PHYS 666: Solid State Physics I

INSTRUCTOR

Michel van Veenendaal

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Office Hours: I am around Tuesdays and Thursdays

Web page with lecture notes: www.niu.edu/~veenendaal/666.htm

PREREQUISITES:

This course will be tough without having done quantum mechanics (560/1 or something equivalent)

Mathematical concepts:

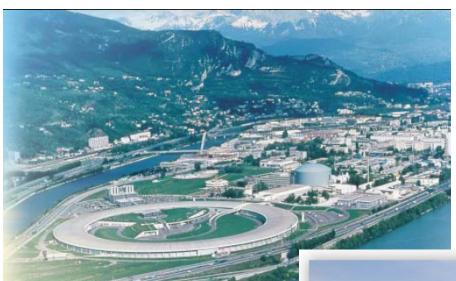
Fourier transforms differential equations (Schrödinger equations) linear algebra (matrices, eigenvalue problems)

- Homework: several homework sets will be given. They will be posted on the web site.
- Midterm: one midterm will be given.

- 1986-90: undergraduate Delft University of Technology (Ir.), the Netherlands
- 1990-94: Ph.D. University of Groningen (Dr.), the Netherlands
- 1994-97: European Synchrotron Radiation Facility, Grenoble, France
- 1997-98: NIU
- 1998-2002: Philips Electronics
- 2002-present: NIU
 - 2002-2008 Associate Professor
 - 2008- Professor
 - o 2009-2013 Presidential Research Professor
- 2005-present: joint with Argonne National Laboratory (Physicist)

Theoretical physicist specialty: condensed matter physics

ESRF



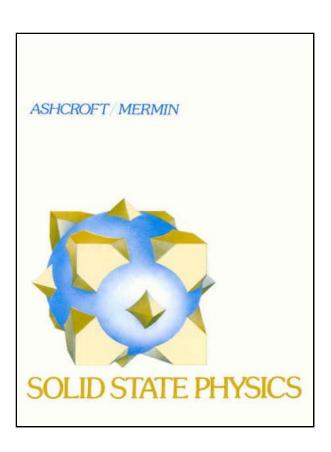
APS



REQUIRED TEXTBOOK:

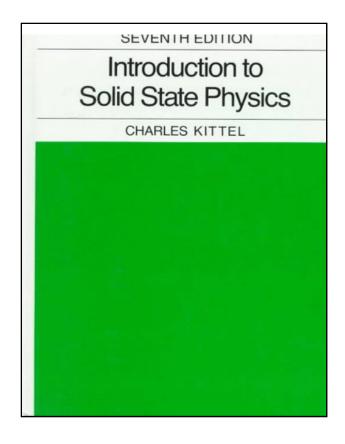
Solid State Physics

by N. W. Ashcroft and N. D. Mermin (Harcourt, 1976).



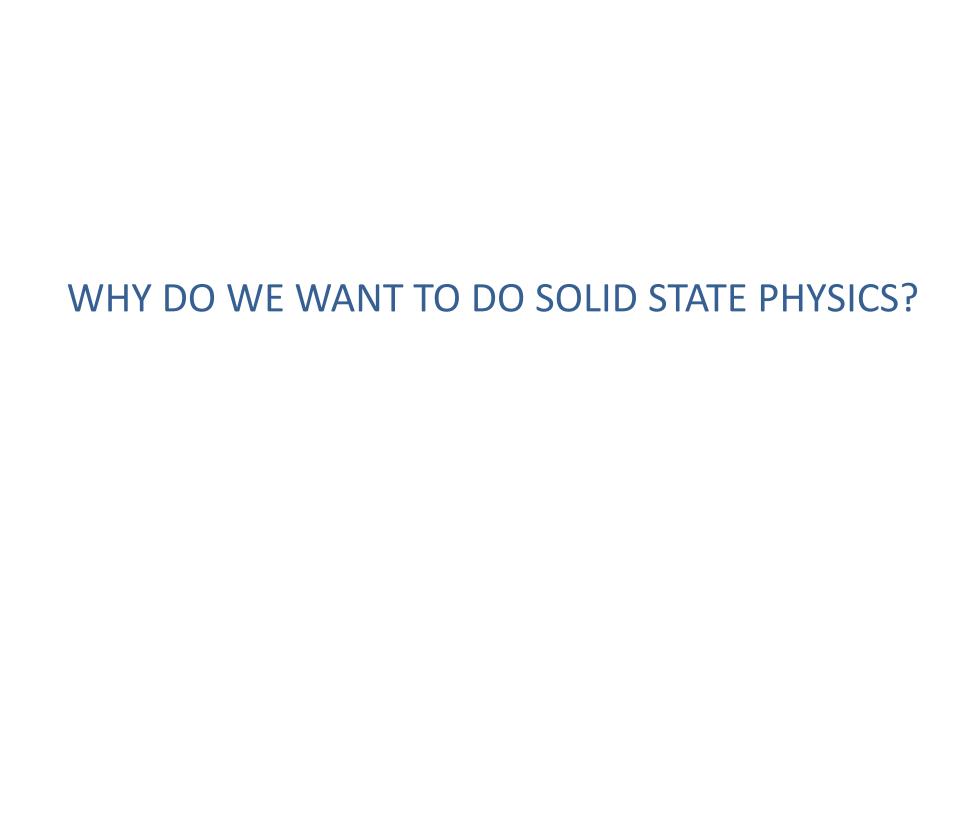
REFERENCED TEXTBOOK

Introduction to Solid State Physics
7th Edition by C. Kittel
(John Wiley & Sons, 1996).



Solid State Physics vs. Condensed-Matter Physics

- Condensed-matter physics is the more modern term
- Condensed-matter physics is broader and applies to concepts that work in solids, but could equally applied to liquid (for example, superconductivity vs. superfluidity, soft-condensed matter)
- 1978 Division of Solid-State Physics of the American Physical Society went to the Division of Condensed-Matter Physics
- 1/3 of U.S. physicists classify themselves as Condensed-Matter Physicists
- Condensed-matter physics is closely related and overlaps with inorganic chemistry, physical chemistry, quantum chemistry, electrical and mechanical.

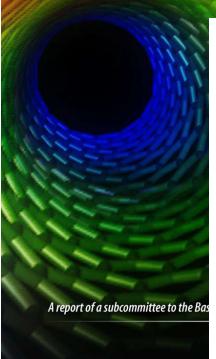


http://www.er.doe.gov/bes/reports/list.html



Steve Chu, Secretary of Energy 1997 Nobel Prize in Physics





Reports from
Basic Energy Sciences
Department of Energy

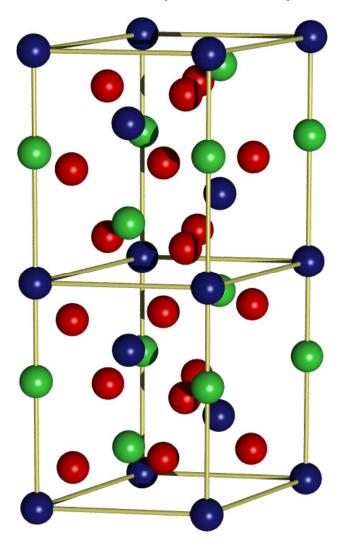
- A significant increase in the rate of discovery, innovation and technological change is needed. BES must lead a bold new initiative focused on solving the critical scientific roadblocks in next-generation, carbon-free energy technologies.
- Significant discoveries will come at the intersection of control science with advanced materials and chemical phenomena, and there is a clear firstmover advantage to those who focus their research efforts here. BES must lead U.S. energy research efforts in this direction lest the U.S. fall behind in global competition for discoveries of future energy sources and systems.
- It will take "dream teams" of highly educated talent, equipped with forefront tools, and focused on the most pressing challenges to increase the rate of discovery. BES must lead the development of these dream teams to close gaps between needs and capabilities in synthesis, characterization, theory, and computation of advanced materials.
- U.S. leadership requires BES to lead a national effort to aggressively recruit the best talent through a series of workforce development and early career programs aimed at inspiring today's students and young researchers to be the discoverers, inventors, and innovators of tomorrow's energy solutions.



| lmagi | ning a Secure, Sustainable Energy Future | 3 | | | |
|-------|--|----|---------------------------|--|--|
| | Materials with Unprecedented Performance | 3 | Nanoscience | | |
| | Making Chemical Change More Selective | 4 | | | |
| | Solar Power | 4 | Catalysis, photosynthesis | | |
| | Returning Carbon to the Earth | 4 | | | |
| | Safer and More Efficient Nuclear Power | 5 | | | |
| | Solar Fuels | 5 | | | |
| | Let There Be (Digital) Light | 6 | | | |
| | Electrical Energy Storage | 6 | Batteries | | |
| | A Solar Economy for Buildings | 6 | | | |
| | Superconductivity and the 21st Century Electric Grid | 7 | Superconductivity | | |
| | A Hybrid Electrical Grid | 8 | | | |
| | Solid-State Lighting | 8 | Solid-state lighting | | |
| | Advanced Transport | 8 | | | |
| | Solar Fuels | 8 | Solar cells | | |
| | Electric Transport | 9 | New electrode materials | | |
| | Advanced Nuclear Energy Systems | 9 | | | |
| | Geological Carbon Sequestration | 9 | | | |
| | Making the Stories Come True | 10 | | | |
| | Basic Materials Research to Commercial Impact | 10 | | | |

WHAT IS A SOLID?

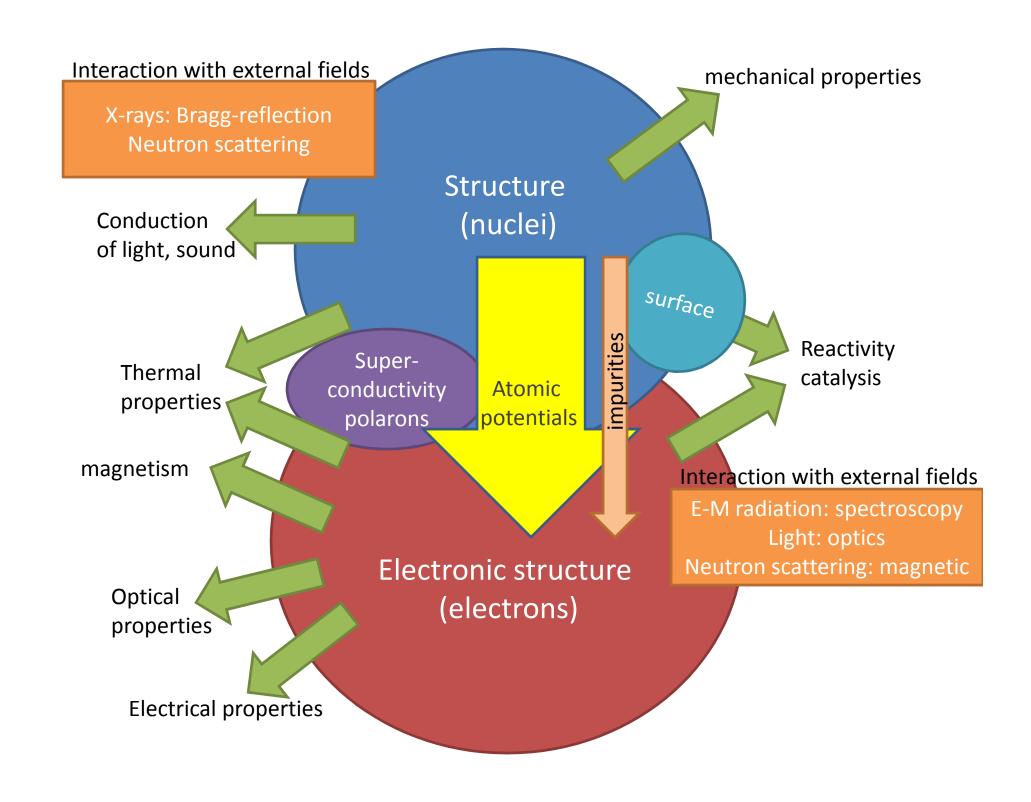
A solid is generally seen as a nice crystal made up of atom



And we will generally be dealing with those

BUT ALSO Amorphous materials heterostuctures Soft condensed matter (X = NH, S)(X = NH/N, S)**Conducting polymers**

Before you are able to deal with this, we have to get through the basics



HISTORY OF SOLIDS....

Whole ages are classified by our ability to control solids





17th century BC.



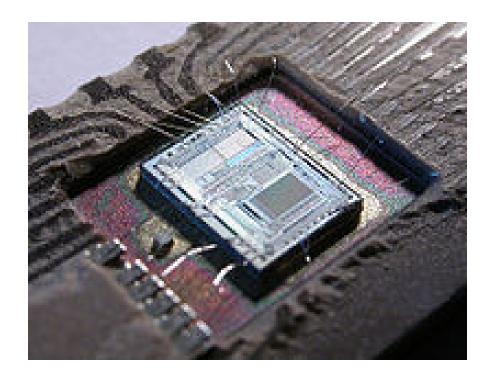
China (1600-1046 BC).

Stone age

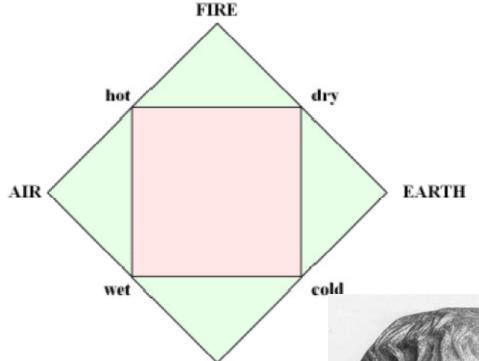
bronze age (3300–1200 BC)

iron age (1200 BC till present?)

Even our information age relies on our ability to manipulate materials (Si)



Ancient cultures:



WATER

Aristotle (384 BC – 322 BC)

Hinduism (Tattva) and Ap/Jala (Water) Water (水) Void/Sky/Heaven Water

Tibetan (Bön) Air Fire Space

Earth

(空)

Earth (地)

Buddhism (Mahābhūta) Vayu/Pavan (Air/Wind) Akasha Agni/Tejas (Aether/Space) (Fire) Prithvi/Bhumi (Earth) Japanese (Godai) Air/Wind (風)

Fire (火)

Modern: solid, liquid, gas, combustion/chemical reactions



Alchemy workshop illustration from Opus medico-chymicum: continens tres tractatus sive basilicas..., Johann Mylius, Francofurtu: Zlemannum a Sande, 1678

People recognized early on the difference in properties between metals

Philosopher's stone turning common metals into gold

EARLIER THEORIES TO DESCRIBE SOLIDS

Obviously, scientists tried to deal with solids before atoms and electron

- Mechanics
- Optical properties
- Thermal conductivity
- Conductive properties

Many of these questions can be addressed without understanding the underlying nature of a material

Of great importance is the strong development of calculus and differential equations starting from Newton and Leibniz, through Euler (1707 –1783), Gauss (1777 –1855) through the French schools (Ecole polytechnique/normale/militaire): Lagrange (1736–1813), Laplace (1749–1827), Fourier (1768–1830), Navier (1785–1836), Cauchy (1789 –1857), Poisson (1781–1840), etc.

Condensed-matter physics tries to connect the properties of the nuclei and electrons to the macroscopically observed quantities

Continuum mechanics

Hooke's law

 $\mathbf{F} = -k\mathbf{x}$

(1676)

Ut tensio, sic vis

As the extension, so the force.





Euler-Bernoulli equation:

(1750)

$$\frac{\partial^2}{\partial x^2} \left(EI \frac{\partial^2 u}{\partial x^2} \right) = w.$$



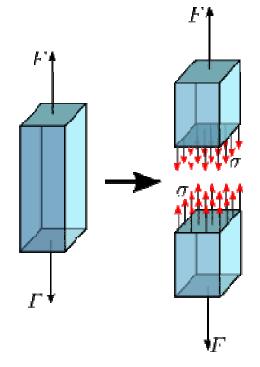
u deflection of the beam at some position x
w is a distributed load or a force per unit length
E is the elastic modulus
I is the second moment of area

Cauchy stress tensor

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \equiv \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \equiv \begin{bmatrix} \sigma_{x} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{y} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{z} \end{bmatrix}$$



Augustin Louis Cauchy (1789 –1857)



(1822)

How are the underlying atomic properties related to the elasticity?

Interactions of radiation and matter

Reflections, color, refraction, absorption are all manifestations of interactions of radiation and matter

Euclid (~300 BC) already wrote a book on Optics



Lenses: Lippershey, Janssen, Galileo

$$\frac{\sin \theta_1}{\sin \theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1}$$

Snell's law is a direct consequence of the electronic properties of the material

What determines the optical properties of a material: opaque, reflecting, transparent?

Late 18th and 19th century: mechanical approach to condensed matter physics

• optical theories by Thomas Young and Jean Fresnel

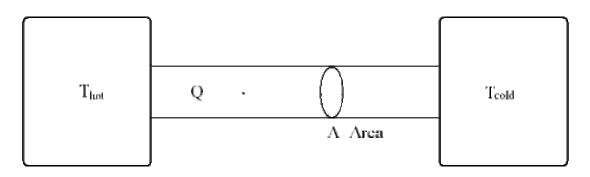




Thomas Young

- A wide variety of theories on elasticity (Navier, Cauchy)
- Theories for heat conductivity by Joseph Fourier

Thermal conductivity



Q heat [Joules]

ΔT T_{hot} T_{cold}

Newton's law of cooling

$$\frac{dQ}{dt} = h \cdot A(T_{\text{env}} - T_0)$$
 (1643-1727)

Fourier's law

$$q_x = -k\frac{dT}{dx} \tag{1822}$$

q is the local heat flux,k is the material's thermal conductivitydT/dx is the temperature gradient







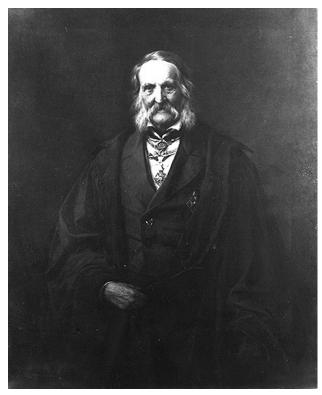
(1768-1830)

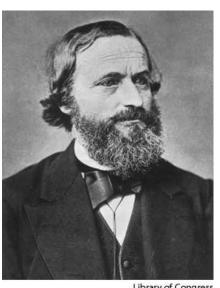
• Interaction between light and matter, theory of birefringence by Franz Neumann

• Early theories of electrical conductivity by, among others, George Ohm and

Gustav Kirchhoff



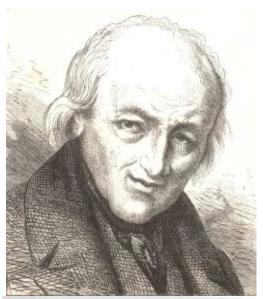




Library of Congress

Crystal structures

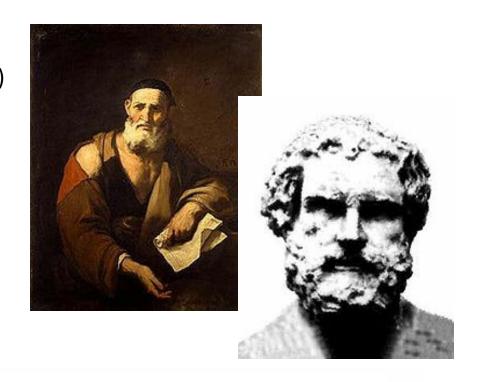
- First scientific approach René-Just Haüy (1743-1822) using an atomistic picture
- Extended by Christian Samuel Weiss, introduced crystallographic axis
- Auguste Bravais: discovered the 14 space lattice types
- Woldemar Voigt classified the 230 different space groups

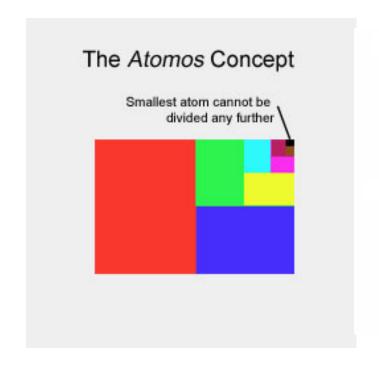


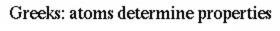


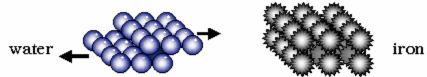
THE RISE (and fall) OF THE ATOMISTIC PICTURE

Leucippus (first half of 5th century BC) Democritus (c. 460 BC – c. 370 BC)









Dalton: atoms determine composition

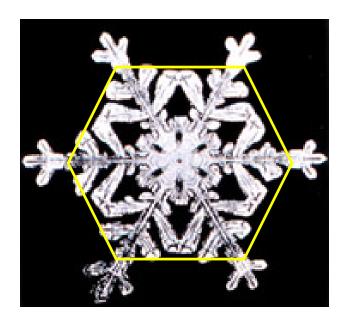


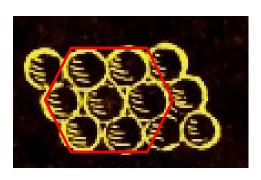
Aristotle: Horror vacui

Johannes Kepler (1571 –1630)

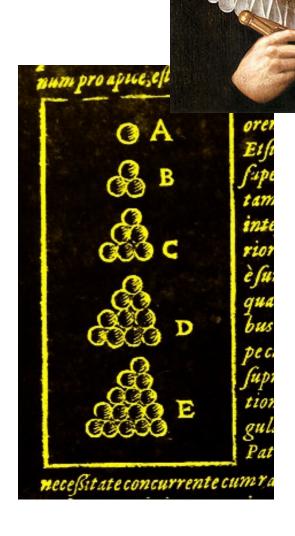
Strena Seu de Nive Sexangula A New Year's Gift of Hexagonal Snow

The Kepler conjecture





(1611)



Corpuscular theory



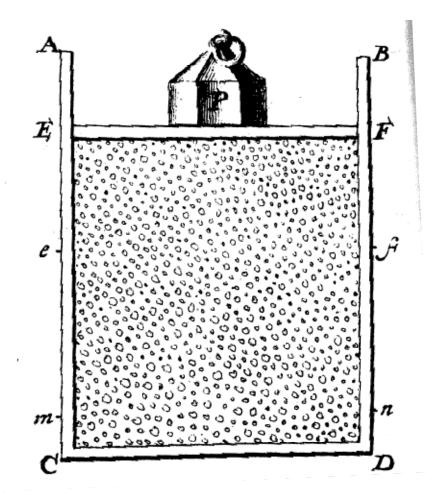


Newton

Boyle (1627 -1691)



Daniel Bernoulli (Groningen, 1700 –1782)



Let the cavity contain very minute corpuscles, which are driven hither and thither with a very rapid motion; so that these corpuscles, when they strike against the piston and sustain it by their repeated impacts, form an elastic uid which will expand of itself if the weight is removed or diminished. . . ".

In physics atomistic ideas were pushed to the background in the late 18th and most of the 19th century

Unreasonable:

Not if one considers the enormous successes of continuum theories in

- Mechanics
- Thermodynamics (i.e. not statistical)
- Electricity and magnetism
- Optics

"Who needs atoms?" reigned during this period.

Not so in chemistry:

I. Law of Conservation of Mass

II. Law of Definite Proportions

Mass relationships during chemical reactions: copper carbonate (CuCO₃) always gives 51.5% copper, 38.8% oxygen, and 9.7% carbon

III. Law of Multiple Proportions

1 g Carbon + 1.33 g O \rightarrow CO 1 g Carbon + 2.66 g O \rightarrow CO₂

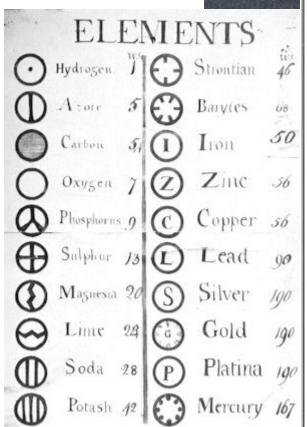
Ratio first and second oxide 1:2

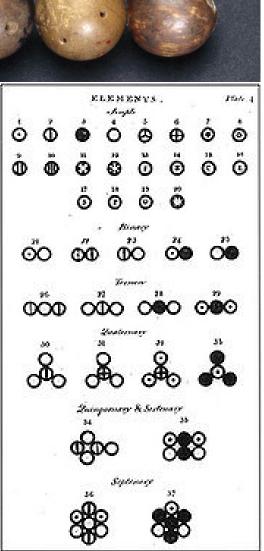
Dalton's law of partial pressures

$$P_{total} = p_1 + p_2 + \dots + p_n$$

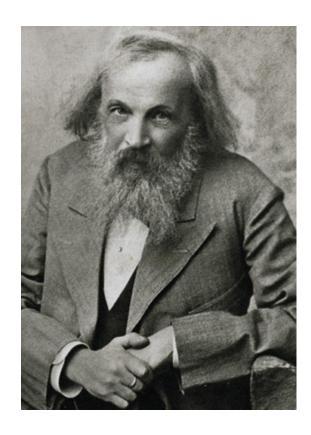


John Dalton (1766 –1844)





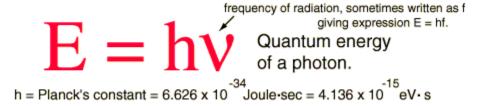
Culmination in Mendeleyev's Periodic table

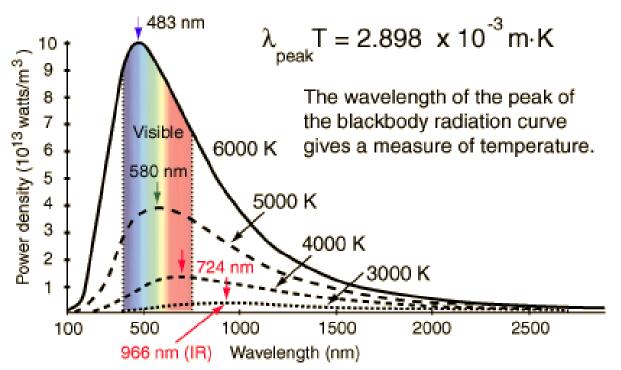


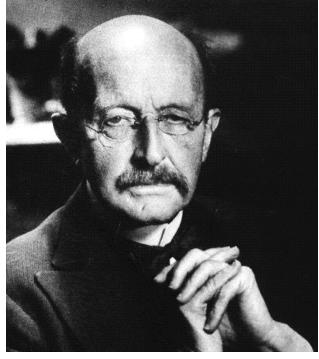
Dmitri Mendeleyev (1834 –1907),

| The Elements | Their Properties in the Free State | The Composition of the Hydrogen and Organo-metallic Compounds | Symbols- and Atomic Weights | The Composition of the Saline Cuides | The Properties of the Saline Oxides | Small Periods or Series |
|--|---|--|---|--|---|----------------------------------|
| Hydrogen Lithium Beryllium Beron Carbon Nitrogen Oxygen Finorine | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | RH _m or B(CH ₃)m [3] m = 1 4 | B A [6] H 1 Li 7 Be 9 B 11 C 12 N 14 O 16 F 19 | R _i O _n [7] 1; *** 2 = 2 - 3 1 - 3 4 1 - 3 - 5 * | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | [11] 1 2 |
| Sedium Magnesium Aluminium Silicon Phoephorus Sulphur Chlorine Potassium Calcium Scandium Titanium | 90° 071 098 23 500° 027 174 14 600° 023 26 11 (1200°) 008 23 12 44° 128 22 14 114° 067 207 15 -75° 18 27 15 (800°) 16 25 - (830°) 16 25 (2500°) (51) (94) | 4 3 - 1 2 - 1 | Na 20 Mg 24 Al 27 Si 28 P 31 S 32 Cl 355 K 39 Ca 40 So 44 Ti 48 | 1† - 2† - 3 4 3 4 1 - 3* 4* 5* 6* 1 1 - 1 - 5* - 7* 1 1† - 2† - 3† - 3† 4 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 4 |
| Vanadium Chronsium Manganese Iron Coball Nickel Copper Zinc Gallium Germanique | (2000') — 5-5 92 (2000') — 5-5 80 (1500') — 7-3 7-8 1400' 012 7-8 7-2 (1400') 013 8-6 6-8 1350' 017 8-7 6-8 1041' 029 8-8 7-2 (200') — 5-26 12 200') — 5-26 12 | | V 51 Cr 52 Mn 55 Fe 56 Co 58 Ni 59 Cu 63 Zn 65 Ga 70 Ge 72 | - 2 3 4 5 - 2 3 4 - 6* - 2 3 3 4 - 6* - 2 3 3 6* - 2 3 3 6* - 2 3 1 1 2 1 - 2 3 - 4 | 249 52 67 274 73 93 | 5 |
| Arsenie Selenium Belomium Buhoibum Strontium Yttrium Zarconium Niobium Molybdenum | \$600° 006 5·7 13 \$17° - 4·8 16 -7° - 5·1 26 \$29° - 1·5 5·7 (800°) - 2·5 35 - (9·4) (16) (1500°) - 4·1 22 - 7·1 13 - 8·6 13 | 3 = - | As 75 Se 79 Br 80 Rb 85 Sr 87 Y 89 Zr 90 Nb 94 Mo 94 | 3 -5. 3 -6. 15. -2+ 3 -4 3 -4. 2 -3 -4. 2 -3 -4. | 41 16 60 48 48 -11 505 45 (-2) 57 45 -02 47 57 +62 44 65 68 | 8 |
| Ruthenium Rhodium Palladium Silver Codmium Indium Indium Indium Indium Codmium Codmium Indium | (2009°) 010 122 84 [1900°) 038 121 86 1500° 012 114 88 950° 013 105 10 390° 051 86 18 176° 046 74 14 230° 023 72 16 432° 012 67 18 452° 017 04 20 114° 49 26 12° 188 71 — 375 36 (600°) 61 23 | 1 3 - 1 1 3 - 1 | Ru 105 Rh 104 Pd 106 Ag 108 Cd 112 In 113 Se 118 Sb 120 Te 125 I 127 Cs 153 Ba 187 La 188 | - 2 3 4 - 6 - 8 - 2 3 4 - 6 1† 2 - 4 - 2+ - 2 3 4 5 - 2 3 4 5 - 3 4 5 6* 1 - 3 4 5 6* 1 - 3 4 5 6* - 3 4 5 6* | Ag ₄ O 75 81 11 815 81 25 In ₉ O ₃ 718 88 27 615 43 28 65 49 26 571 68 47 | 7 |
| Cerium | (1500°) — 66 21 (800°) — 65 22 — — (69) (25) — — 104 18 (1500°) — 191 96 | | Ce 140 Di 142 (14) Yb 178 (1) Ta 182 W 184 | 3 4 3 -5 5 6 | 918 43 (-2) 75 59 46 69 67 8 | 10 |
| Osmium Iridium Platinum Gold Mercury Thallium Lead Bismuth | (3500°) 007 224 85 2000° 007 224 85 1772° 005 215 92 1045° 014 193 10 -39° - 136 15 284° 031 118 17 386° 020 113 13 268° 034 98 22 | | Ou 191 Ir 193 Pt 196 An 198 Hg 200 Tl 204 Pb 206 Bi 208 | 3 4 -6 -82 3 4 -6 -8 1 2 3 4 1 -3 4 1 -3 -43 3 -5 | Au ₂ O (12'3) (43) (15) 11'1 39 43 Tl ₂ O ₃ (97) (47) (43 89 43 42 | 0 |
| Thorismy | 111 21 | The state of the s | Th 132 | 4 | 986 34 26 | 12 |

REVOLUTION IN PHYSICS







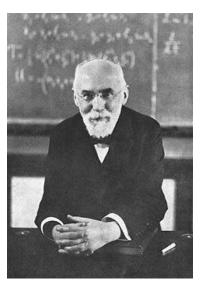
Energy per unit volume per unit frequency $S_{\upsilon} = \frac{8\pi h}{c^3} \frac{\upsilon^3}{e^{h\upsilon/kT}-1}$

Energy per unit volume per unit
$$S_{\lambda} = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}$$
 wavelength

Classical electron theory

• discovery of electron J. J. Thompson, Lorentz

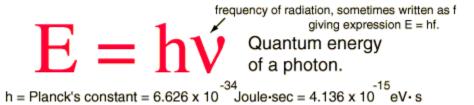


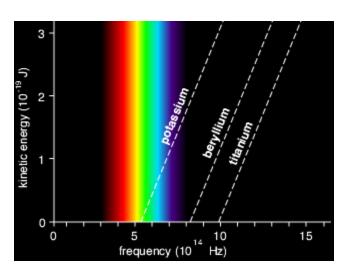


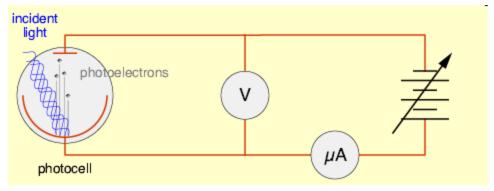
•Drude model

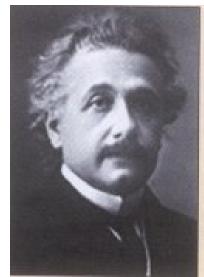
Treats electrons as a gas following Boltzmann statistics as opposed to Fermi-Dirac statistics. Quantities of by several orders of magnitude (gets a lucky break with Wiedemann-Franz law)











MODERN SOLID STATE PHYSICS

Solid state physics based on atoms generally based on quantum-mechanics (although sometimes classical mechanics)

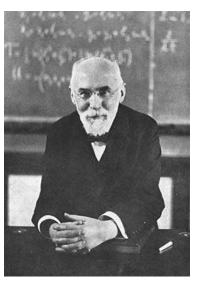
Classical electron theory

• Drude model (1900)

Treats electrons as a gas following Boltzmann statistics as opposed to Fermi-Dirac statistics.

Quantities of by several orders of magnitude (gets a lucky break with Wiedemann-Franz law)





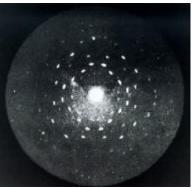
Paul Drude (1863 –1906)

X-ray diffraction

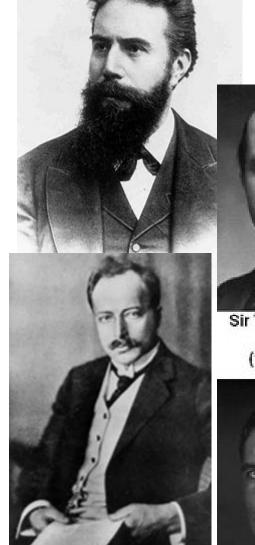
1895: discovery of X-rays by Wilhelm Röntgen (Nobel 1901)

1912: discovery of X-ray diffraction by Max von Laue, Nobel 1914 (other contributors

Ewald, Sommerfeld)



1913: interpretation by William and Lawrence Bragg, Nobel 1915



Sir William Henry Bragg (1862 - 1942)



William Lawrence Bragg (1890 - 1971)

First applications of quantum mechanics

Specific heat of solids: The change in internal energy with respect to temperature

experiments by Nernst





Einstein $E(k)=\omega_0$



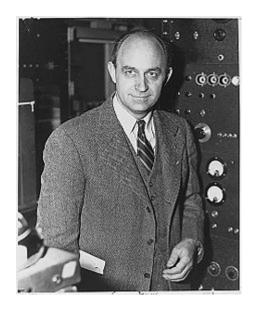
W. Nanct

Walther Nernst (1864 –1941)

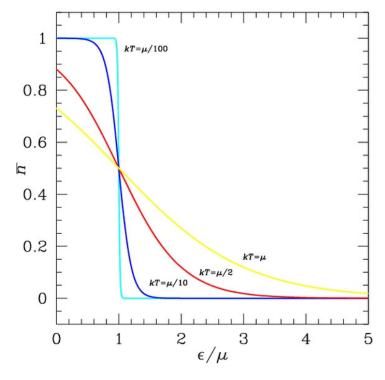


Peter Debye (1884 –1966) Nobel Chem 1936 E(k)~k

Fermi-Dirac statistics







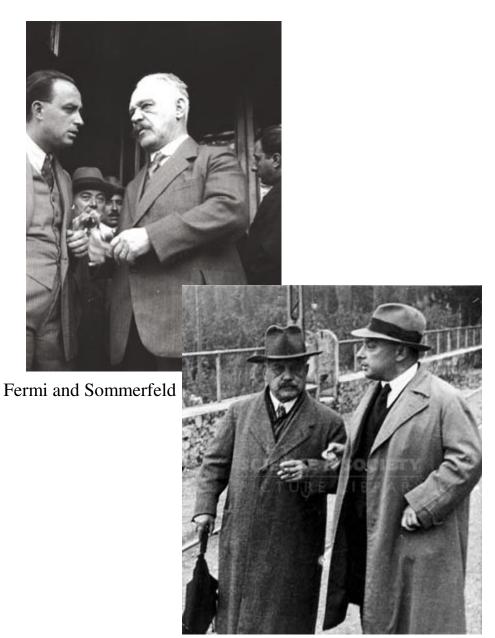
Sommerfeld theory including Fermi-Dirac statistics

Specific heat much smaller since very few electrons participate in the conduction

Solves dilemma of Drude-Lorentz theory

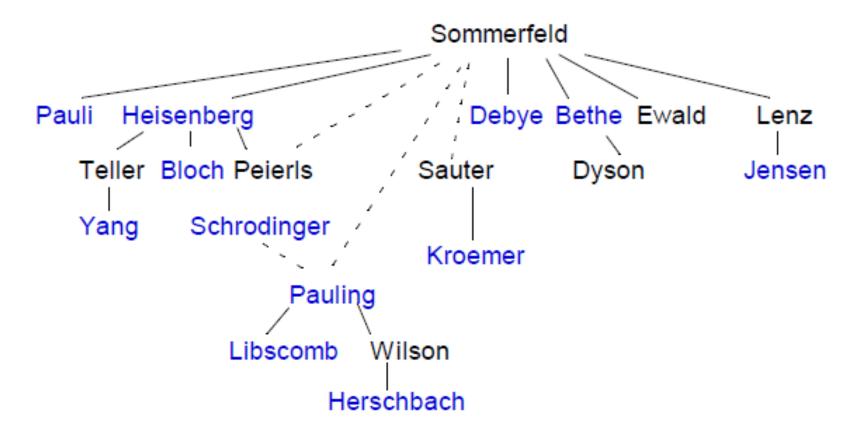
Completely ignores the presence of ions!

Still fails to describe many properties...



Sommerfeld and Pauli

In addition, Sommerfeld was a star in producing world-class scientists (a selection)

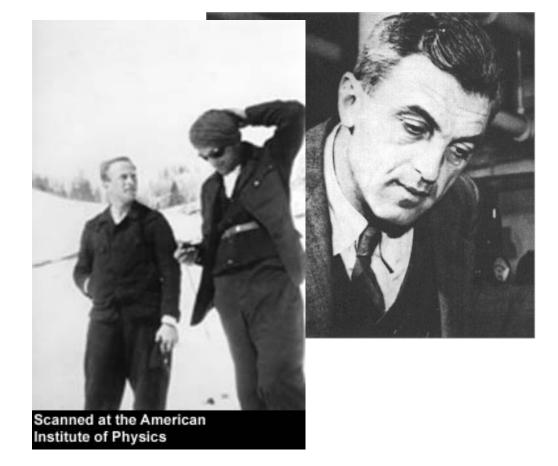


Albert Einstein told Sommerfeld: "What I especially admire about you is that you have, as it were, pounded out of the soil such a large number of young talents."

Bloch's theorem

Inclusion of the ions in the theory of metals

Inclusion of translational symmetry is essential



(Bloch's theorem)

Bloch and Heisenberg

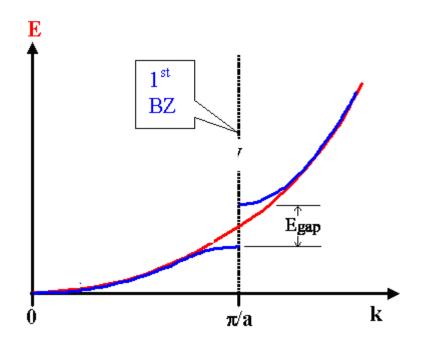
$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}}, \qquad \psi_{\mathbf{n}\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{n}\mathbf{k}}(\mathbf{r}),$$

$$u_{\mathbf{n}\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{n}\mathbf{k}}(\mathbf{r})$$
Free electrons
Bloch electrons

Band gaps and Brillouin zones

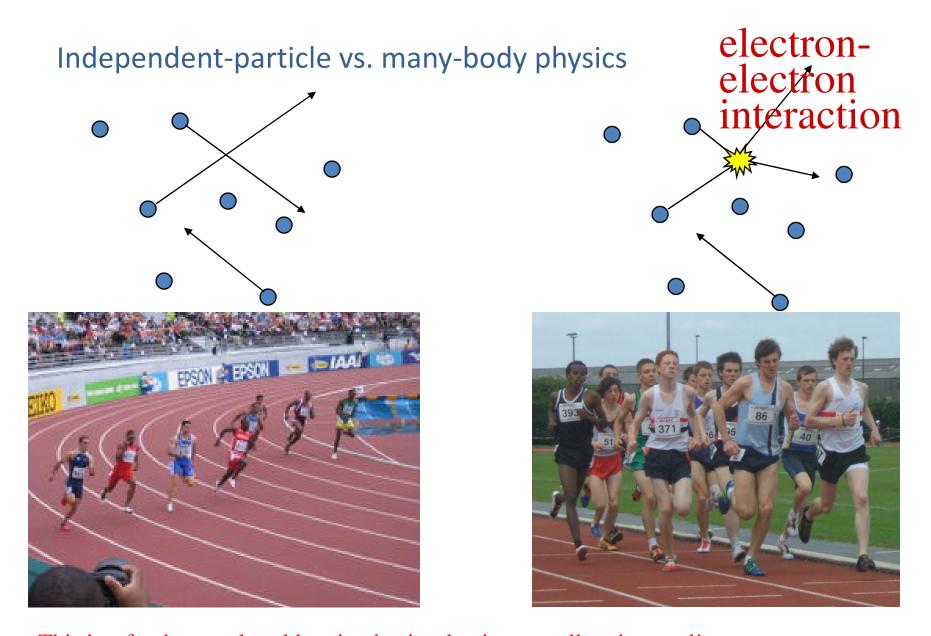


Sir Rudolf Peierls, (1907–1995),





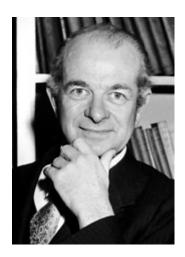
Léon Brillouin (1889 –1969)



This is a fundamental problem in physics that is not well understood!

There are very extensive codes based on the independent-particle approximation

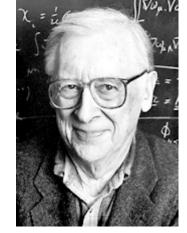
- Density functional theory
- Local Density Approximation
- Molecular orbital theory
- Quantum chemistry



Linus Pauling (1901-1994)

Nobel chem 1954



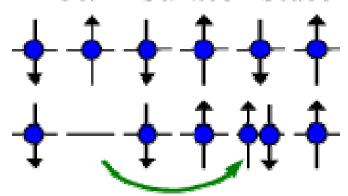


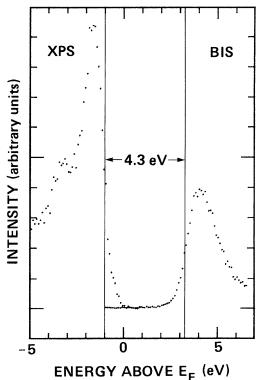
Walter Kohn (1923) John Pople (1925-2004) Nobel chem 1998

However, often we have to deal with many-body effects

• Effects where electron-electron interactions are important

Mott-insulator state











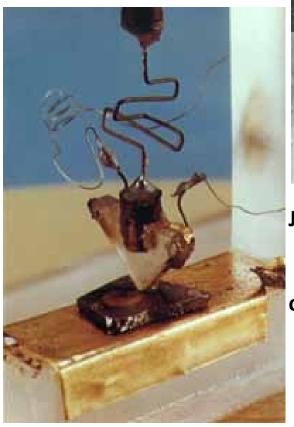
Philip W. Anderson (1923) John van Vleck (1899-1980) Sir Nevill Mott (1905-1996) Nobel 1977

Why is NiO an insulator and not a metal?

WHAT IS THIS?



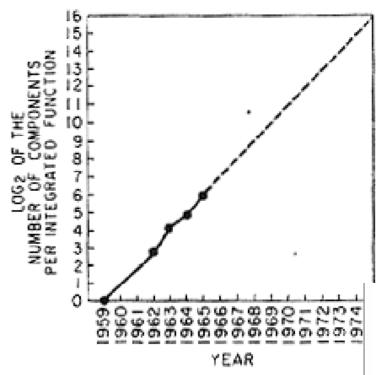
The first transistor! Bell-Labs (1947)





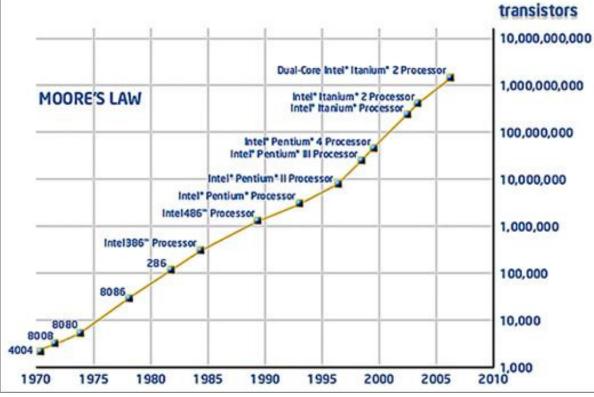
John Bardeen, Walter Brattain, and William Shockley working on the first transistor

Nobelprize 1956

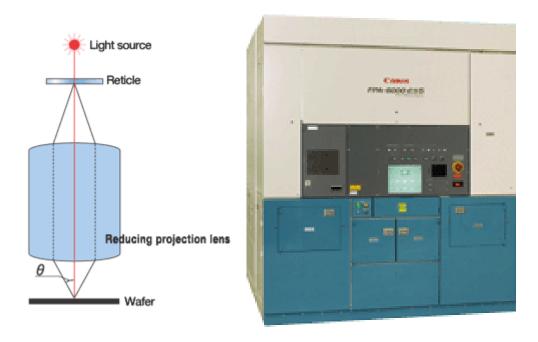


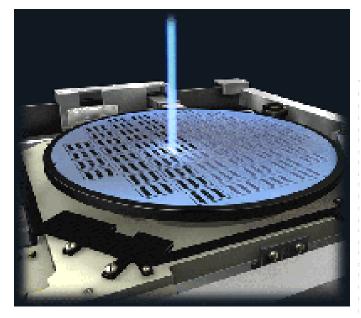
Moore's Law



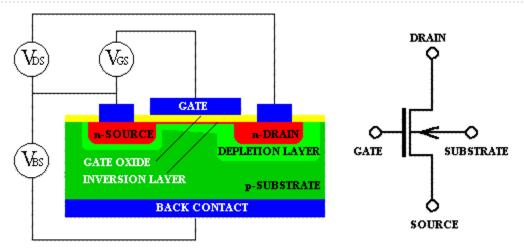


Optical lithography

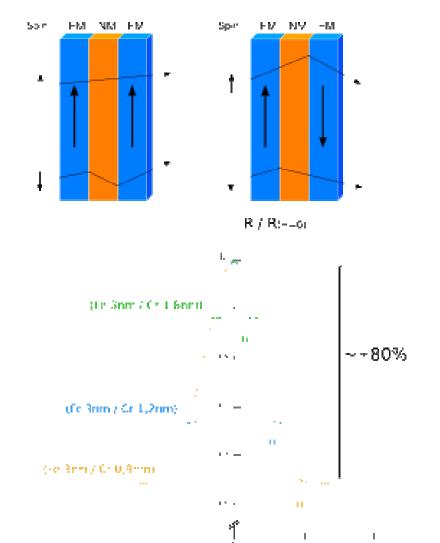




 $RES = k_1 \, \lambda \, / \, NA$



Other device technology: giant magnetoresistance



H (Mainss).



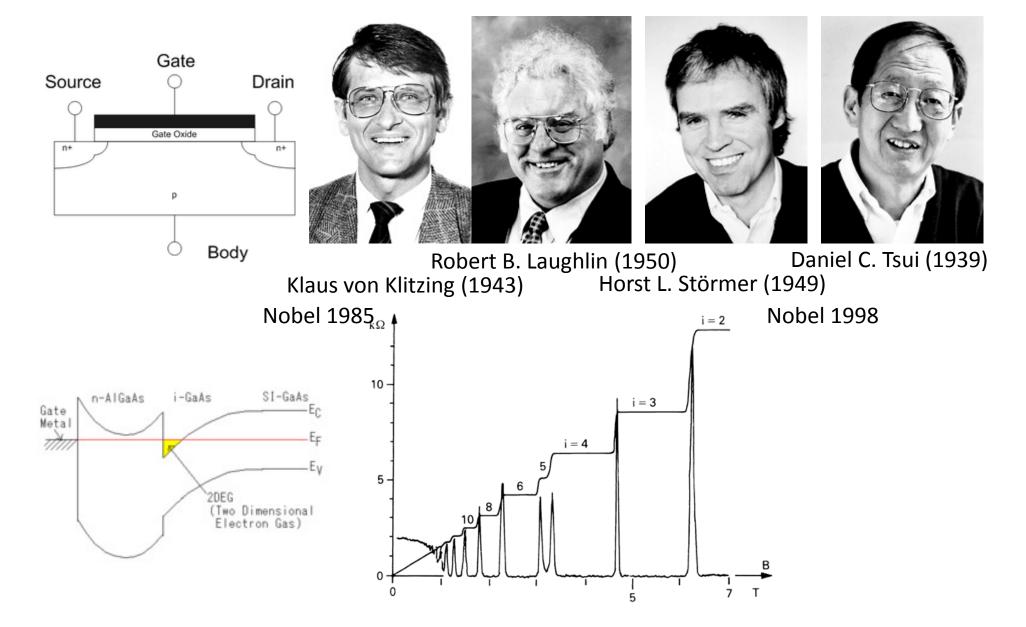


Albert Fert (1938) Peter Grünberg (1939) Nobel 2007



Read heads of hard drives

More exotic phenomena (only at low temperatures) Quantized resistance, quantum Hall effect, fractional quantum Hall effect



EMERGENT PHENOMENA

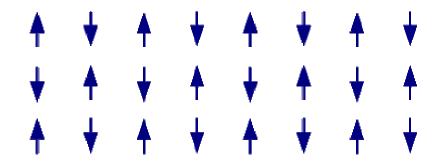
The whole is greater than the sum of its parts.

Sometimes when you put things together new order appears

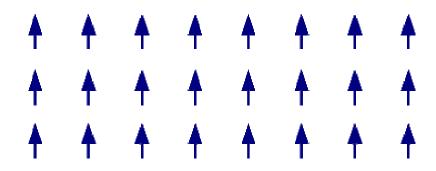
- Magnetism
- Superconductivity
- Superfluidity



An example: Antiferromagnetism









Louis Néel (1904 –2000)

Nobel 1970

)

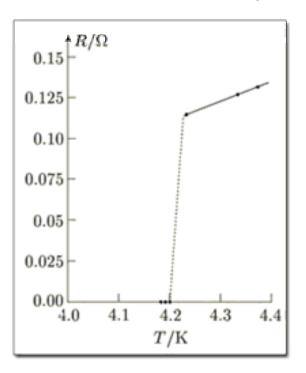
Experimental developments:

Low-temperature physics:

Kamerlingh-Onnes

1908: Liquefaction of Helium

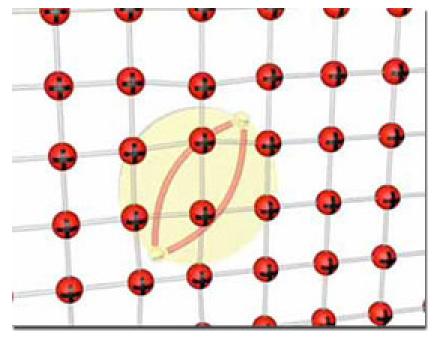
1911: Discovery of superconductivity





Heike Kamerlingh Onnes (1853 –1926) Nobel 1913

Only explained in 1957:



Cooper pairs



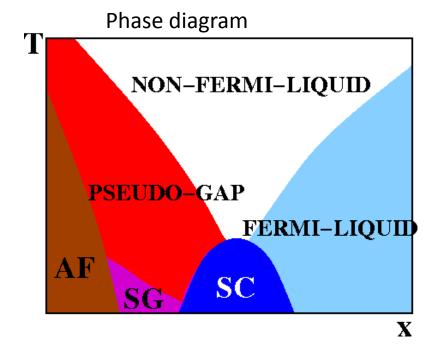
John Bardeen (1908 –1991)

Leon Cooper (1930) John Robert Schrieffer (1931)

Nobel 1972

Johannes Georg Bednorz (1950)

High temperature superconductivity





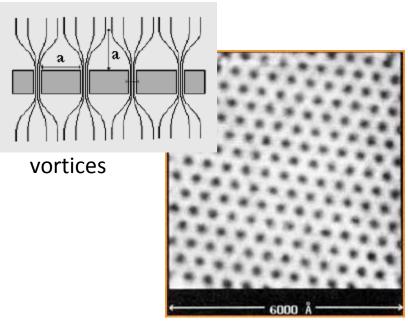
Karl Alexander Müller (1927)

Nobel 1987



Still under debate....

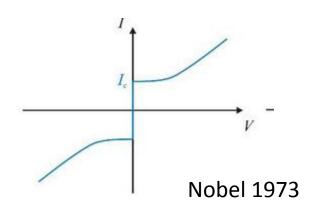
Infinitely fascinating, apparently, superconductors





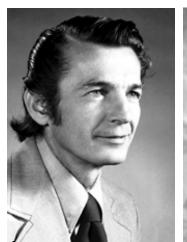
Alexei Abrikosov (1928-) Nobel prize 2004

Plus all kinds of interesting junction effects





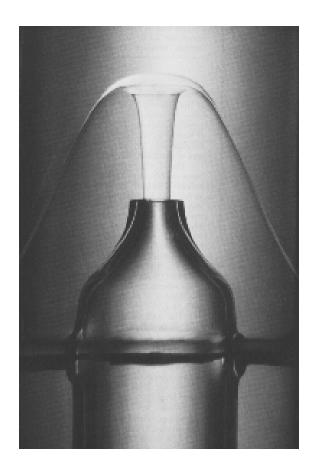




Leona Esaki (1925)

Ivar Giaever (1929)

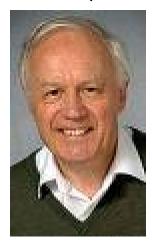
A strongly related phenomena (especially theoretically) is superfluidity



Helium II



Lev Landau (1908 –1968) Nobel 1962



Sir Anthony Leggett, KBE, FRS (1938-) Nobel 2004