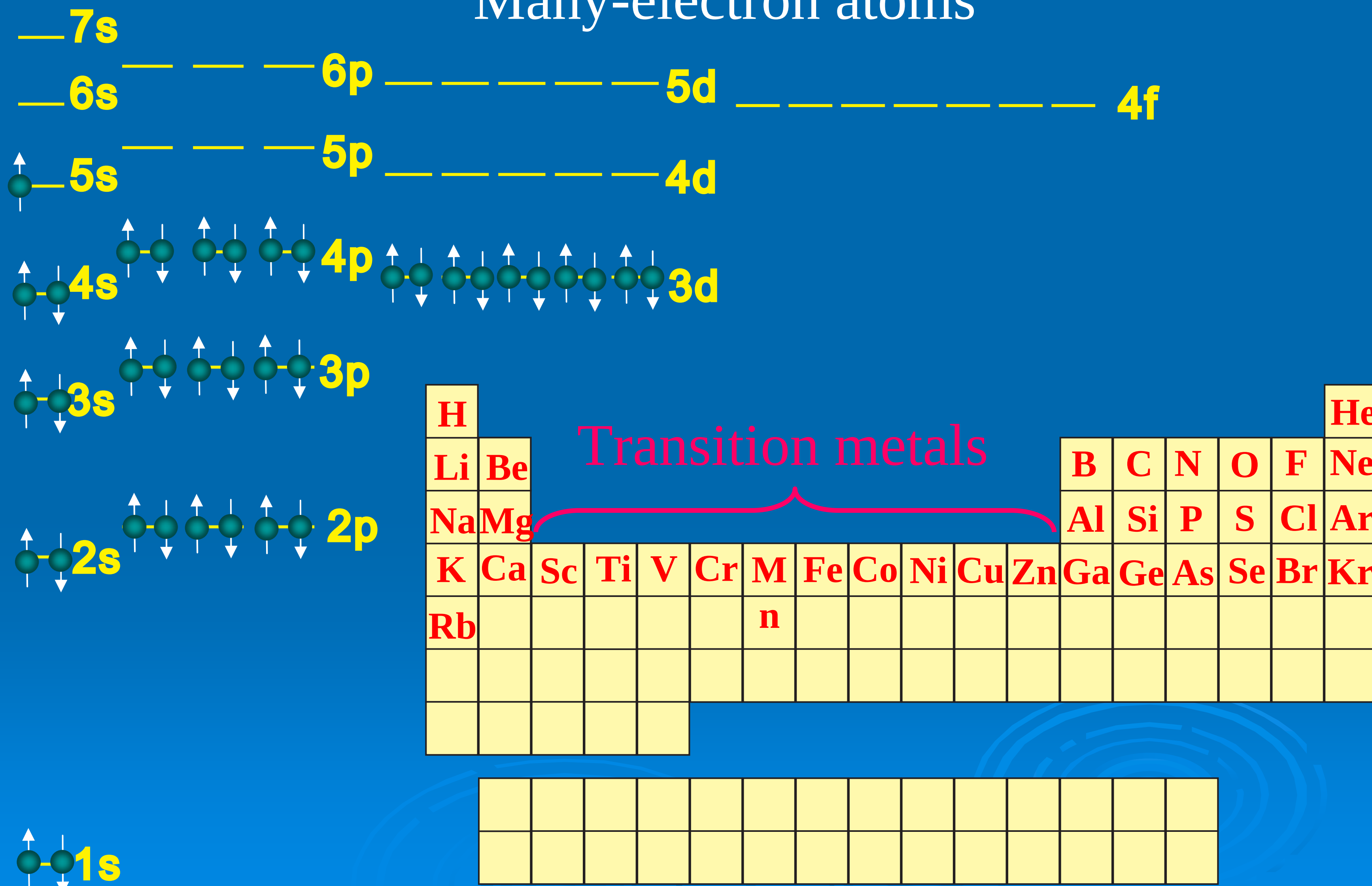


（3）Macroscopic sample possesses entire magnetization.



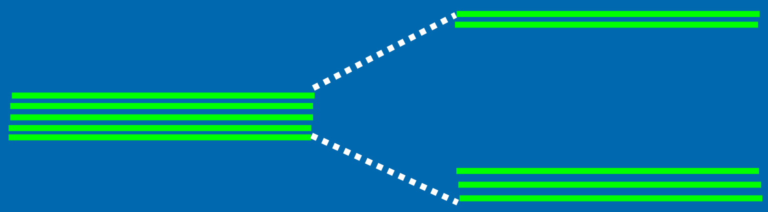
Occupying Process of Electron Energy Levels

Many-electron atoms



Magnetic Moments in Atoms (Ion and Molecule)

d-orbital in atoms
The spin ↑ and spin ↓ have five rooms in each.

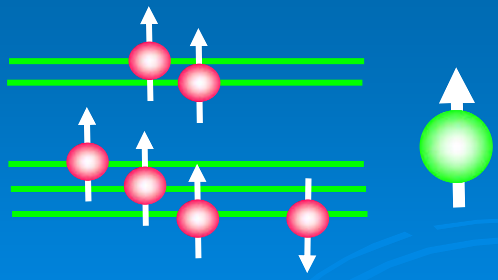


The five energy levels may split depending on their environment (crystal field).

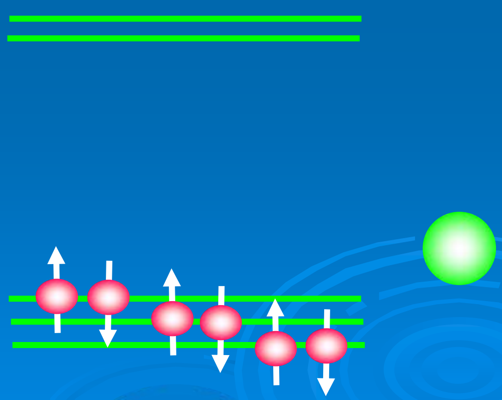
How are the electrons filled here?

To avoid interelectron Coulomb repulsion as much as possible, the electrons should be aligned in the same spin direction. (Hund’s Rule)

Fe^{2+}(six d electrons example)



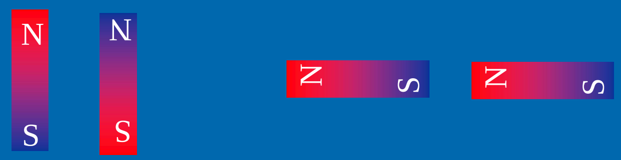
Relatively small split



Large split

Alignment of Magnetic Moments in Atoms

What is the aligning force of the atom's magnetic moment?



~~Is it the magnetic dipole interaction In classical electromagnetism?~~

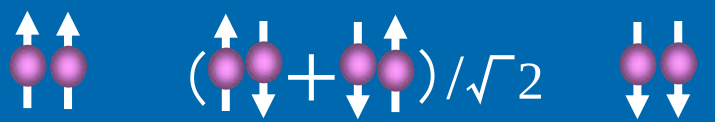
Too weak as the interaction (energy<1K)

Quantum-mechanical effect

Exchange interaction

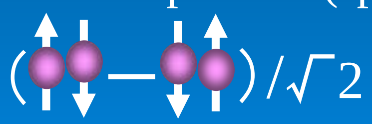
(difference of Coulomb interactions due to spin direction)

Two spins are in parallel (spin-triplet term)



Difference in Coulomb interaction energy (exchange interaction)

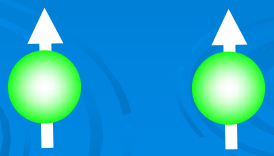
Two spins are antiparallel (spin-singlet term)



$$\text{Energy} = -J\,\mathbf{s}_1 \cdot \mathbf{s}_2$$

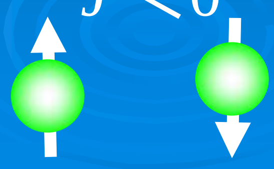
Ferromagnetic

$J > 0$

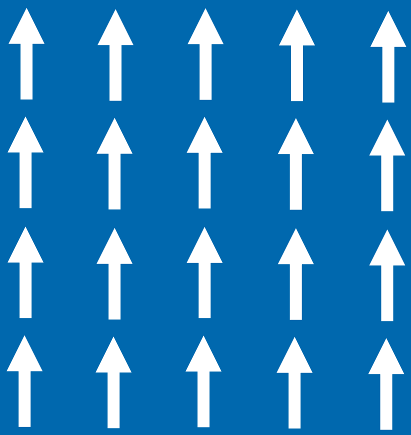


Antiferromagnetic

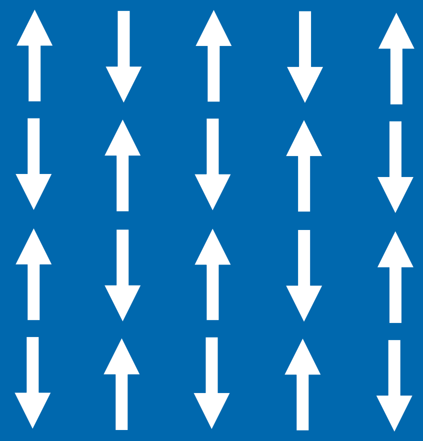
$J < 0$



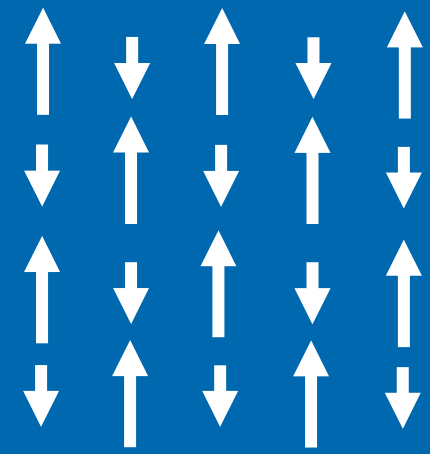
Varieties of Magnetic Bodies



Ferromagnetic
(Includes macroscopic Magnetization.)

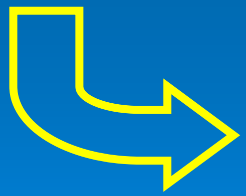


Antiferromagnetic
(No macroscopic magnetization.)

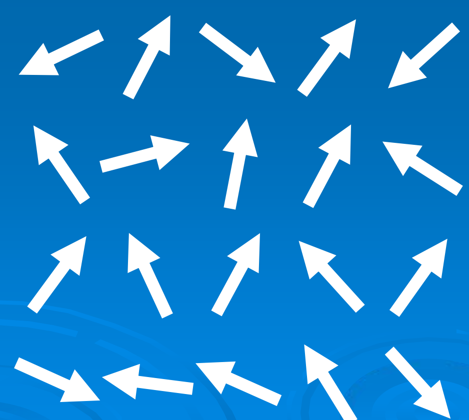


Ferrimagnetic
(Includes macroscopic Magnetization.)

Ordered state



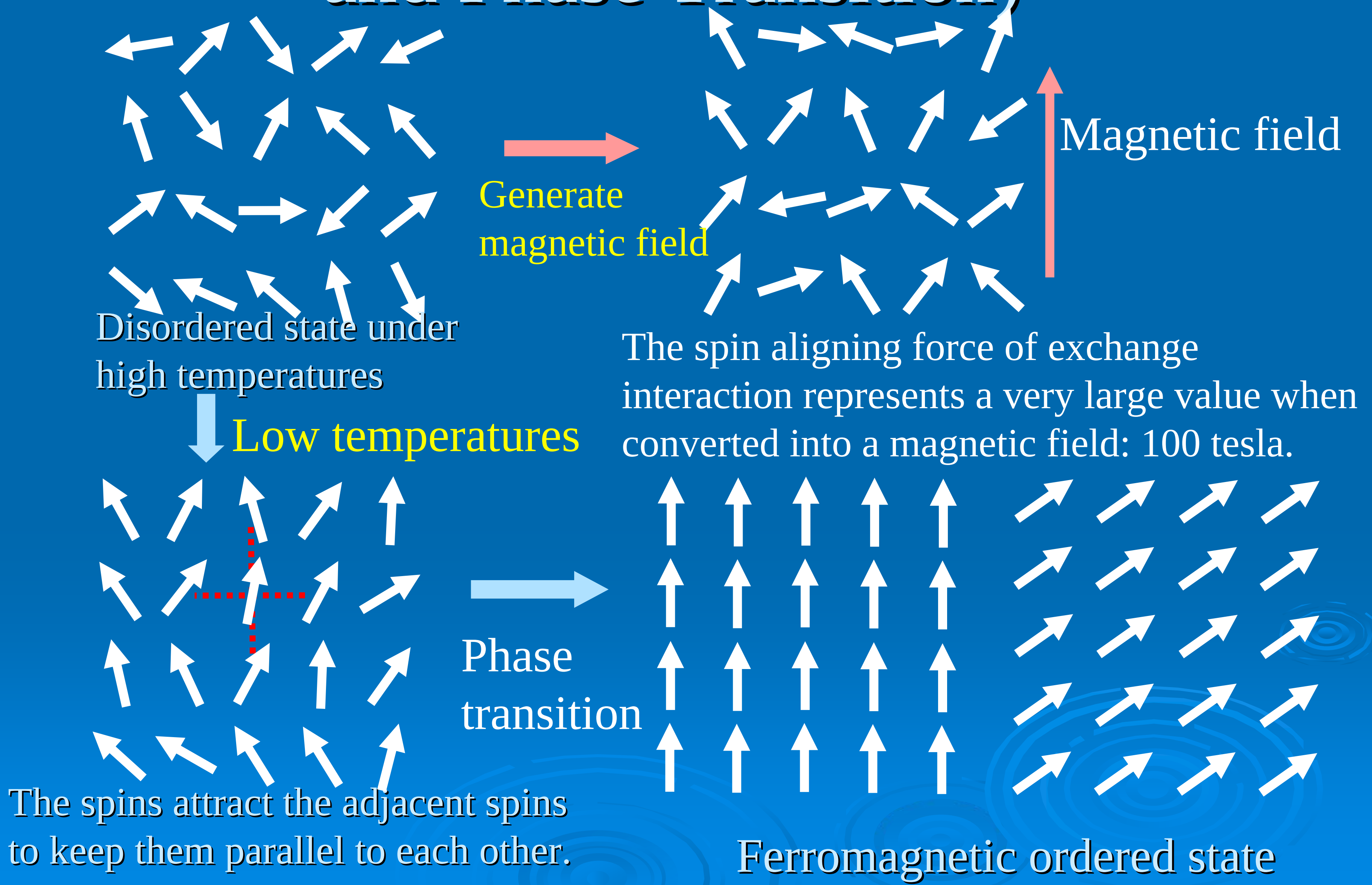
Under high temperatures



Disordered state

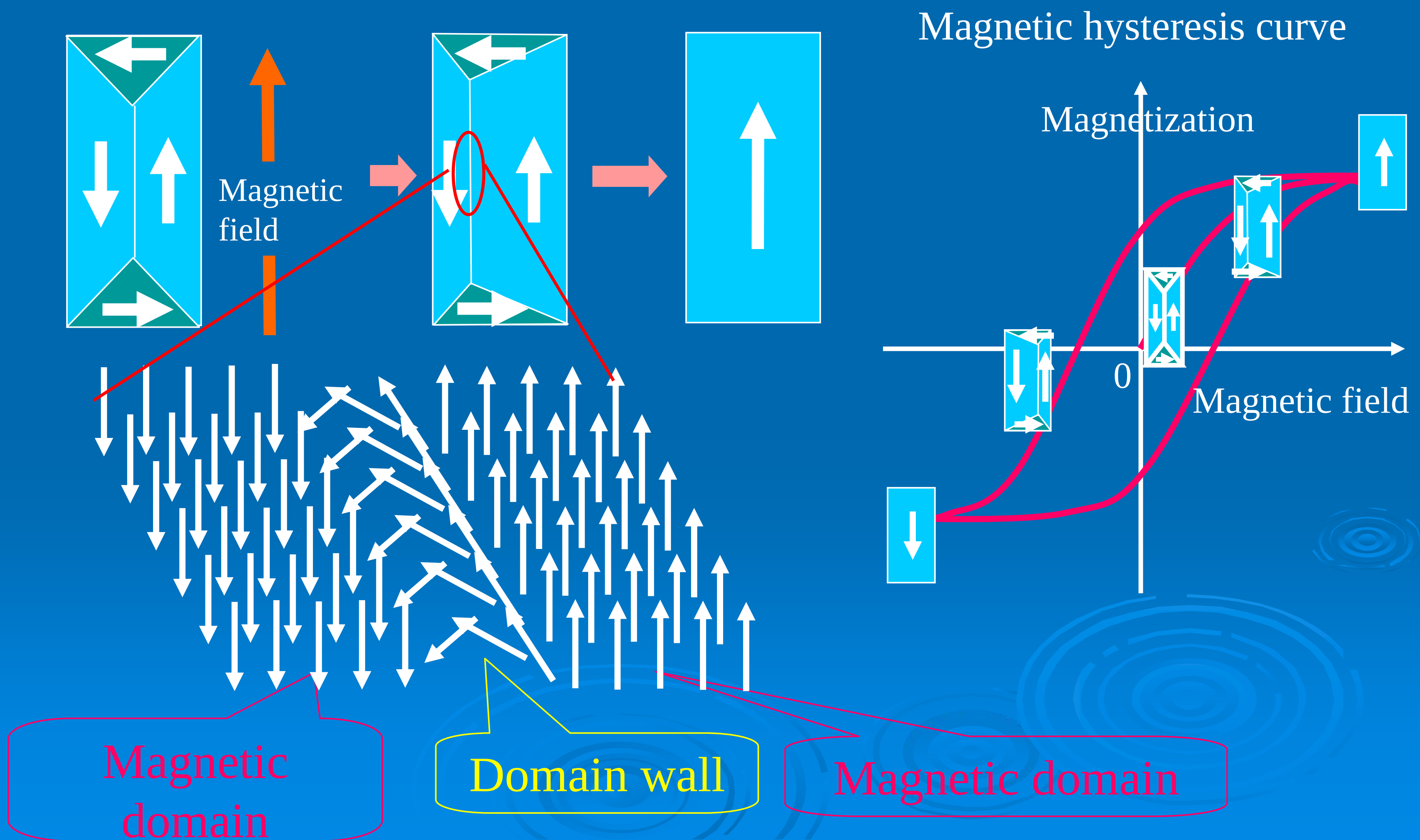
Paramagnetic (No macroscopic magnetization.)

Magnetic Order (Corporative Phenomenon and Phase Transition)



Magnetic Domains and Domain Walls

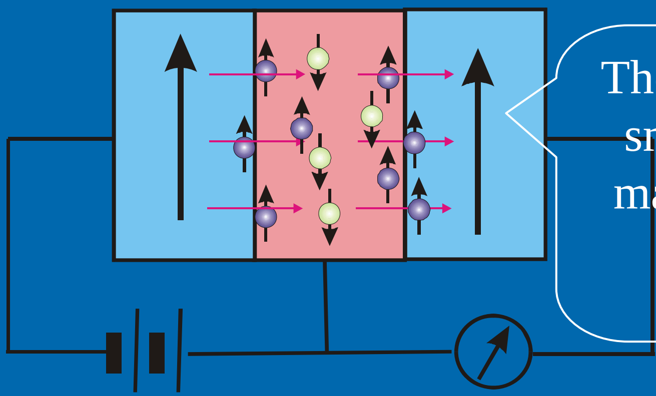
Magnetizing process of ferromagnetic bodies



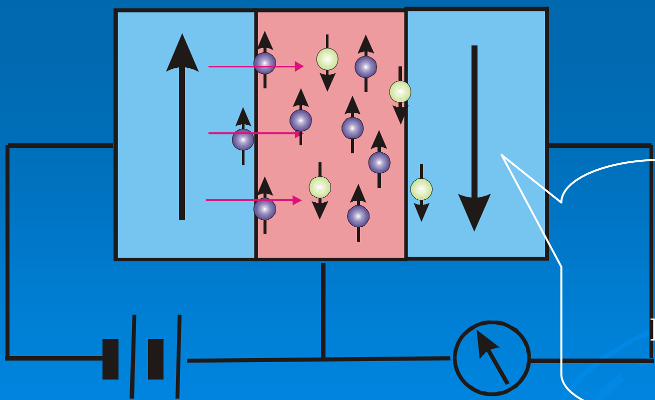
Spintronics

Electronics: takes advantage of the freedom in electron charges.
Spintronics: takes advantage of both the freedom in electron charges and in spin.

Spin-valve device

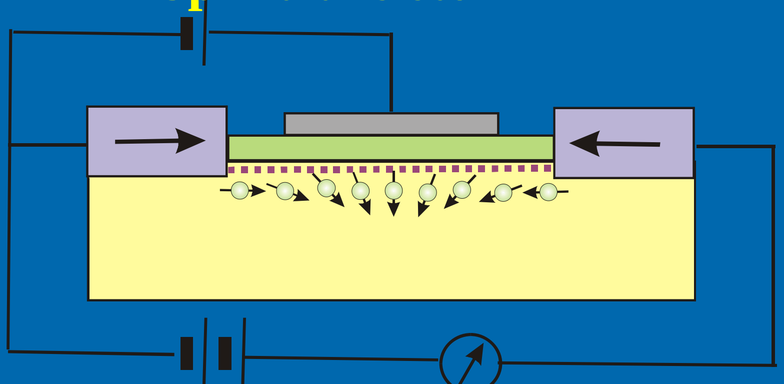


The current flows smoothly when magnetization is in the same direction.

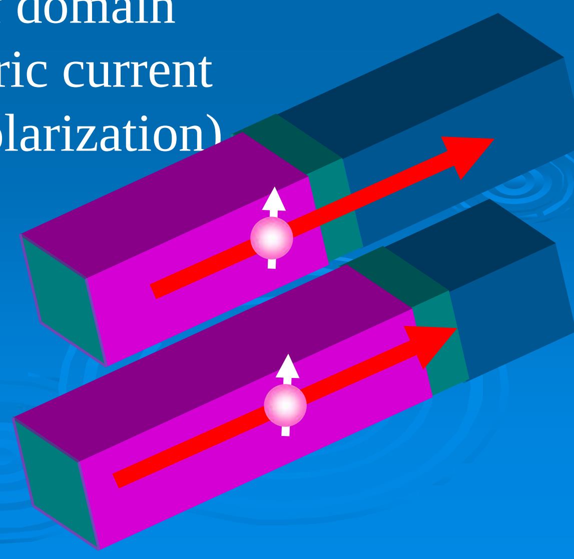


The current flows less smoothly when magnetization is in the opposite direction.

Spin transistor



Activation of domain wall by electric current flow (spin polarization)



Superconductivity

Superconductivity of Elements

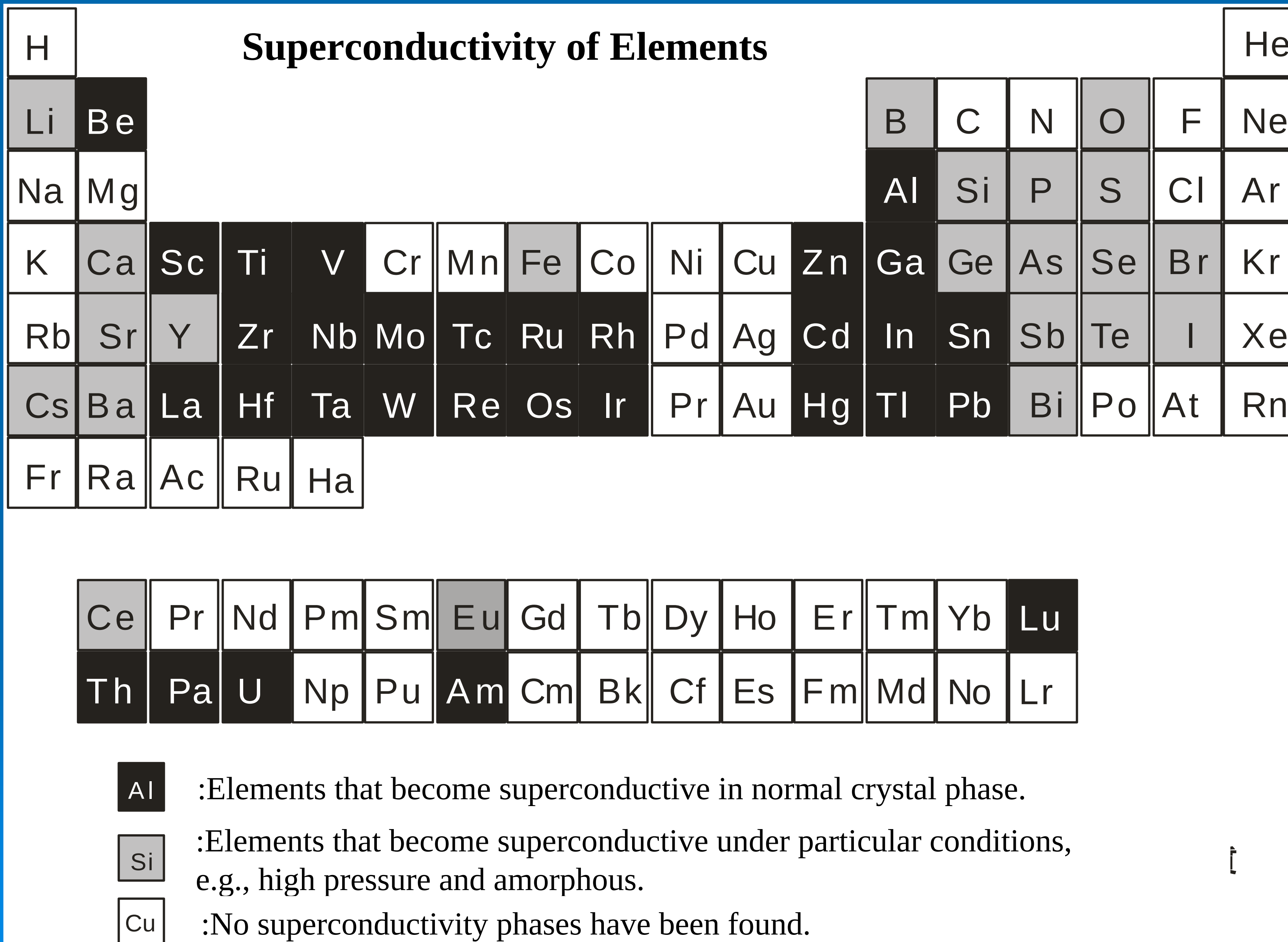
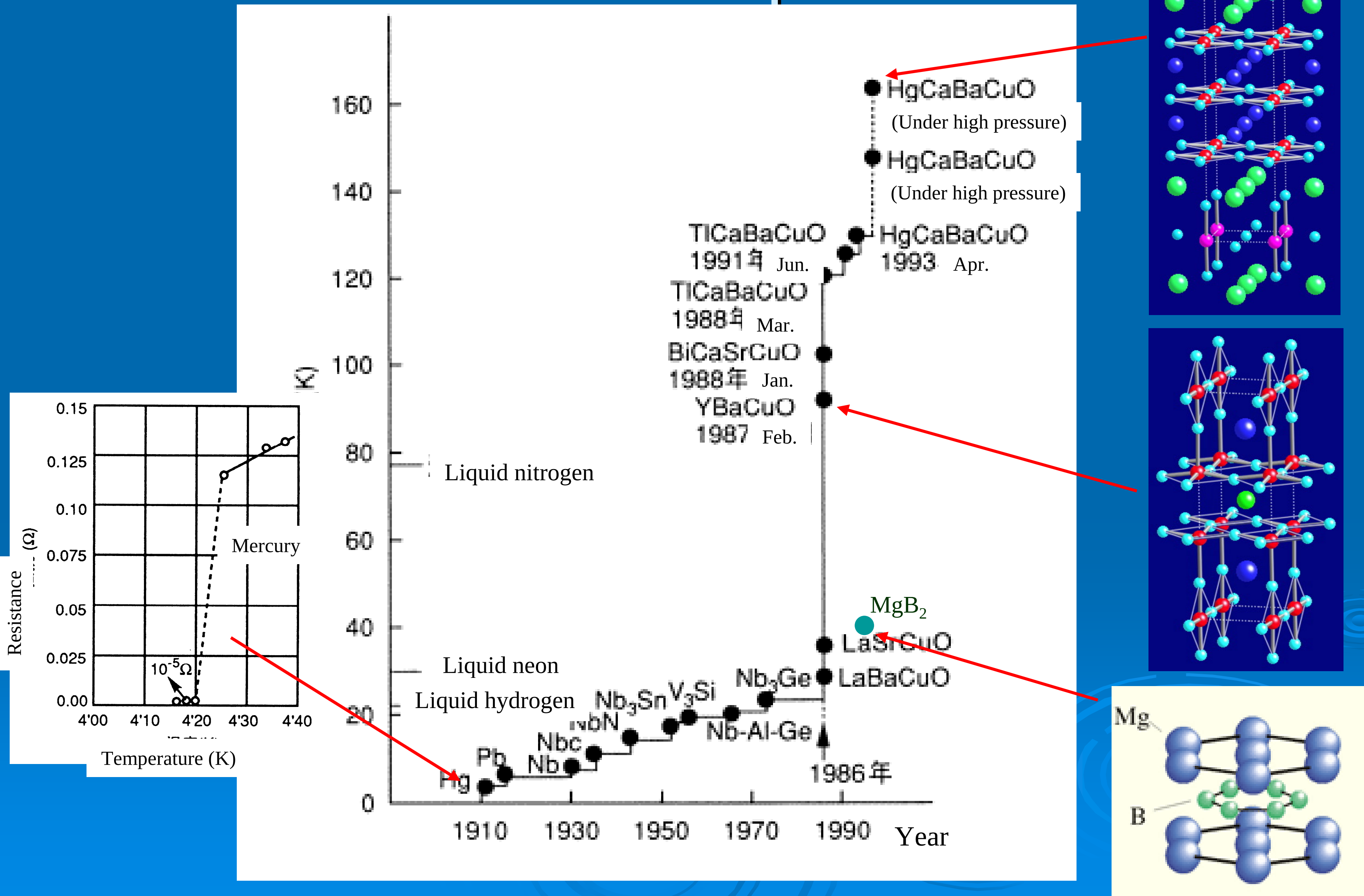
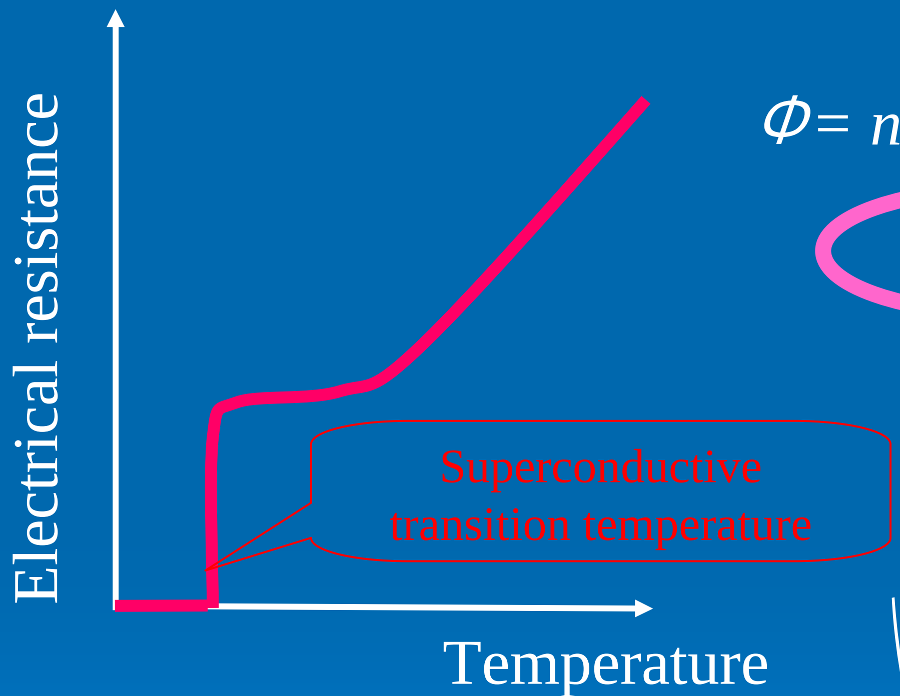


Diagram of Superconducting Transition Temperatures

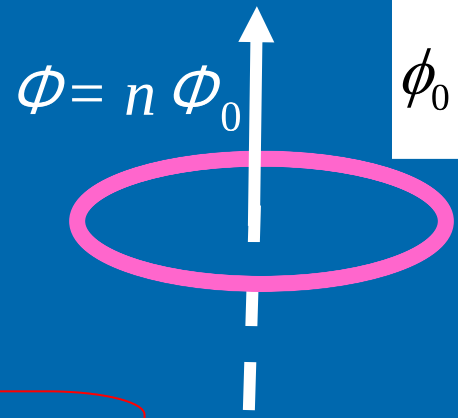


Basic Properties of Superconductivity

Perfect conductor (zero resistance)

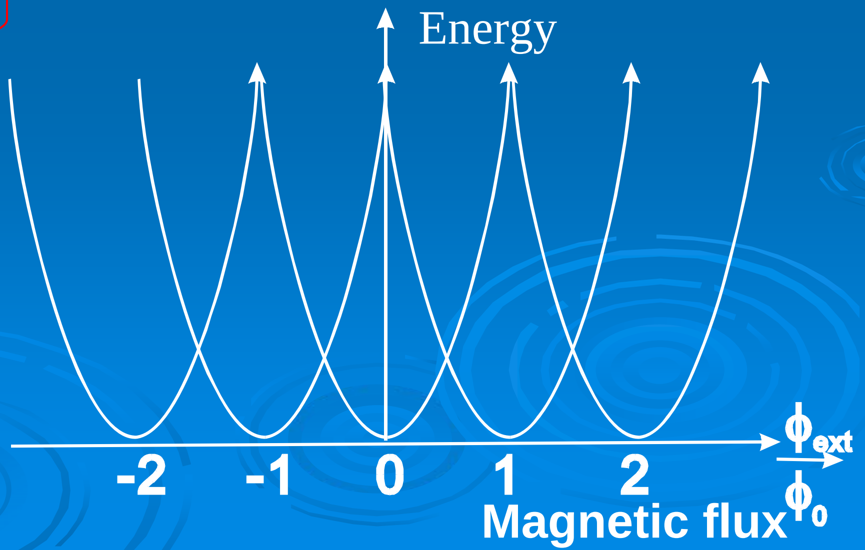


Quantization of magnetic flux

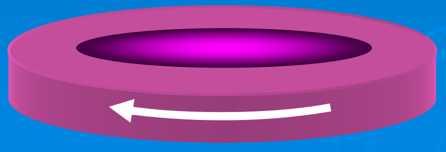


$$\phi_0 = \frac{h}{2e} = 2.07 \times 10^{-15}\,\mathrm{Wb}$$

It is same as the quantization of circulation (vortex) at superfluidity.



Perfect conductor



Superconductor ≠ Perfect Conductor

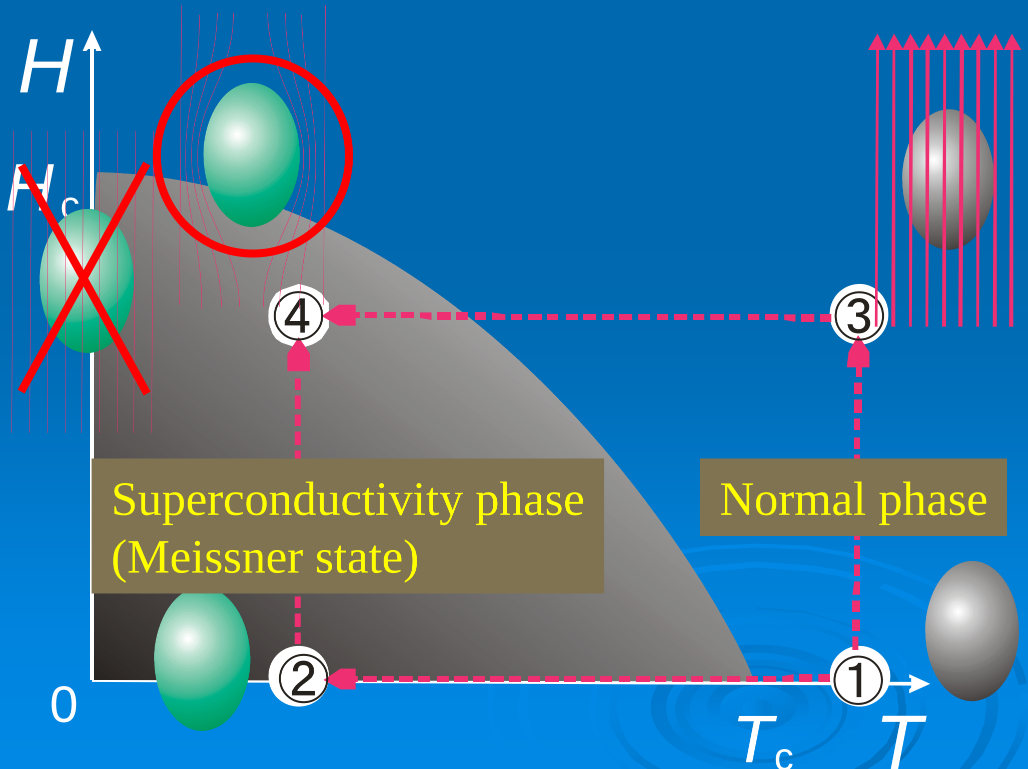
Although a shielding current can flow when the field is electrified in a Conductor (Lenz's law), damping occurs immediately due to the resistance.

⬇

A perfect conductor allows a shielding current to flow continually without damping.

⬇

In this case, the state depends on how the field is electrified.

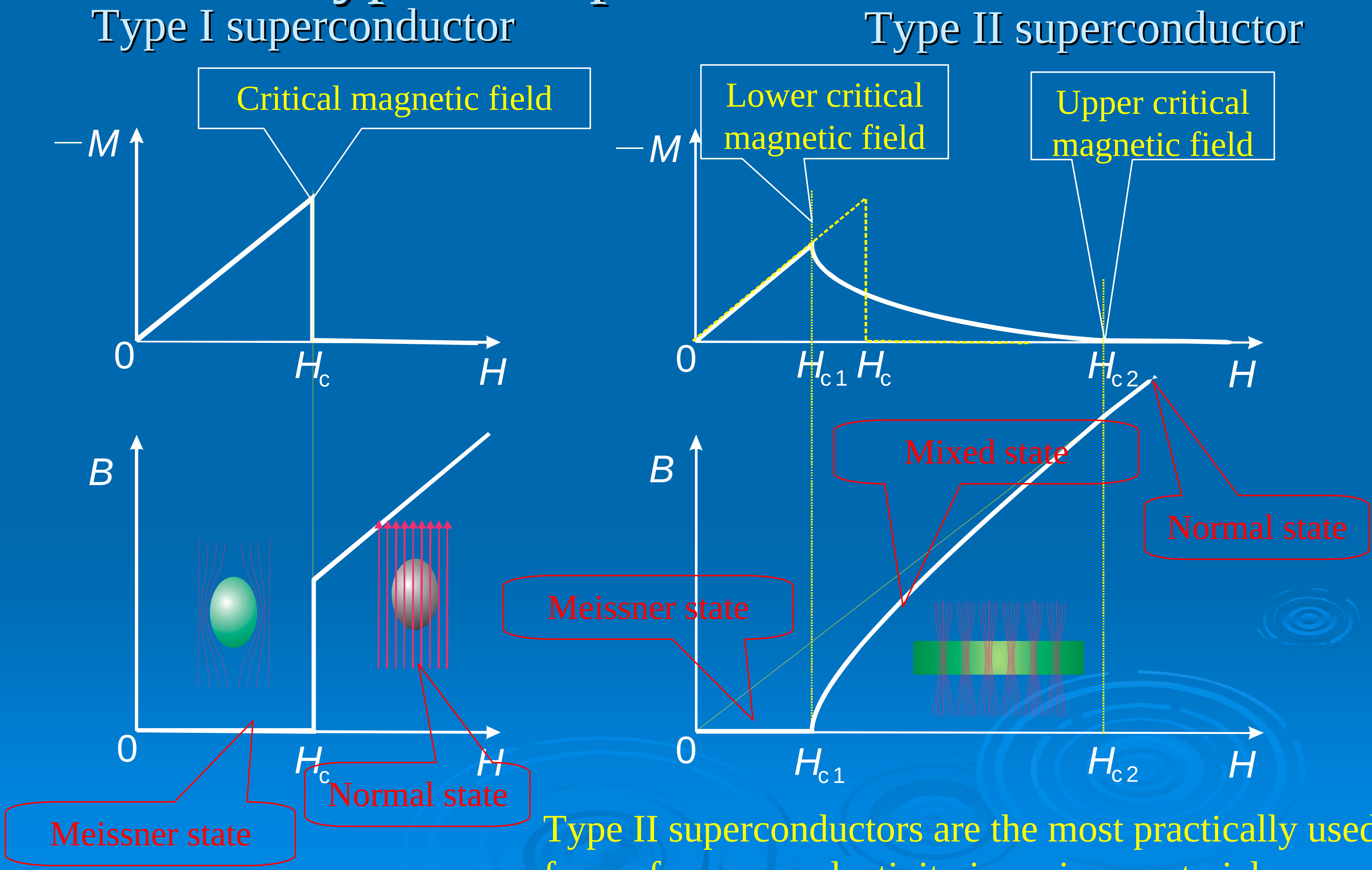


Meissner effect (total diamagnetism)

The magnetic field is completely excluded in a superconductor.

The shielding current of superconductors is a current under thermal equilibrium state.

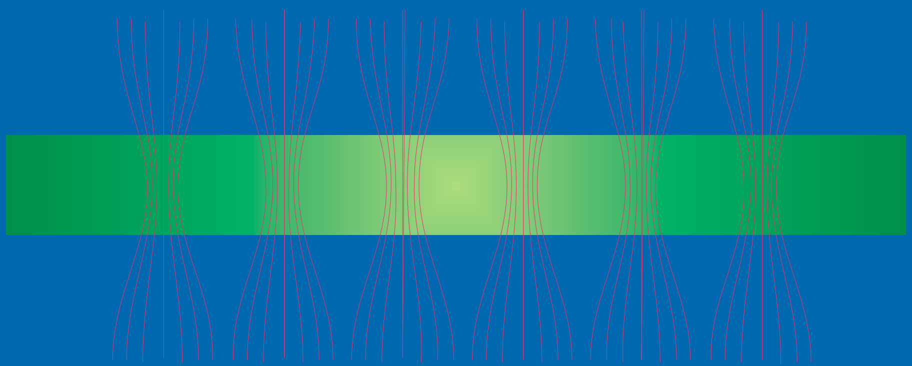
Type I Superconductors and Type II Superconductors



Type II superconductors are the most practically used form of super conductivity in various materials.

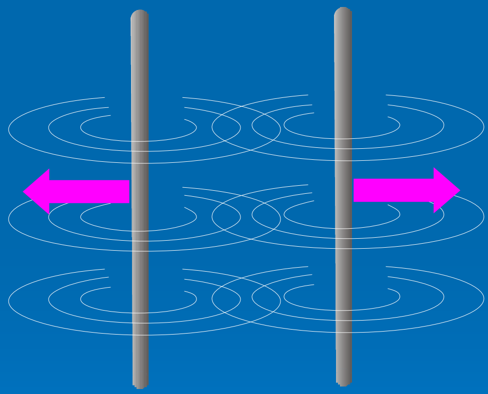
Quantum Magnetic Flux (Vortex Filament)

The mixed state of Type II superconductors.



Quantum magnetic flux
(vortex filament)

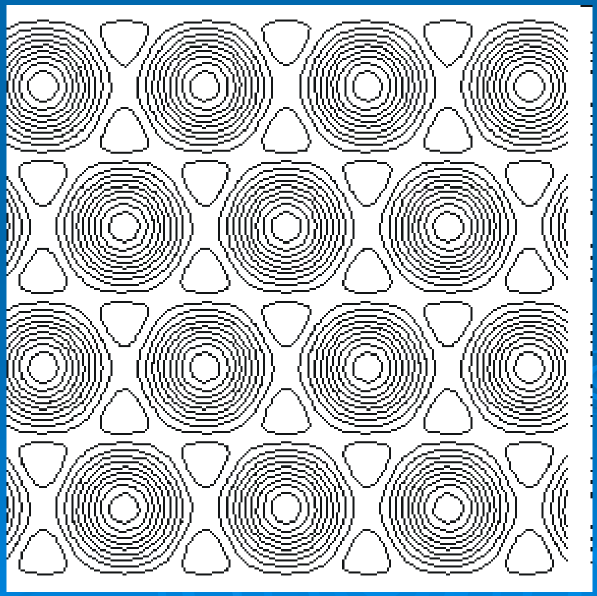
$$\phi_0 = \frac{h}{2e} = 2.07\times10^{-15}\,\mathrm{Wb}$$



Repulsive force is acted
on between the vortex filaments.

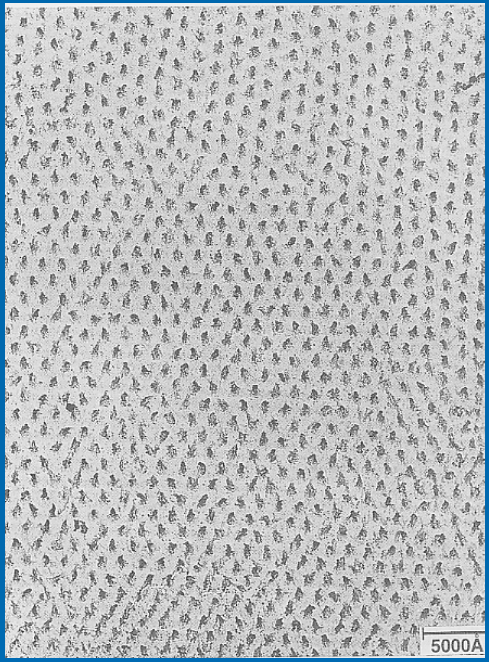
⇓

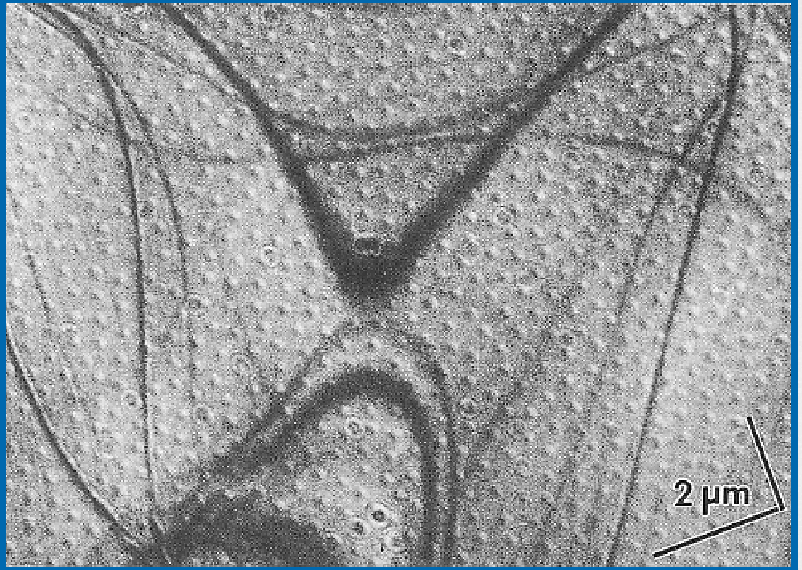
Triangular lattice

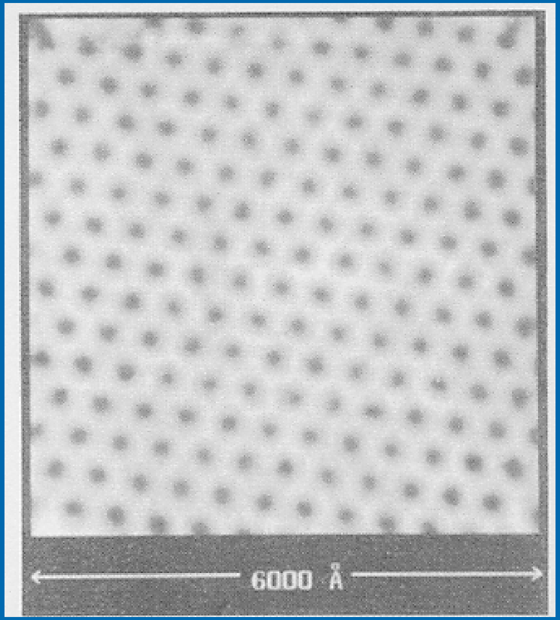


Magnetic flux lattice
(Abrikosov lattice)

Observation of Magnetic Flux Lattices





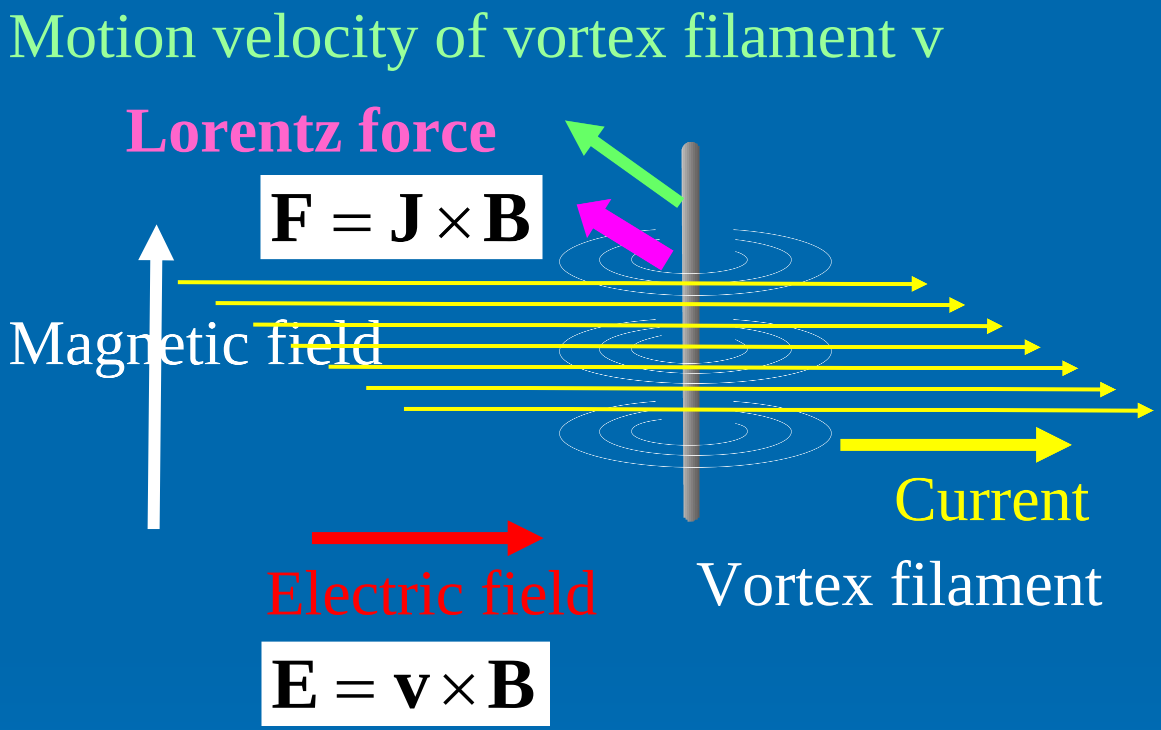


Bitter method
(Essmann & Traueble,1968) ‡

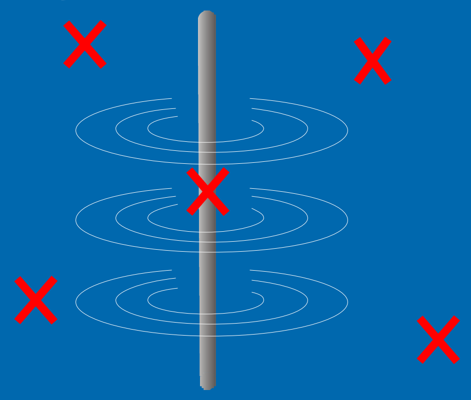
Lorentz microscope
(Akira Sotomura,1992) ‡

Scanning tunnel microscope
(Hess, 1989) ‡

Lorentz Force and Pinning for Vortex Filaments



Pinning of vortex filament



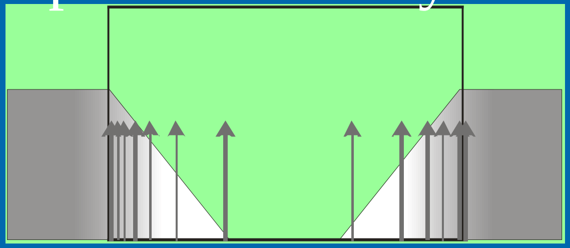
Energy dissipation does not occur if the vortex filament is not pinned tightly.

Electric field occurs when the vortex filaments start to move.
Generation of an electric field in the direction of current implies that there is a non-zero electric resistance (energy dissipation) being generated.

Lorentz force vs. pinning:
Electric current density where vortex filament starts moving
$\Rightarrow$ Critical electric current density

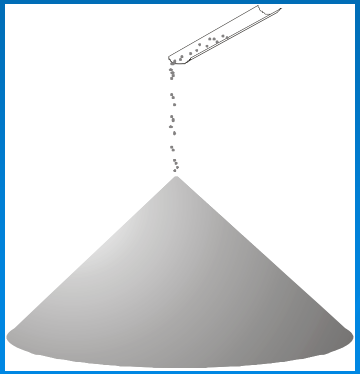
"Hard" Superconductivity

Strong pinning of vortex filament in superconductivity.

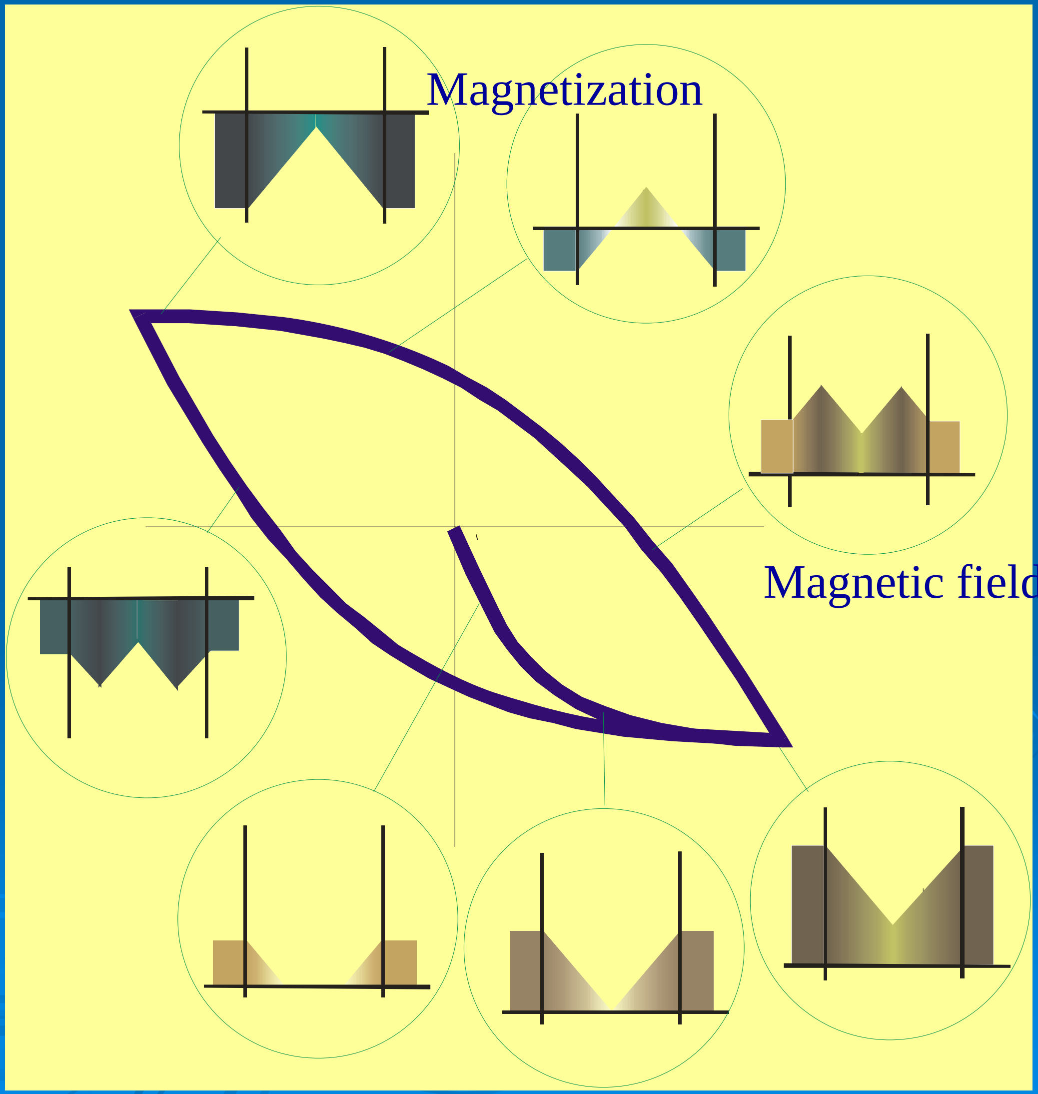


Shielding current flows until it reaches the critical current
⇒The gradient for magnetic flux is being determined.

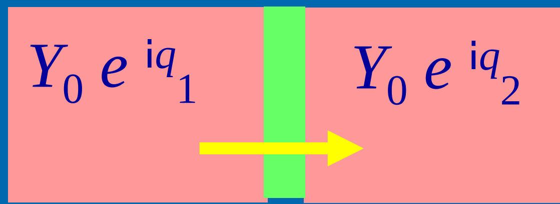
Formation of a sand hill
(Critical self-organization state)



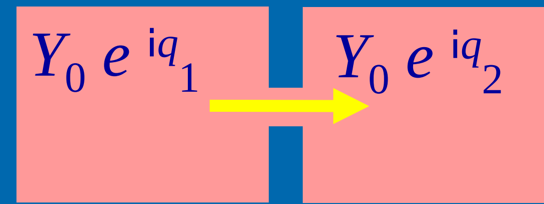
Magnetic hysteresis curve



Josephson Junction



Tunnel junction

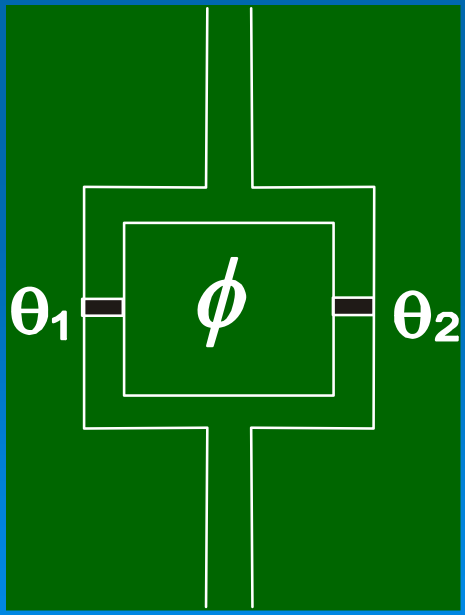


Weak bonding

Josephson current:
The phase difference between junctions.

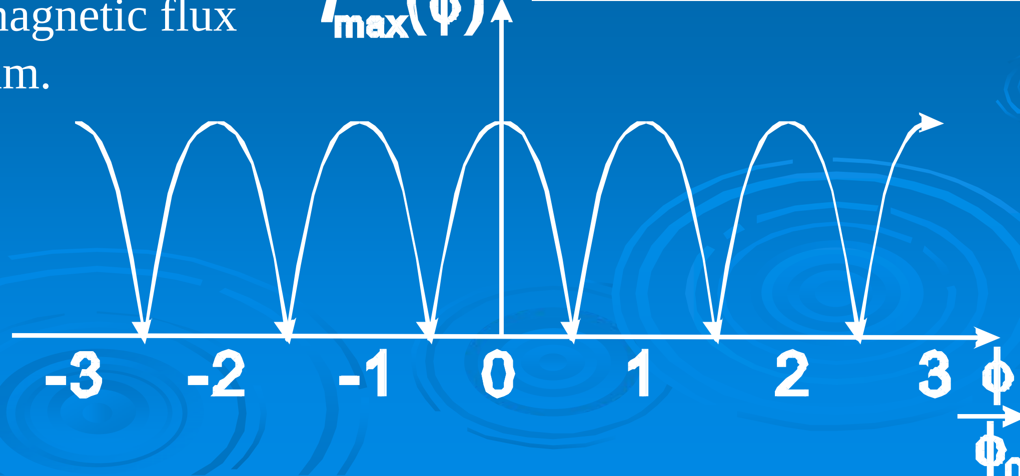
$$J = J_c \sin(\theta_1 - \theta_2)$$

Superconducting quantum interference device (SQUID)



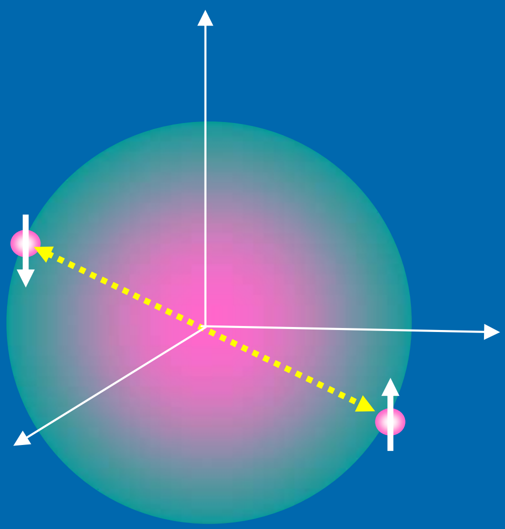
Superconducting current in a circuit periodically changes by unit; magnetic flux quantum.

$$I_{\max} = 2 I_c \left| \cos\left(2\pi \frac{\phi}{\phi_0} \right) \right|$$



The Mechanism of Superconductivity

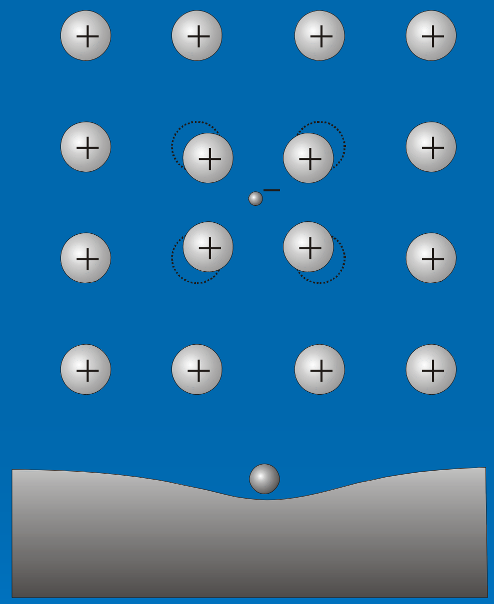
Formation of Cooper pair

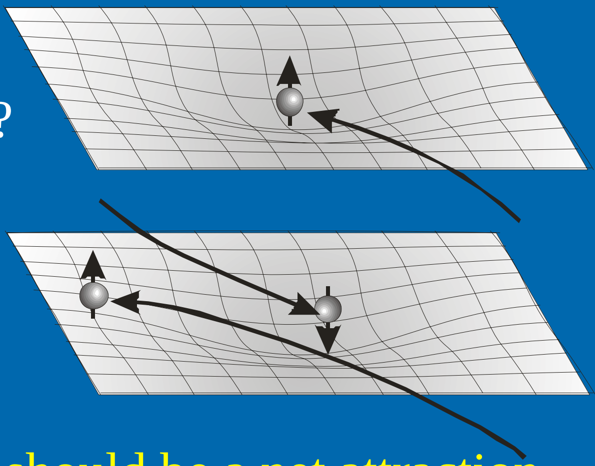


A bound state (Cooper pair) is formed when gravity is acted on the Fermi surface of the two electrons.

What about the origin of gravity?

Electron-lattice interaction





There should be a net attraction from the interaction of the electron lattice as long as the interelectron attraction remains greater than the Coulomb repulsion.

Superconductivity transition temperature

$$T_{\mathrm{c}} = 1.14\Theta_{\mathrm{D}} \exp\left(-\frac{1}{N(0)V}\right)$$

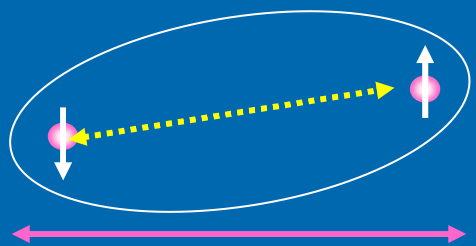
Bardeen-Cooper-Schrieffer (BCS) Mechanism

Interelectron attraction is greater than the interelectron Coulomb repulsion force.

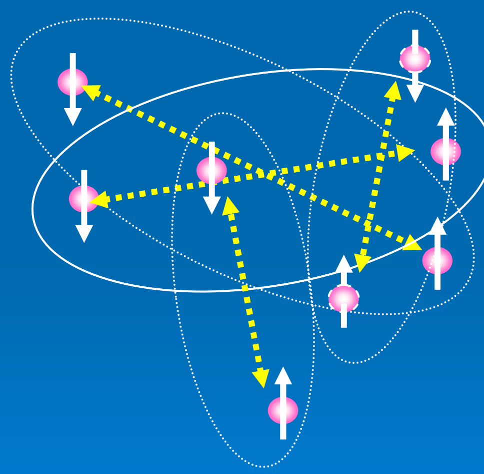
Formation of Cooper pair

Bose-Einstein condensation of the Cooper pair
⇒ Superconductivity state

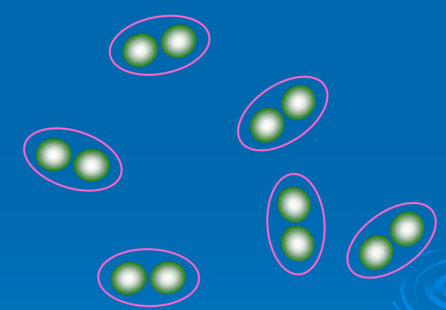
Size of Cooper pair



Coherence length



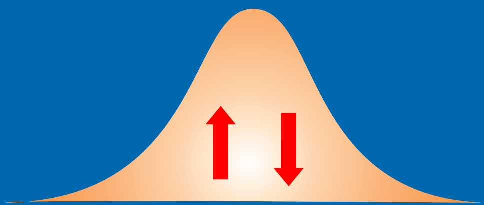
Cooper pairs are in a superposition state.



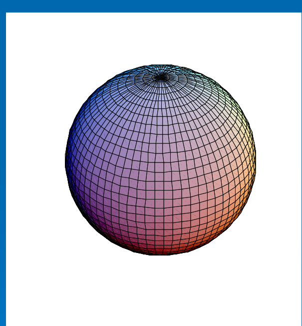
For ordinary molecules, the size of molecules are smaller than the interparticle distances.

Anisotropic Superconductors

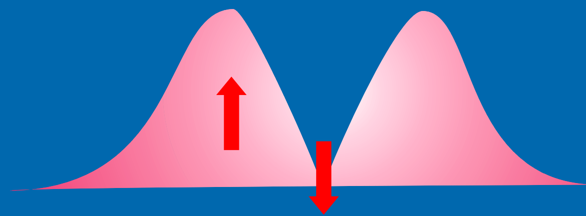
Symmetric properties of Cooper pairs.



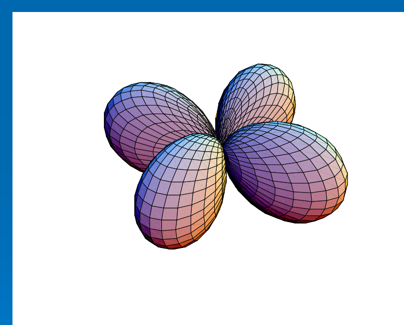
s wave (l = 0)
(Spin-singlet term)



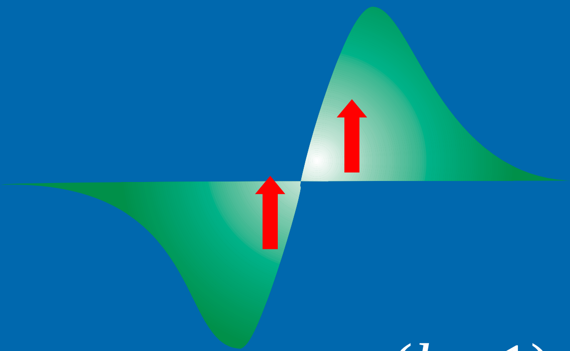
Most common superconductor.



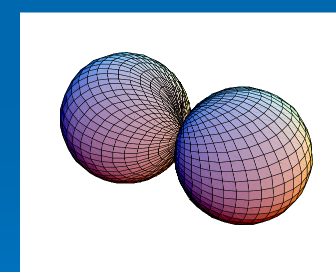
d wave (l = 2)
(Spin-singlet term)



E.g., Copper oxide high-temperature superconductor.



p wave (l = 1)
(Spin-triplet term)



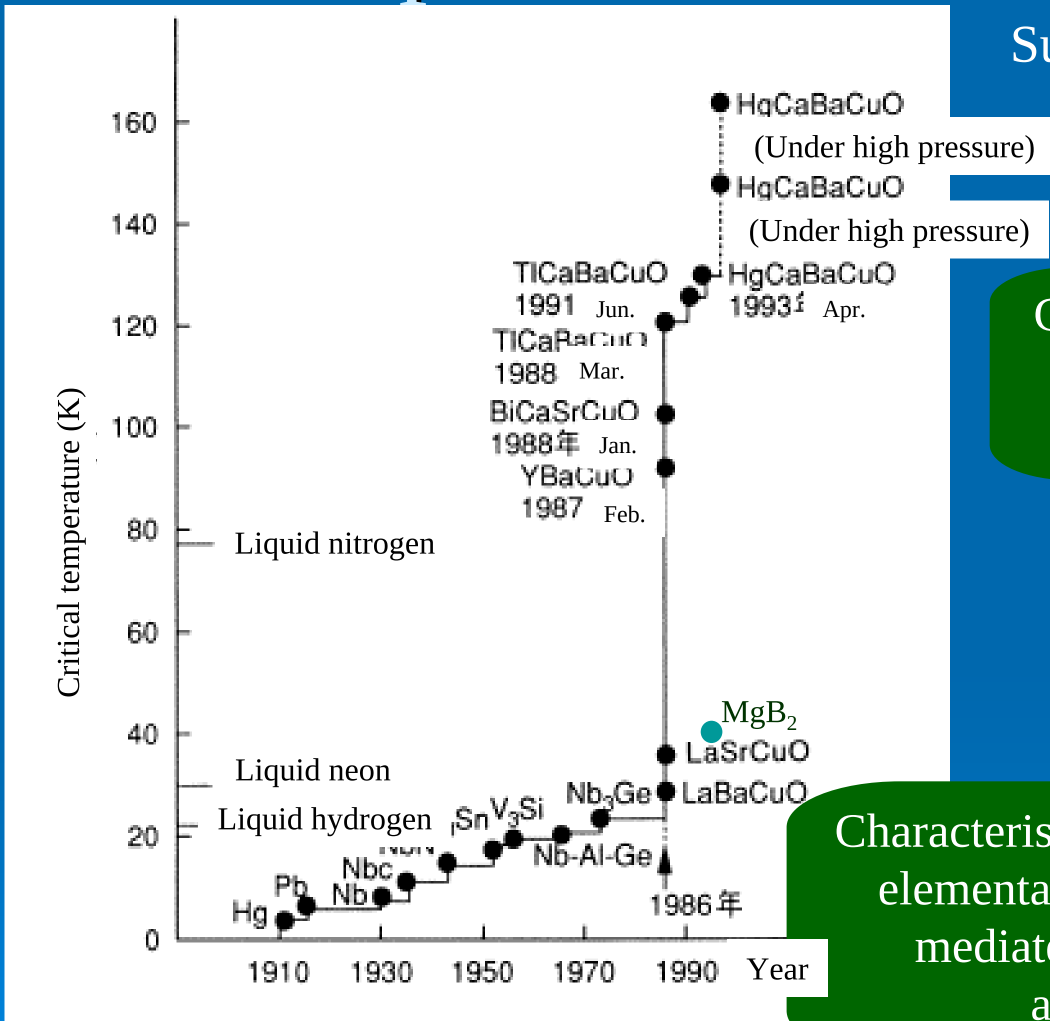
Ruthenium oxide
UPt_3 and superfluidity of ^3He.

Exotic Superconductors

- Copper oxide superconductors（$YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$）
- Sr_2RuO_4
- Heavy electron systems (UPt_3 and $CeCu_2Si_2$)
- Organic superconductors

  (($(TMTSF)_2PF_6$ and $(BEDT\text{-}TTF)_2Cu(NCS)_4$)
- MgB_2
- Alkali-doped fullerene K_3C_{60}
- Boron-doped diamonds

Is Room Temperature Superconductivity Possible?



Superconductivity transition temperature

$$T_c = 1.14\Theta_D \exp\left(-\frac{1}{N(0)V}\right)$$

Characteristic energy scale for lattice oscillation.

Intensity of electron-lattice interaction.

Is the limit around ~30K?

$$T_c \approx T^* \exp\left(-\frac{1}{\lambda}\right)$$

Characteristic energy scale for elementary excitation that mediates interelectron attraction.

Intensity of interaction.

Room temperature superconductivity:
there is no evidence to prove its impossibility.

Summary

- Properties of electrons in a solid state (band structure)
  - Band and Gap
- Metals, insulator, and semiconductors
  - Conduction carriers
  - Metal insulator transition, Mott insulators, and strongly-correlated electron systems.
- Magnetism
  - Magnetic moments in atoms ⇒ exchange interaction ⇒magnetic domain structure.
  - Spintronics
- Superconductivity
  - Basic properties of superconductors
  - BCS mechanism
  - Exotic superconductors

University Lecture
Science of Material

Lecture 6 What is Condensed Matter Physics?

Lecture 7 Quantum Mechanics and Artificial Materials
-- High-tech and the State-of-the-art Physics

Lecture 8 Atom Control and Quantum Control
--Nano-science and Quantum Information

Lecture 9 Diverse Matter and Physical Properties

The University of Tokyo,
The Institute For Solid State Physics

Yasuhiro Iye

Condensed Matter Physics (Material Science)

- Study of the dynamic properties (physical properties) in dynamic matter based on the understanding of the fundamental principles in physics (quantum mechanics).
- The "game of catch" between experiment and theory.
- Experiments that can approach the very essence of quantum mechanics have already been performed.
- Basic study of materials such as electron devices and optical communications that are fundamental for modern civilization will be covered in the lectures by Dr. Komiyama.