Quantum Mechanics & Materials Science

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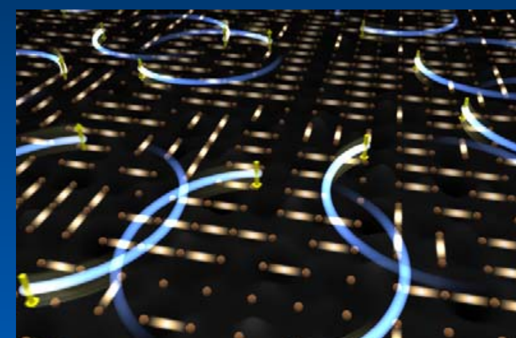
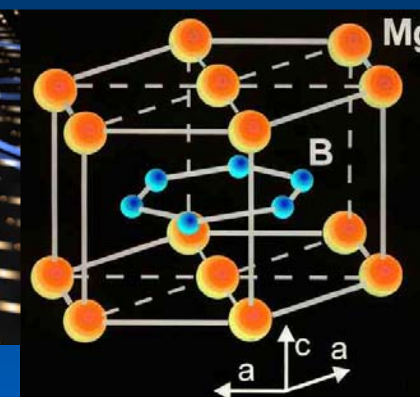
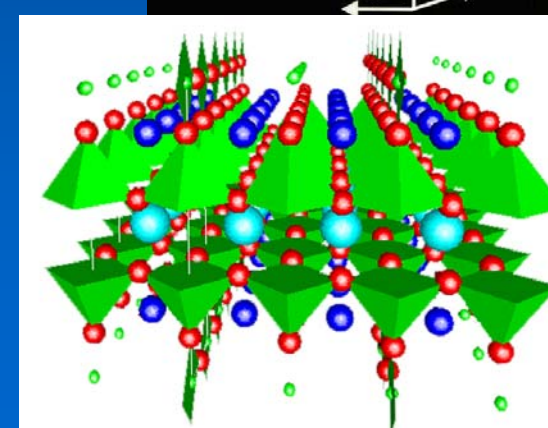




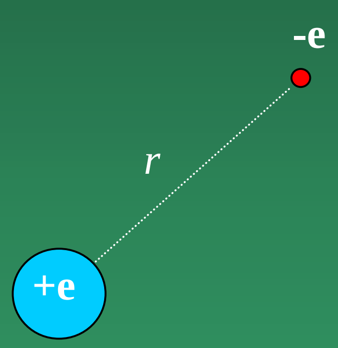


Describing Atomic Structure

One of the triumphs of quantum mechanics is its ability to explain
ATOMIC STRUCTURE

* This **CANNOT** be accounted for using the principles of classical physics

* **HYDROGEN** has the simplest atom and consists of a single negative charged **ELECTRON** and a central positive charged **NUCLEUS**



THE HYDROGEN ATOM

Coulomb Force Between the Electron & Proton:

$$F(r) = -\frac{e^2}{4\pi\varepsilon_o r^2}$$

an attractive force!

Potential Energy of Electron at a Distance r From the Nucleus:

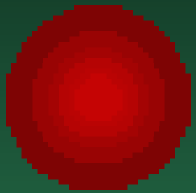
$$V(r) = V(\infty) - \int_{\infty}^{r} F(r)dr = 0 + \frac{e^2}{4\pi\varepsilon_o}\int_{\infty}^{r}\frac{dr}{r^2} = -\frac{e^2}{4\pi\varepsilon_o r}$$

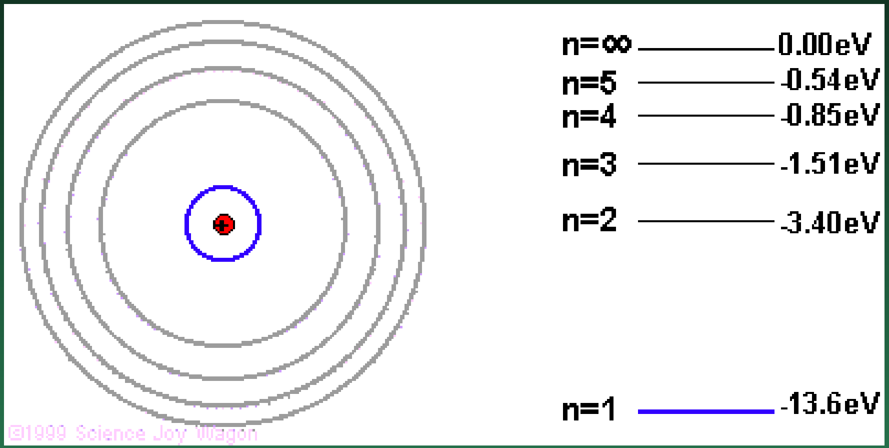
The Bohr Atom

In 1912, Niels Bohr suggested that electrons ***orbit*** around the nucleus.

⇒ However, the electrons can only be in ***special orbits***!

Niels Hendrik David Bohr
Nobel Prize in physics, 1922





$$E_n = -\frac{13.6\,\text{eV}}{n^2}$$

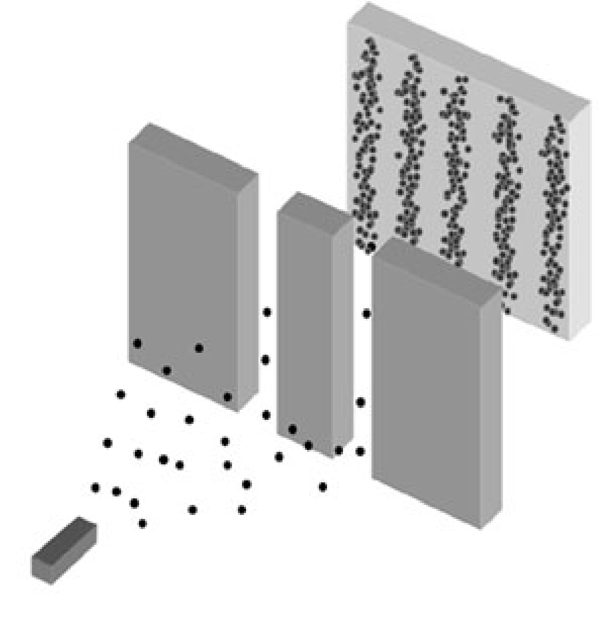
Different orbits correspond to different energies and the **energy** of the electron can only change by a small discrete amount called **"quanta".**

In actuality, electrons don't fly around the nucleus in little circles, and consequently the Bohr model fails to describe many properties of atoms.

Wave Nature of the Electron

If you perform an experiment to see where the electron is, then you find a ***"particle-like"*** electron. But otherwise the electron is a ***wave*** that carries information about where the electron is probably located.

$\Rightarrow$ When you aren't looking for it, the electron isn't in any particular place!



In quantum mechanics, the information about the likelihood of an electron being detected at a position x at time t is governed by a ***probability wave function***:

$$\Psi(x,t) = \underline{A(x,t)}\exp[\underline{iS(x,t)/\hbar}]$$

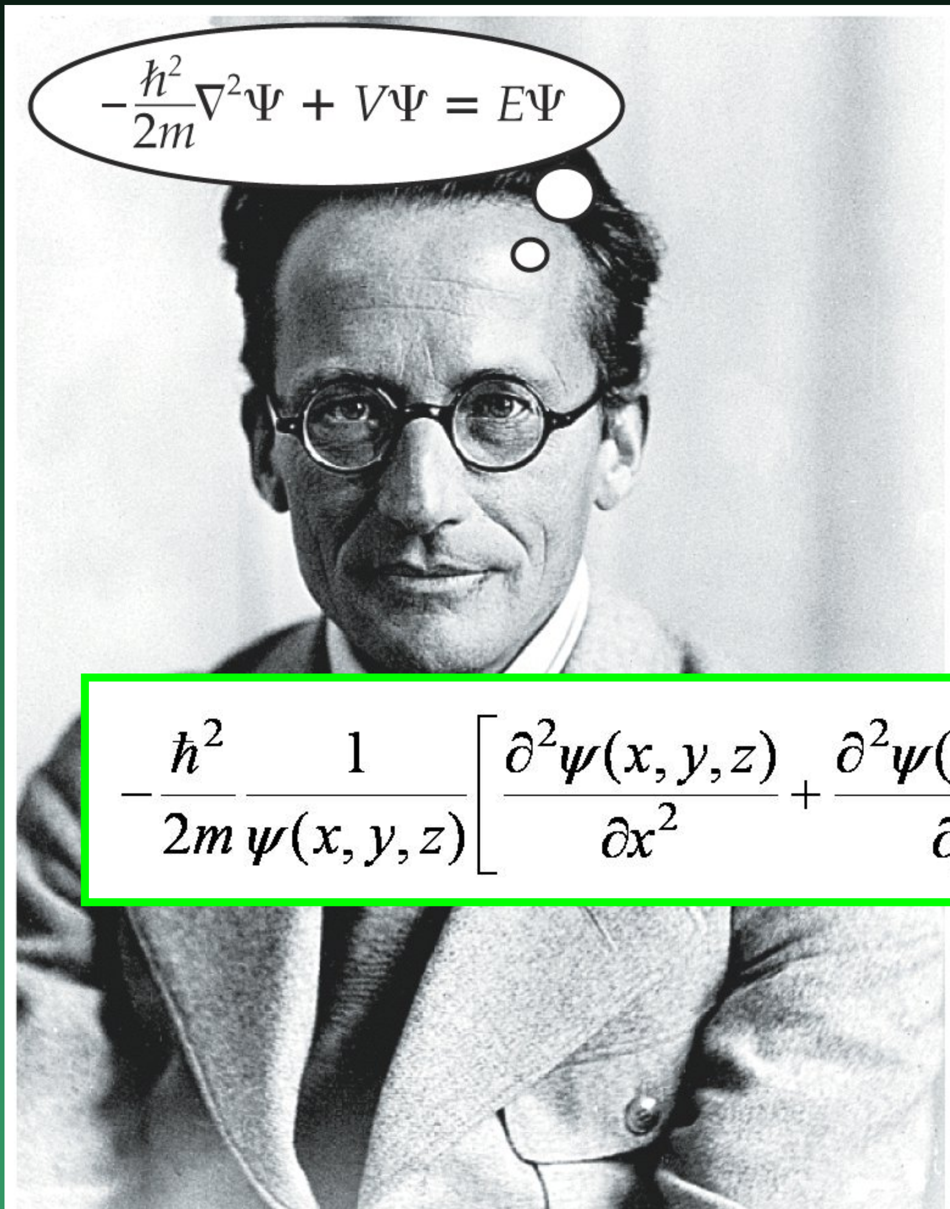
Amplitude **factor which is the square-root of the probability**

$$|\Psi(x,t)|^2 = A^2(x,t)$$

Phase **factor, which has no physical meaning**

The phase is important when we add amplitudes, so interference takes place.

The Schrödinger Equation



Schrödinger: If electrons are waves, their postion and motion in space must obey a wave equation.

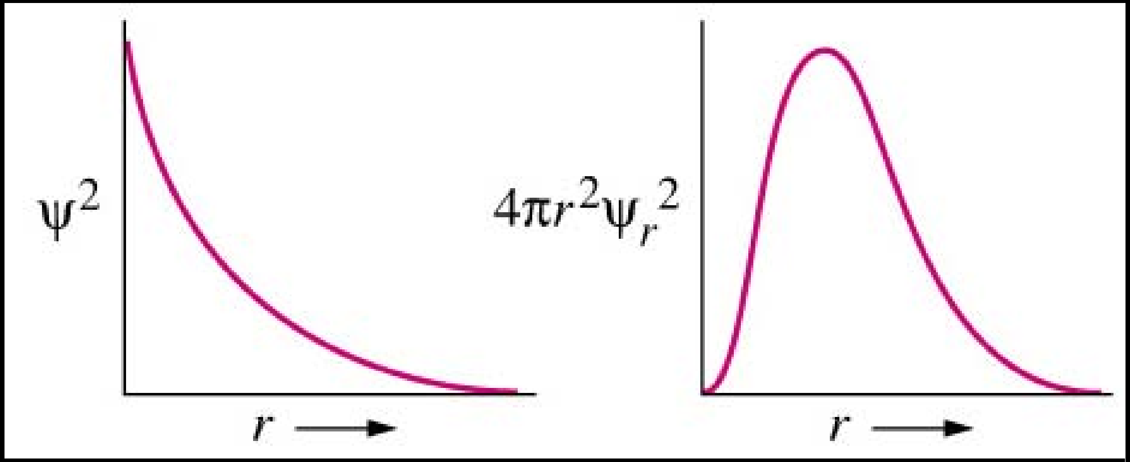
Solutions of wave equations yield wavefunctions, Ψ, which contain the information required to describe ALL of the properties of the wave.

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x,y,z)}\left[\frac{\partial^2\psi(x,y,z)}{\partial x^2}+\frac{\partial^2\psi(x,y,z)}{\partial y^2}+\frac{\partial^2\psi(x,y,z)}{\partial z^2}\right]=E-V(r)$$

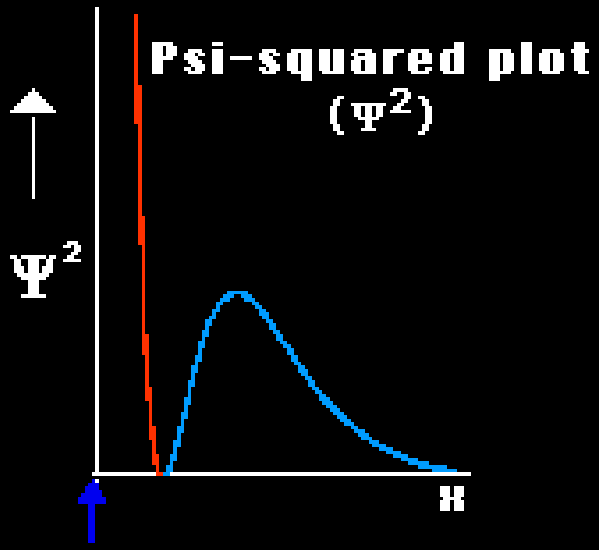
$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

The “position” of the electron is spread over space and is not well defined.

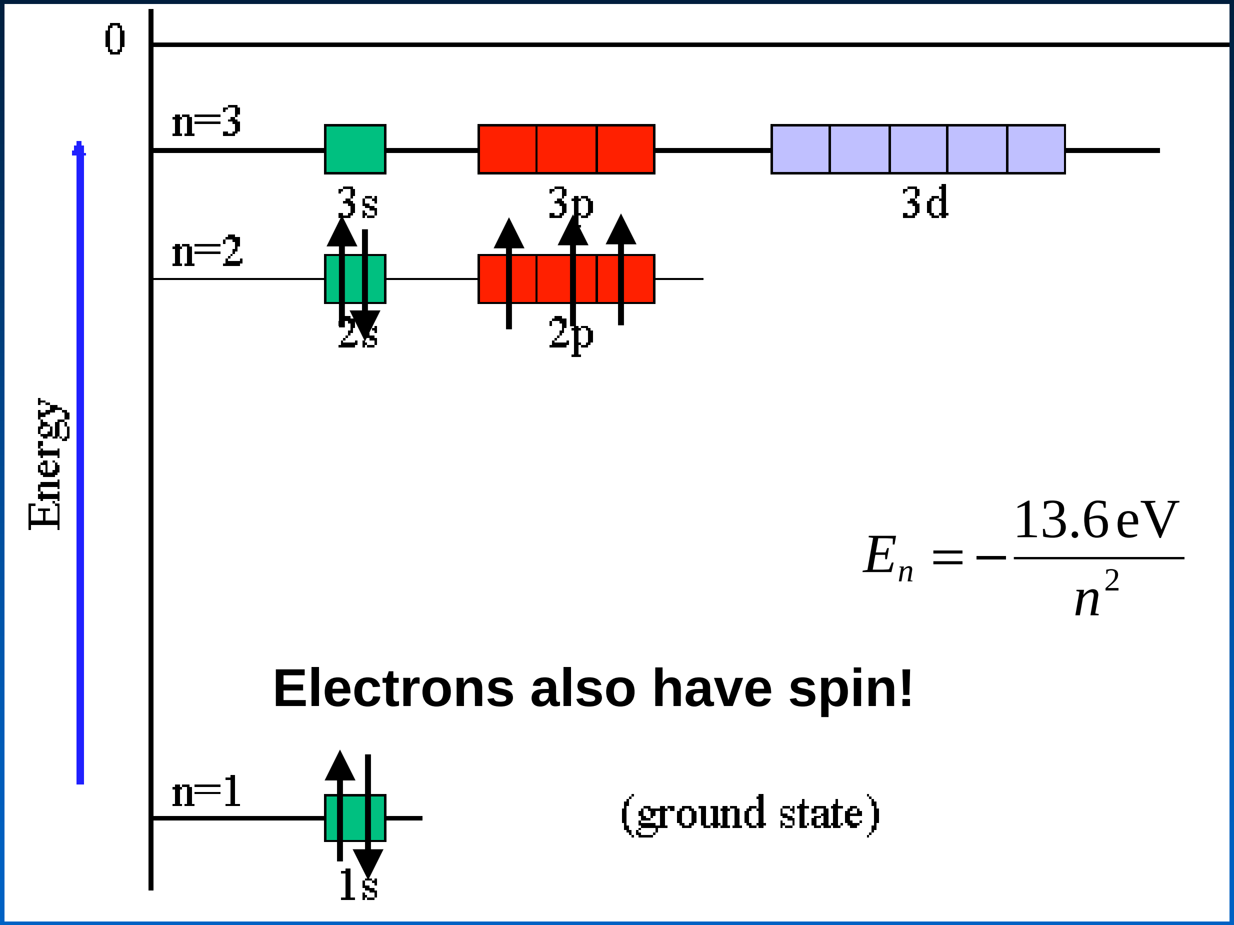
1s electron (ground state)



2s electron (first excited state)



The solutions of the Schrödinger equation lead to ***quantum numbers*** (associated with the quantization of energy and angular momentum), which provide the address of the electron in the atom!



An electron may be promoted from the ground state to an excited state by absorbing an appropriate quantum of energy.

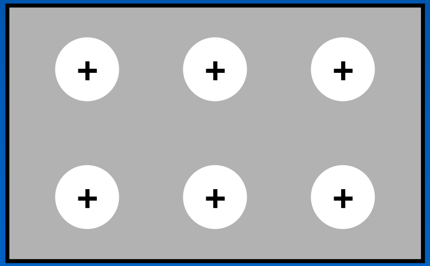
Metallic Crystals

Metals are **GOOD** electrical conductors and typically correspond to those elements whose shells are **OVERFILLED** by just one or two electrons

$$\Rightarrow \mathrm{Na}: 1s^2\, 2s^2\, 2p^6\, 3s^1$$

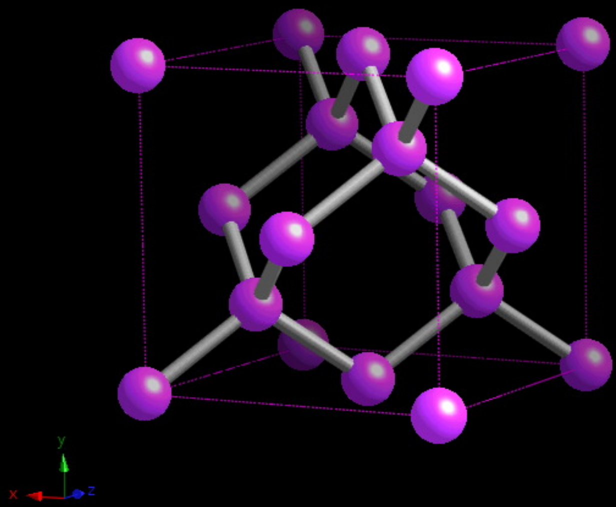
$$\Rightarrow \mathrm{Cu}: 1s^2\, 2s^2\, 2p^6\, 3s^2\, 3p^6\, 3d^{10}\, 4s^1$$

In metals these extra **VALENCE** electrons are SURRENDERED by each atom, thus forming a **SEA** of charge that may wander **FREELY** through the crystal and so **CONDUCT** electricity

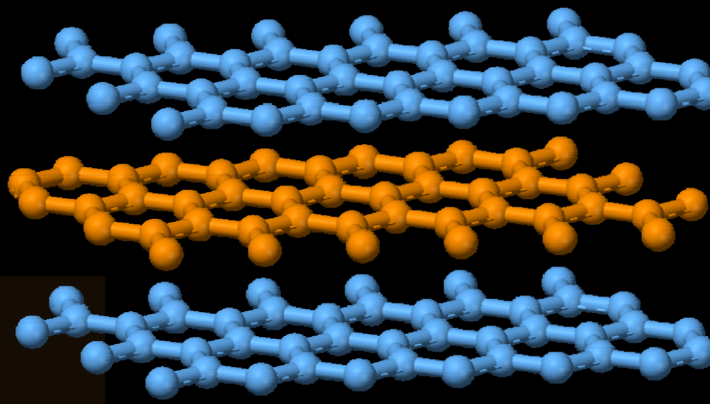


SCHEMATIC MODEL OF A METAL CRYSTAL
THE IONIZED ATOMIC CORES SIT AT FIXED POSITIONS WHILE THE GREY REGIONS REPRESENT THE ELECTRON GAS THAT IS SPREAD UNIFORMLY THROUGH THE CRYSTAL

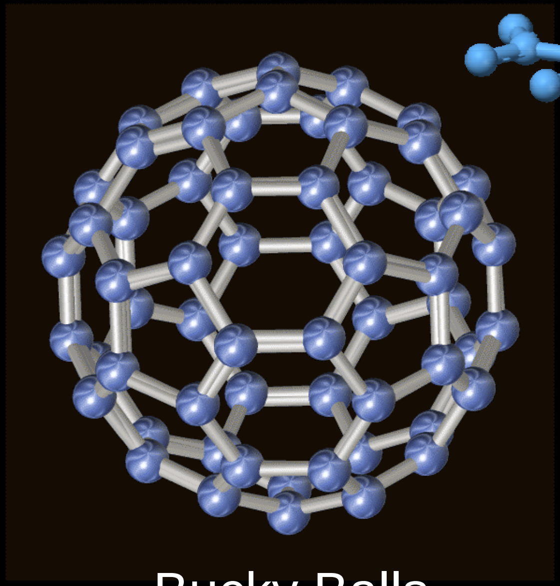
Materials Made of Pure Carbon (C)



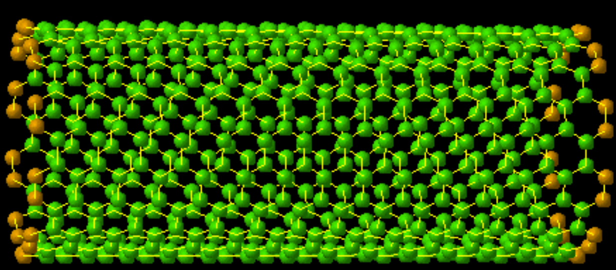
Diamond



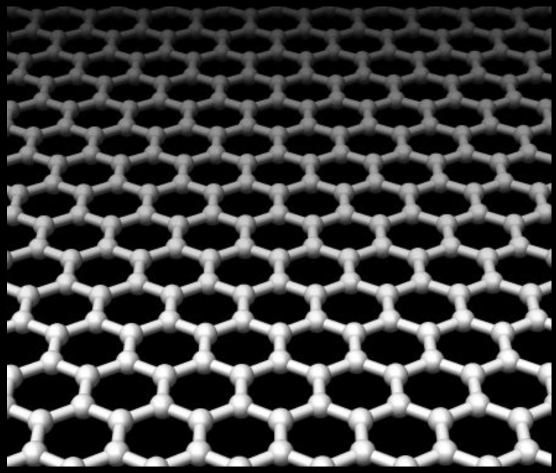
Graphite



Bucky Balls



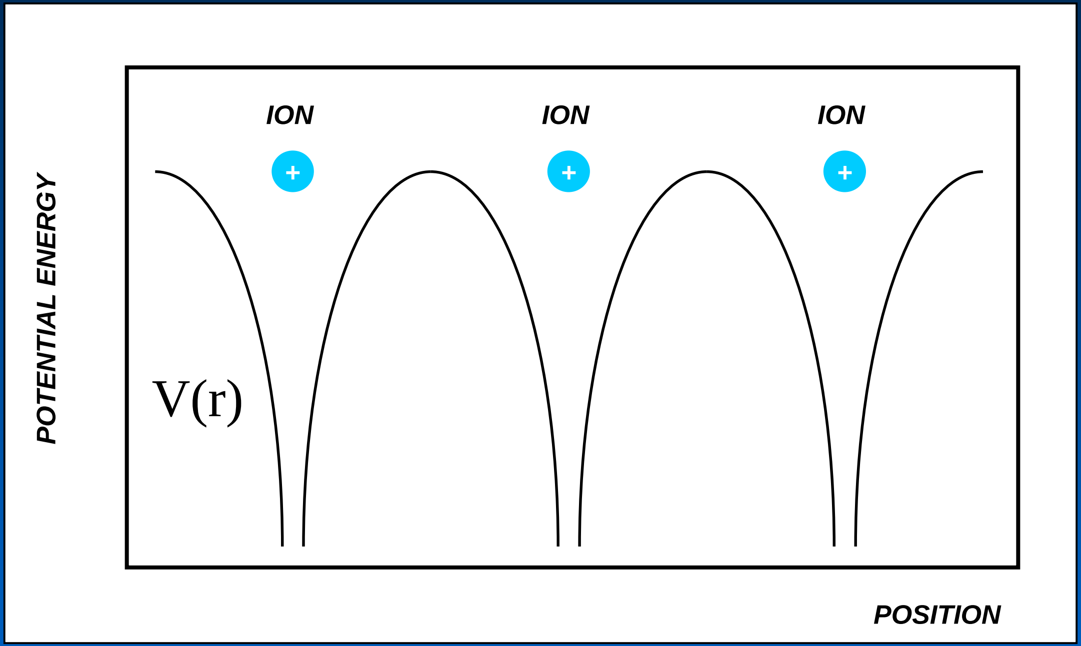
Nanotubes



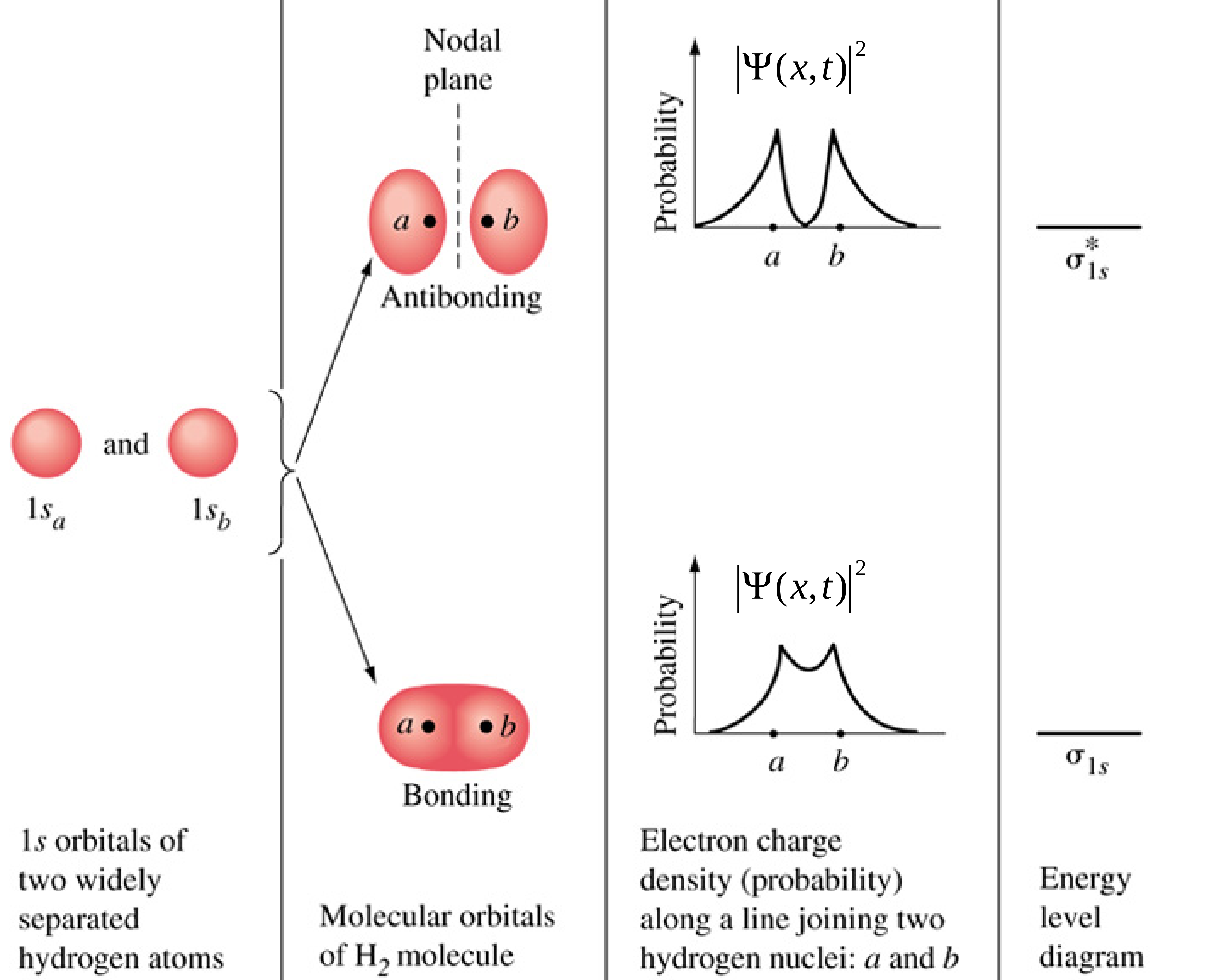
Graphene

Electrons in Solid Materials

Inside a solid, electrons move in a ***periodic potential*** $\boldsymbol{V(r)}$ due to the positive ion cores that are arranged in a periodic array (*i.e.* crystal lattice).



Solving the Schrödinger equation in this case is not so easy!

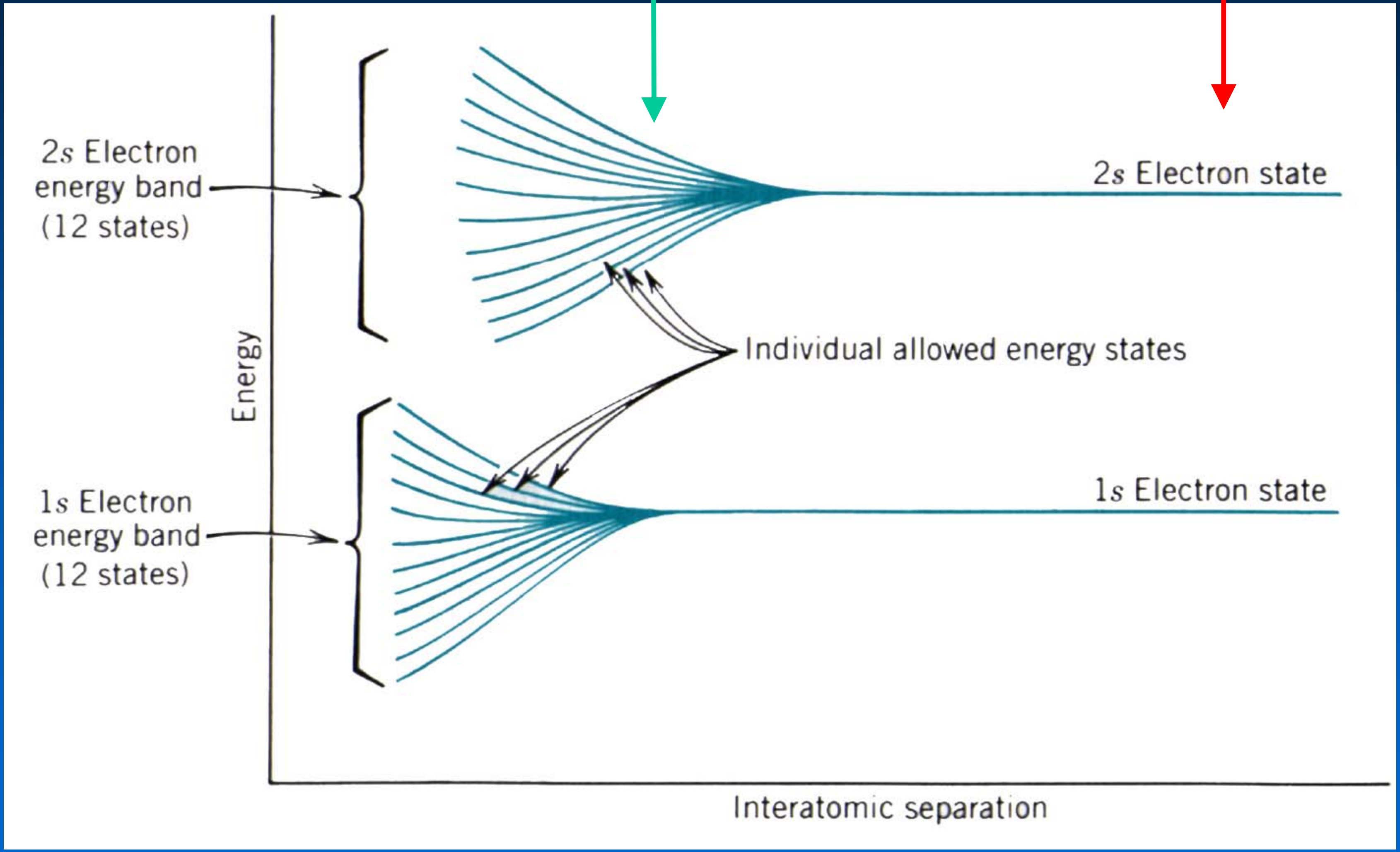


Nodal plane
a
b
Antibonding
and
1s_a
1s_b
Bonding
a
b
|Ψ(x,t)|^2
Probability
a
b
|Ψ(x,t)|^2
Probability
a
b
σ*_1s
σ_1s
1s orbitals of two widely separated hydrogen atoms
Molecular orbitals of H_2 molecule
Electron charge density (probability) along a line joining two hydrogen nuclei: a and b
Energy level diagram

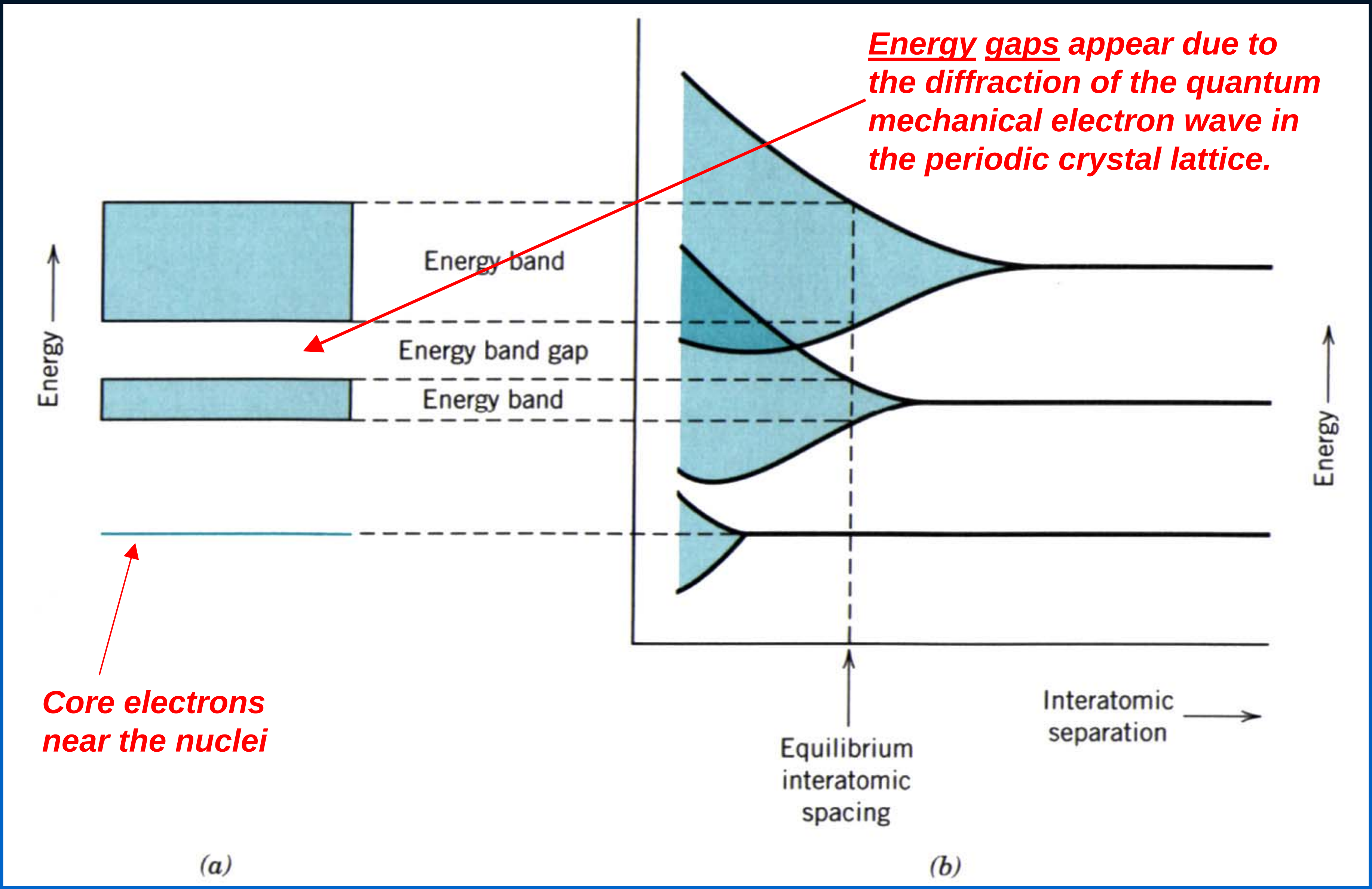
Example: 12 atoms brought together to form a solid

If the atoms are pushed together to form a solid, the electrons of neighboring atoms will interact and the allowed energy levels will broaden into *energy bands*.

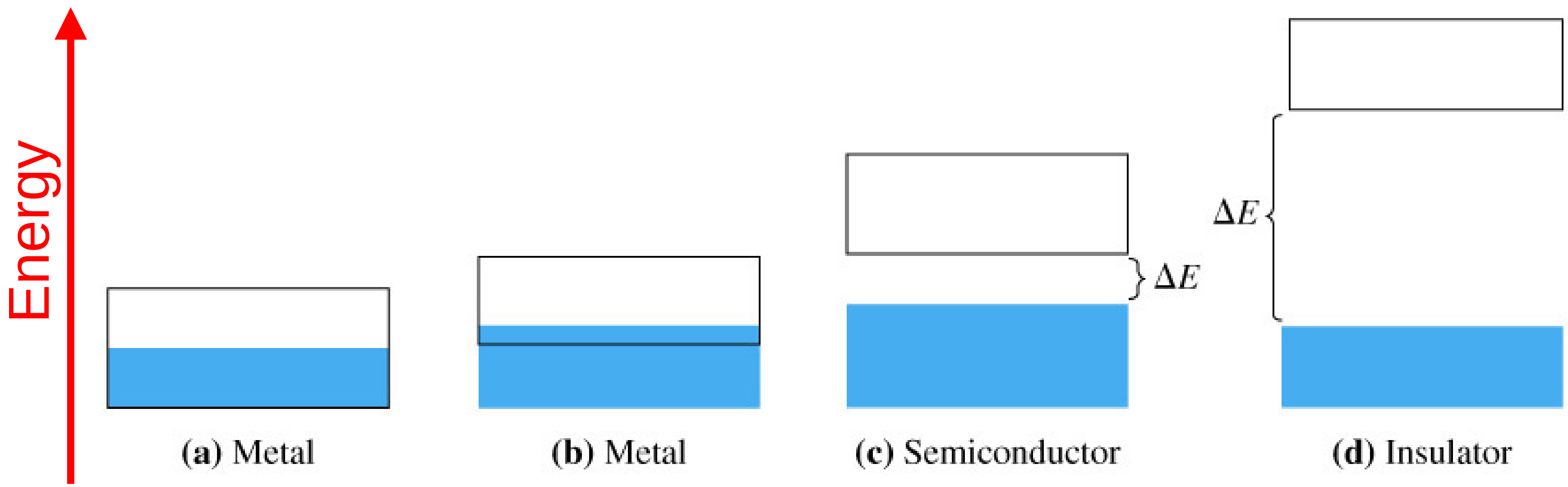
Allowed energy levels of ***isolated*** atoms.



In a real solid there are zillions of atoms!



The band structure of a solid determines how well it conducts electricity.



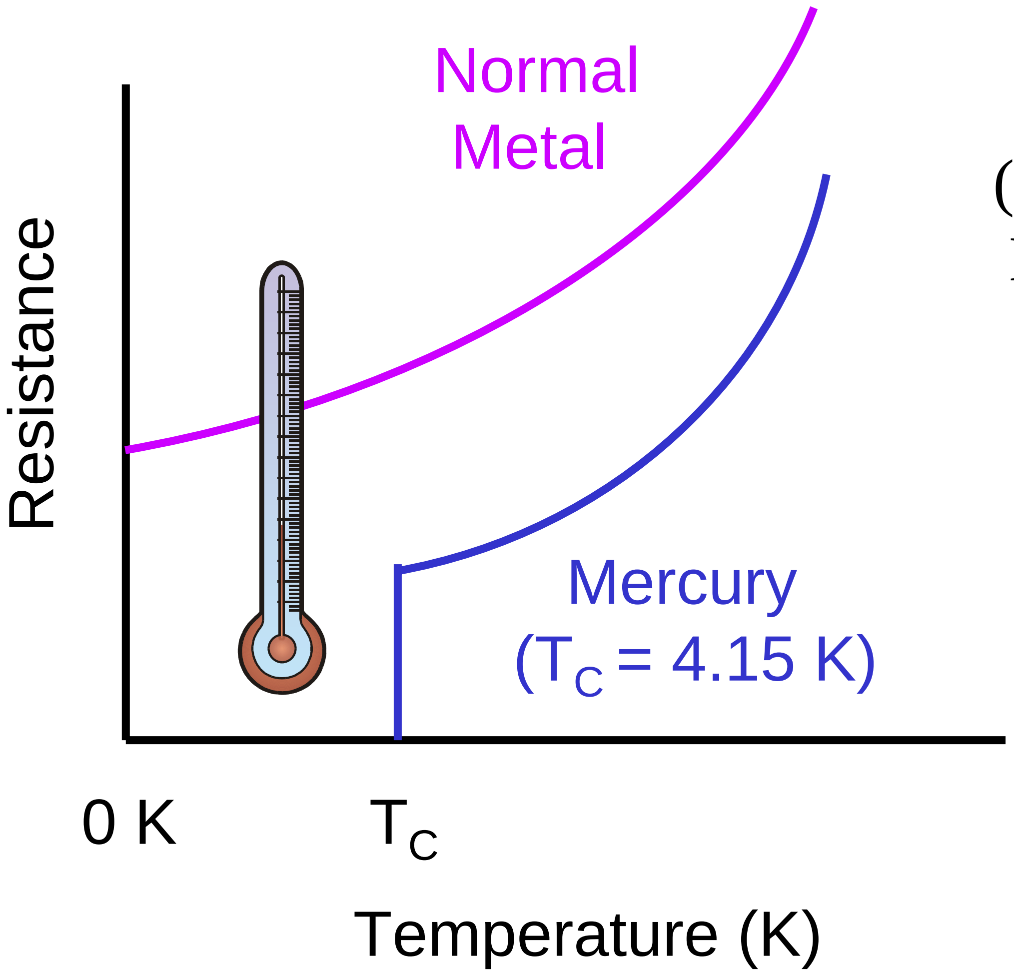
Electrical Resistance in a Metal

Resistance to the flow of electrical current is caused by ***scattering*** of electrons.

- scattering from lattice vibrations (phonons)
- scattering from defects and impurities
- scattering from electrons

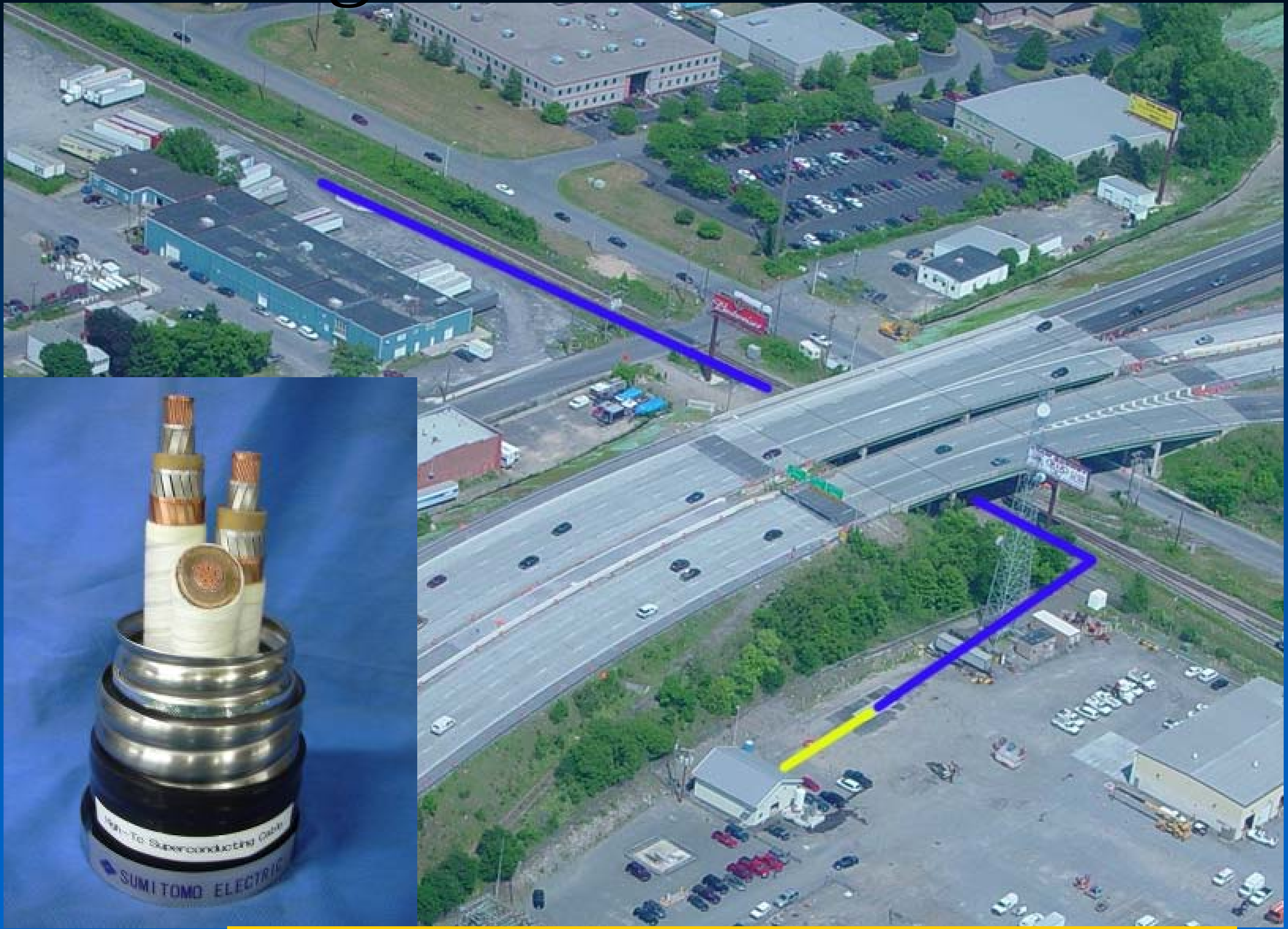
Resistance causes ***losses*** in the transmission of electric power and ***heating*** that limits the amount of electric power that can be transmitted.

Superconductivity



(1911) Dutch physicist
H. Kamerlingh-Onnes

Large HTS Power cable



Bi-2223 cable -Albany New York – commissioned fall 2006
February 2008 updated with YBCO section

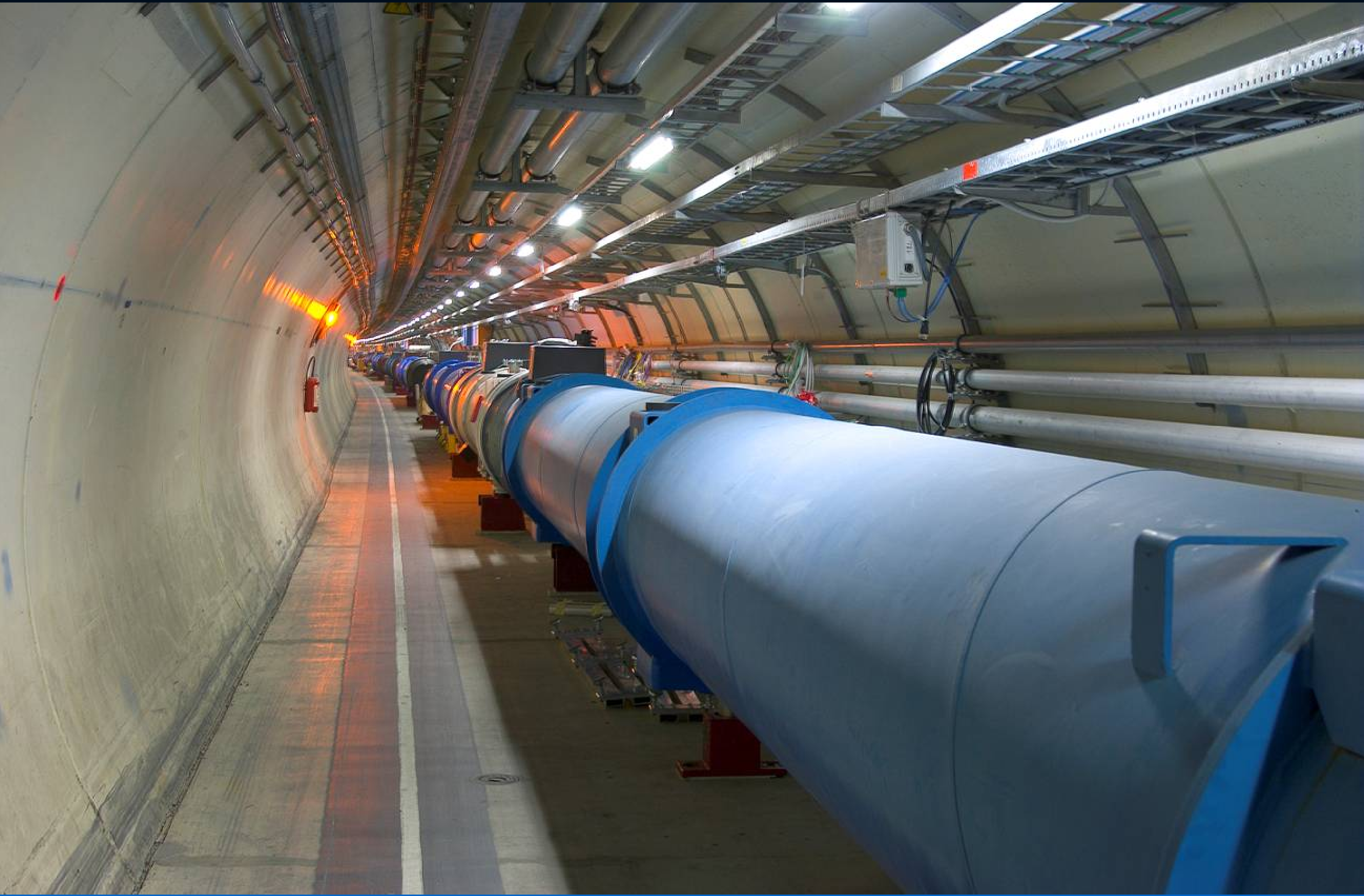
Superconducting magnets

MRI machine

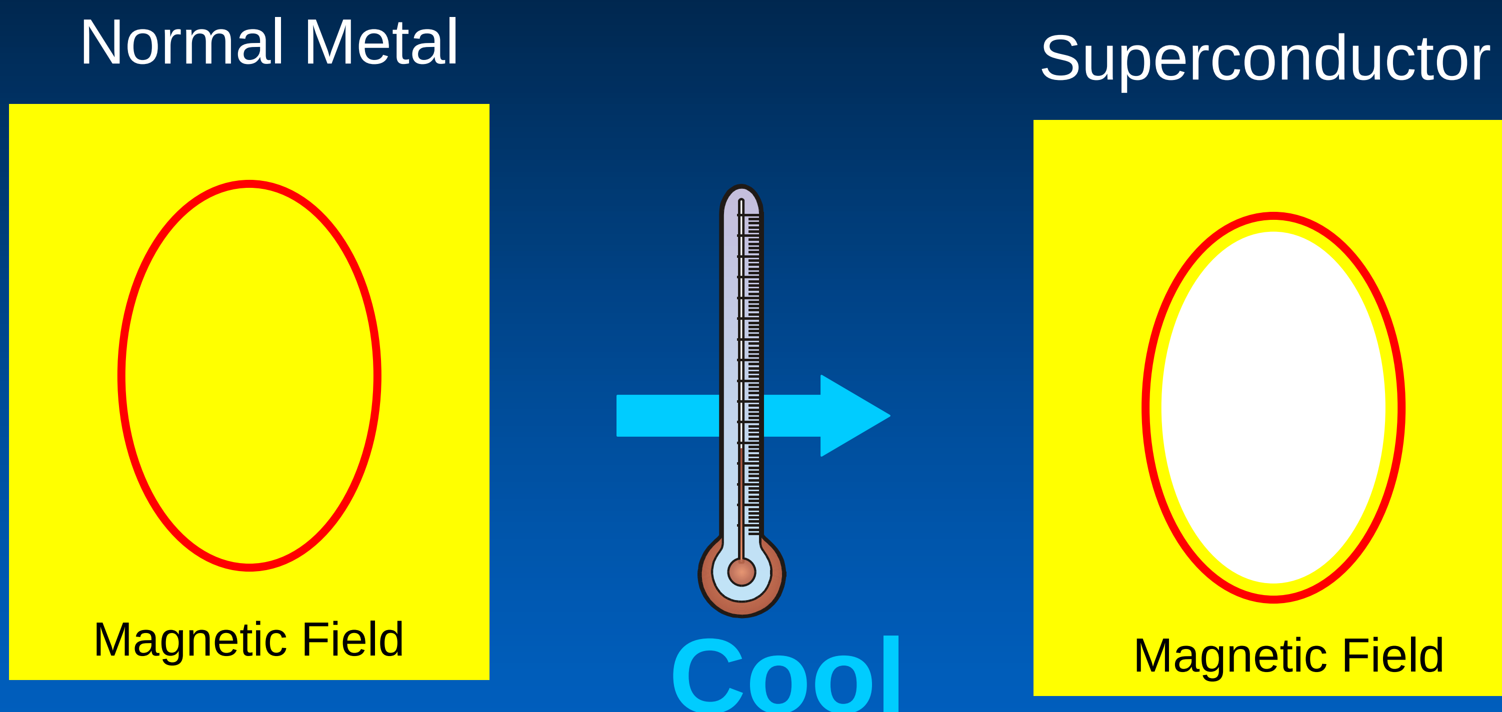
The 27 km Large Hadron Collider (LHC) at CERN in Geneva, Switzerland

By colliding protons at the enormous energy of 14 trillion electron volts, or TeV, it should be powerful enough to create the Higgs for a fleeting fraction of a second.

Inside the 27 km tunnel…



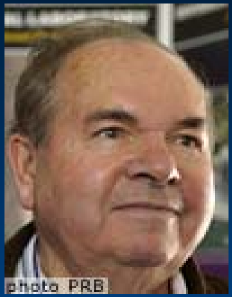
Magnetic Flux Expulsion: "Meissner Effect"

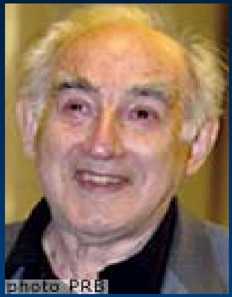


Magnetic Levitation

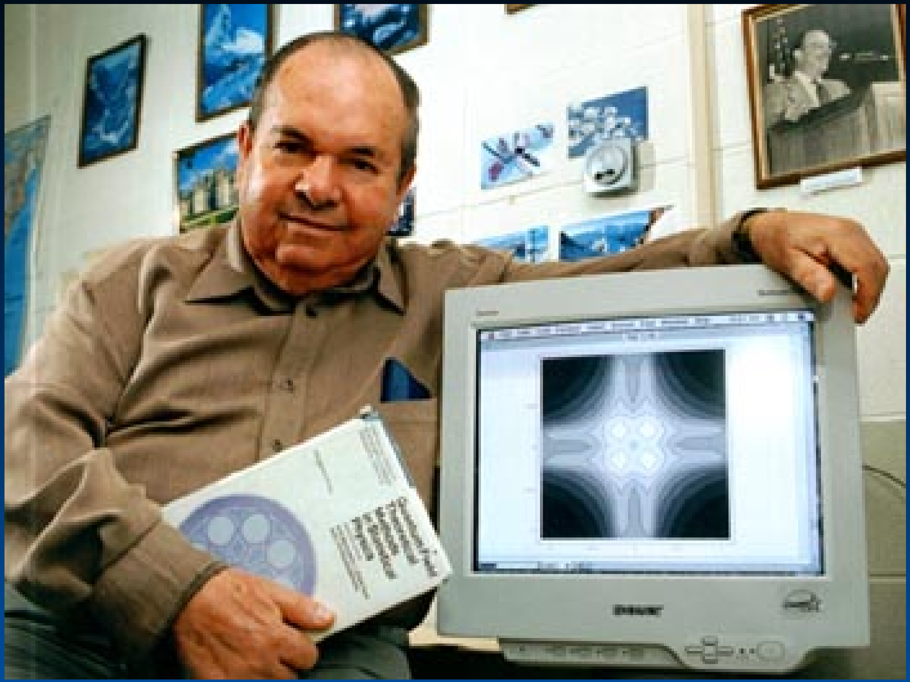
Maglev Train, Shanghai
(500 km/h)

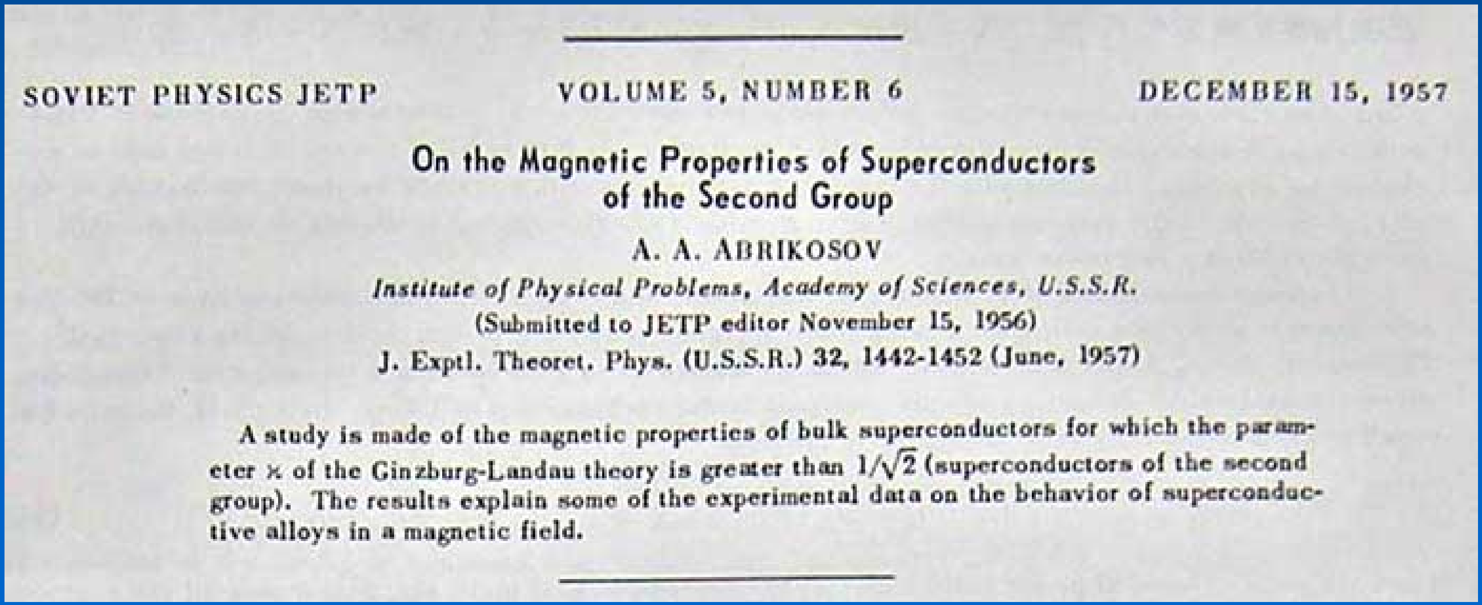
2003 Nobel Prize in Physics





A.A. Abrikosov **V.L. Ginzburg** **A.J. Leggett**





SOVIET PHYSICS JETP VOLUME 5, NUMBER 6 DECEMBER 15, 1957

On the Magnetic Properties of Superconductors of the Second Group

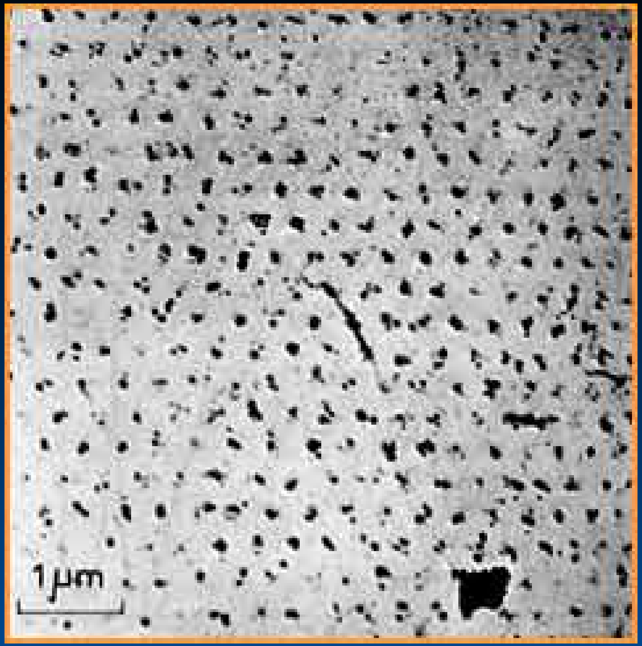
A. A. ABRIKOSOV

Institute of Physical Problems, Academy of Sciences, U.S.S.R.

(Submitted to JETP editor November 15, 1956)

J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 1442-1452 (June, 1957)

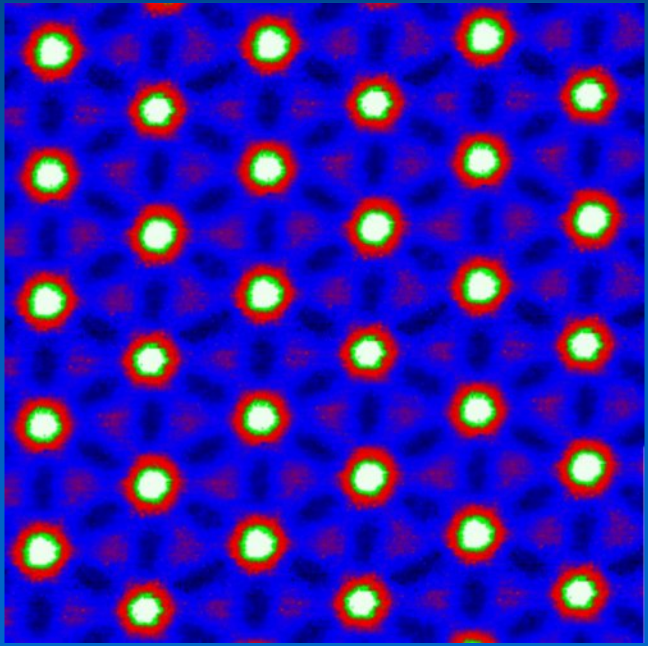
A study is made of the magnetic properties of bulk superconductors for which the parameter $\varkappa$ of the Ginzburg-Landau theory is greater than $1/\sqrt{2}$ (superconductors of the second group). The results explain some of the experimental data on the behavior of superconductive alloys in a magnetic field.



First observation of the Abrikosov Vortex Lattice

Bitter Decoration

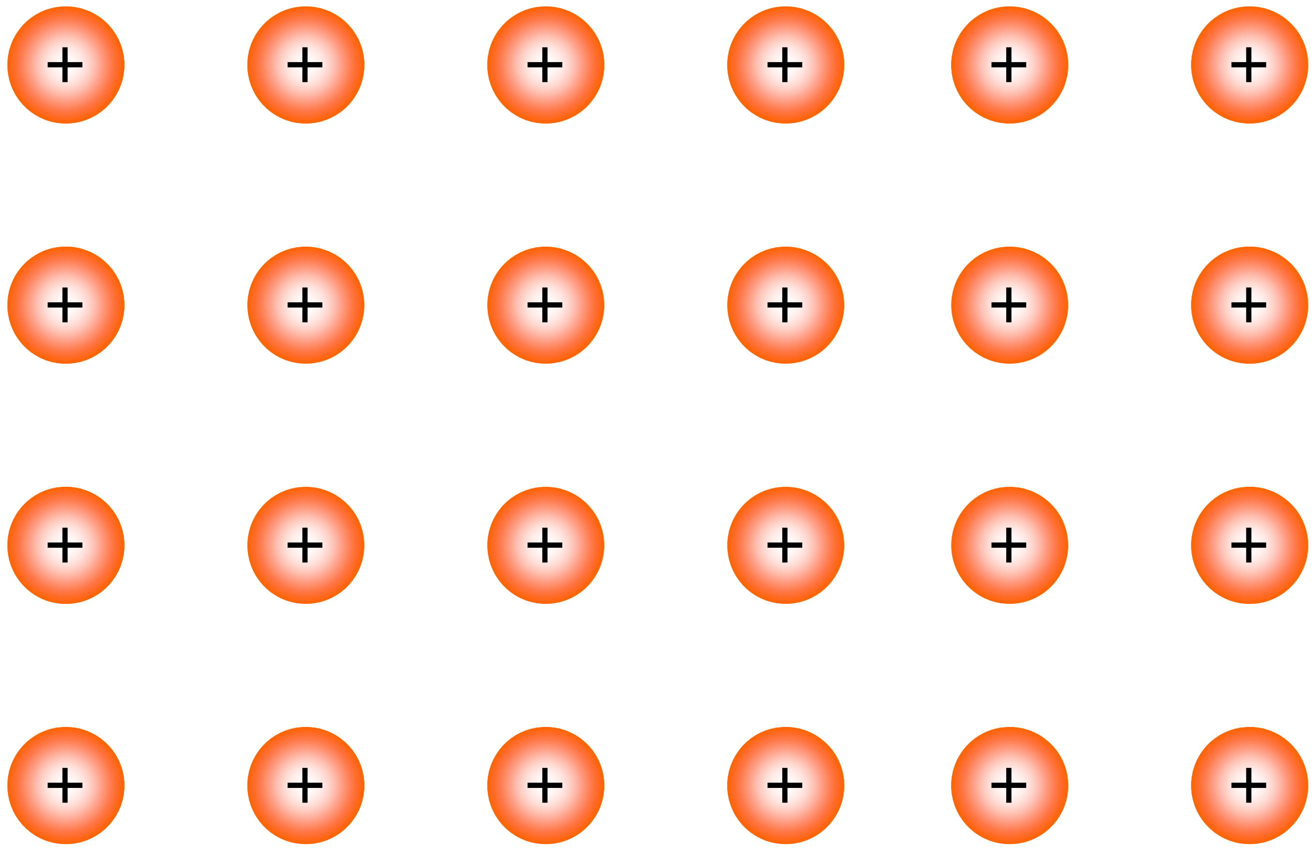
U. Essmann and H. Trauble
Physics Letters 25A, 526 (1967)



Modern Image of the Abrikosov Vortex Lattice

STM

J.C. Davis *et al.*



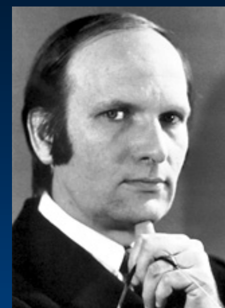
“Cooper Pair”

BCS Theory of Superconductivity

1972 Nobel Prize in Physics

J. Bardeen

L.N. Cooper



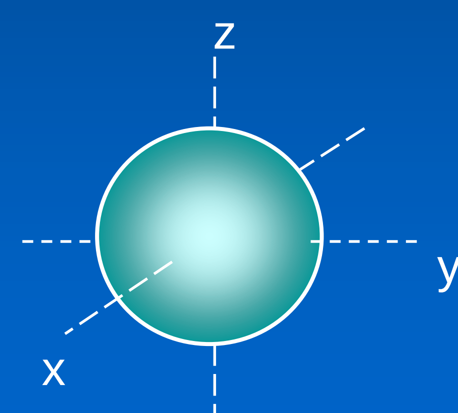
J.R. Schrieffer

General idea - Electrons pair up ("Cooper pairs") and form a ***coherent quantum state***, making it impossible to deflect the motion of one pair without involving all the others.

Zero resistance and the expulsion of magnetic flux require that the Cooper pairs share the same phase $\Rightarrow$ **"quantum phase coherence"**

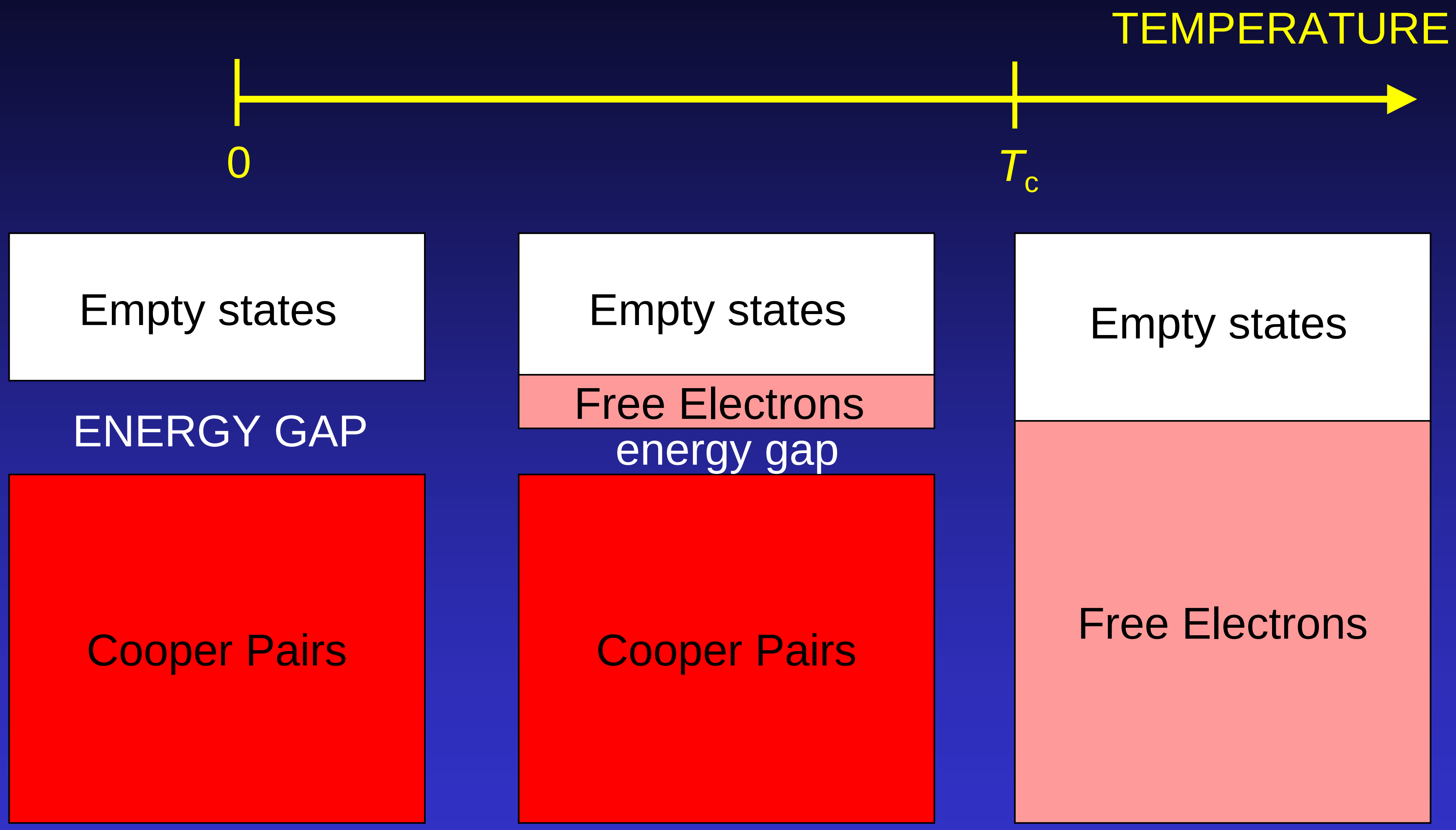
The superconducting state is characterized by a complex ***macroscopic wave function***:

$$\Psi(\vec{r}) = \underbrace{|\Psi_0|}_{\text{Amplitude}}\, e^{\underbrace{i\theta(\vec{r})}_{\text{Phase}}}$$



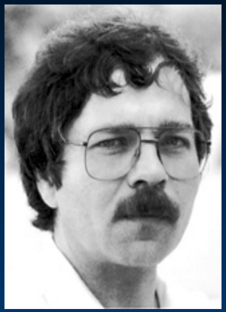
***s*-wave pairing symmetry**

BCS Superconductor

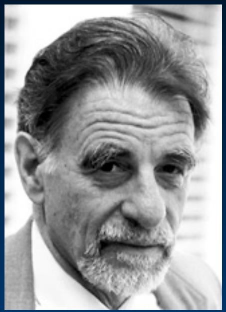


High-Temperature Superconductivity

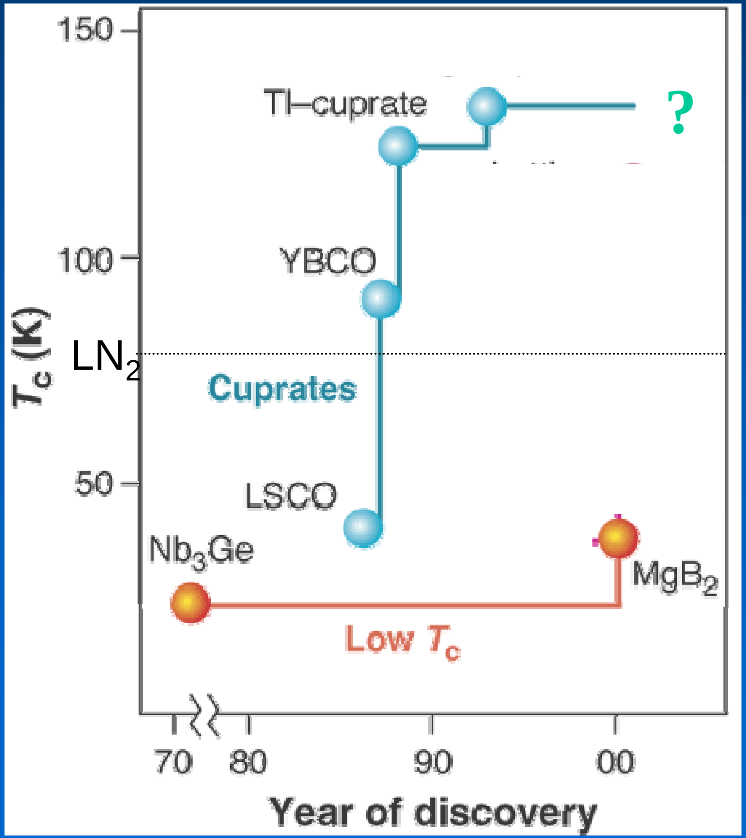
1987 Nobel Prize in Physics

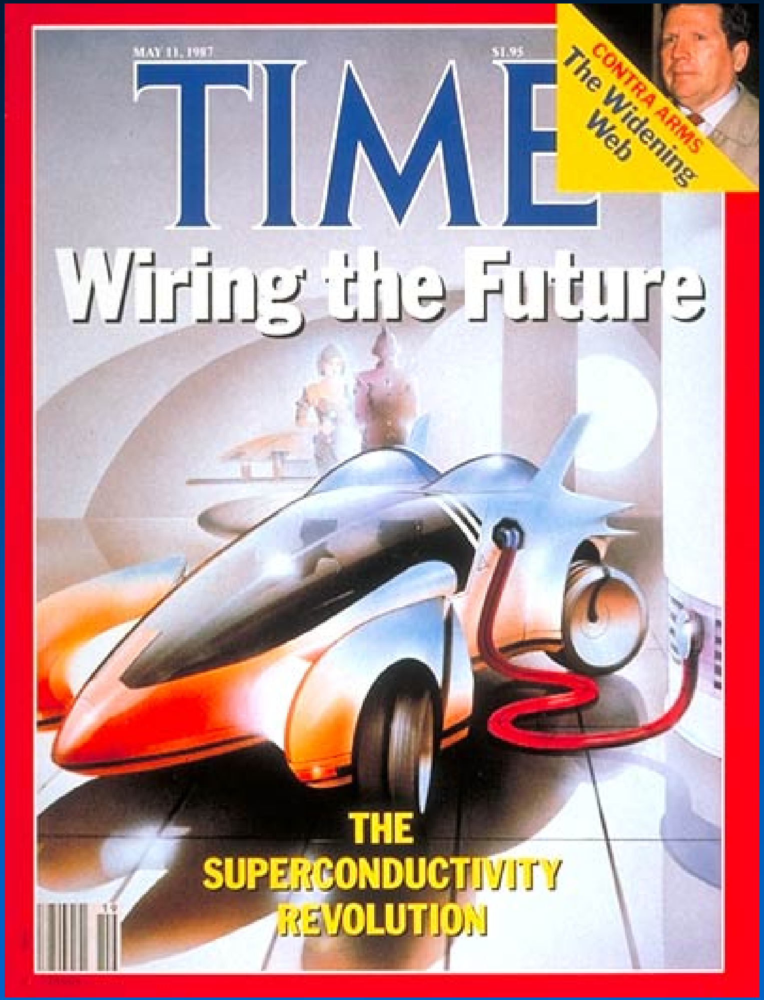


J.G. Bednorz



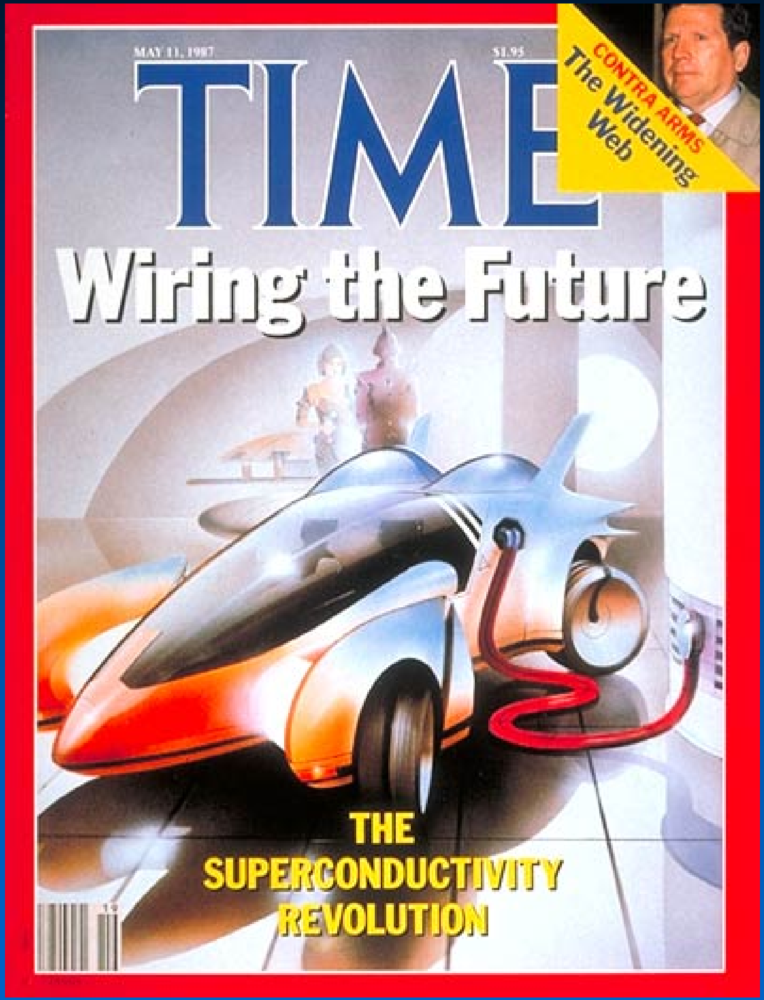
K.A. Müeller





Time Magazine May 11, 1987

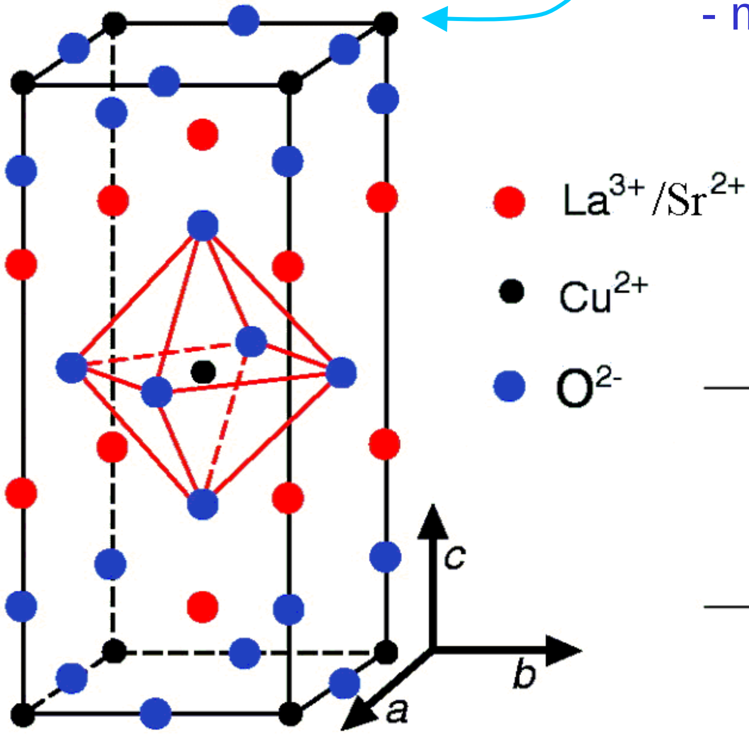
High-Temperature Superconductivity



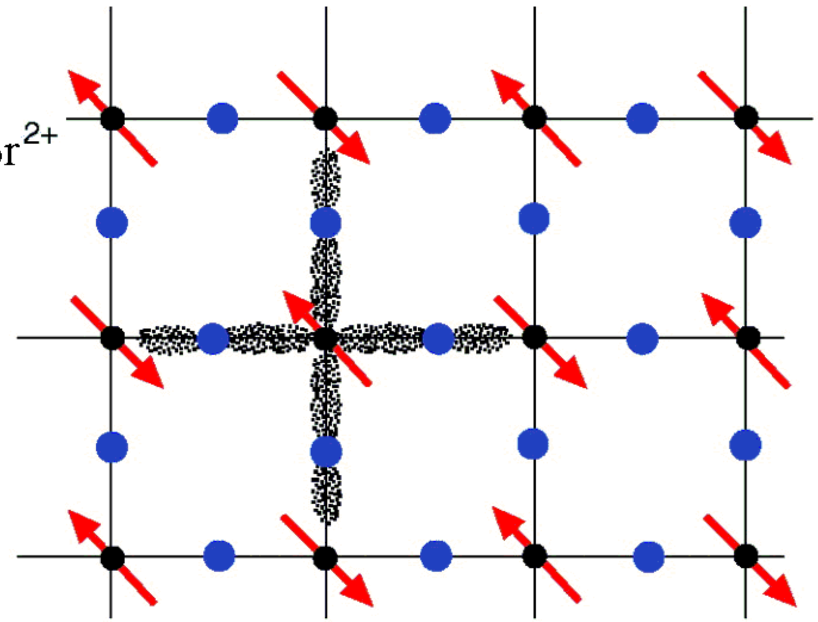
Time Magazine May 11, 1987

High-T_c Cuprates

$La_{2-x}Sr_xCuO_4$

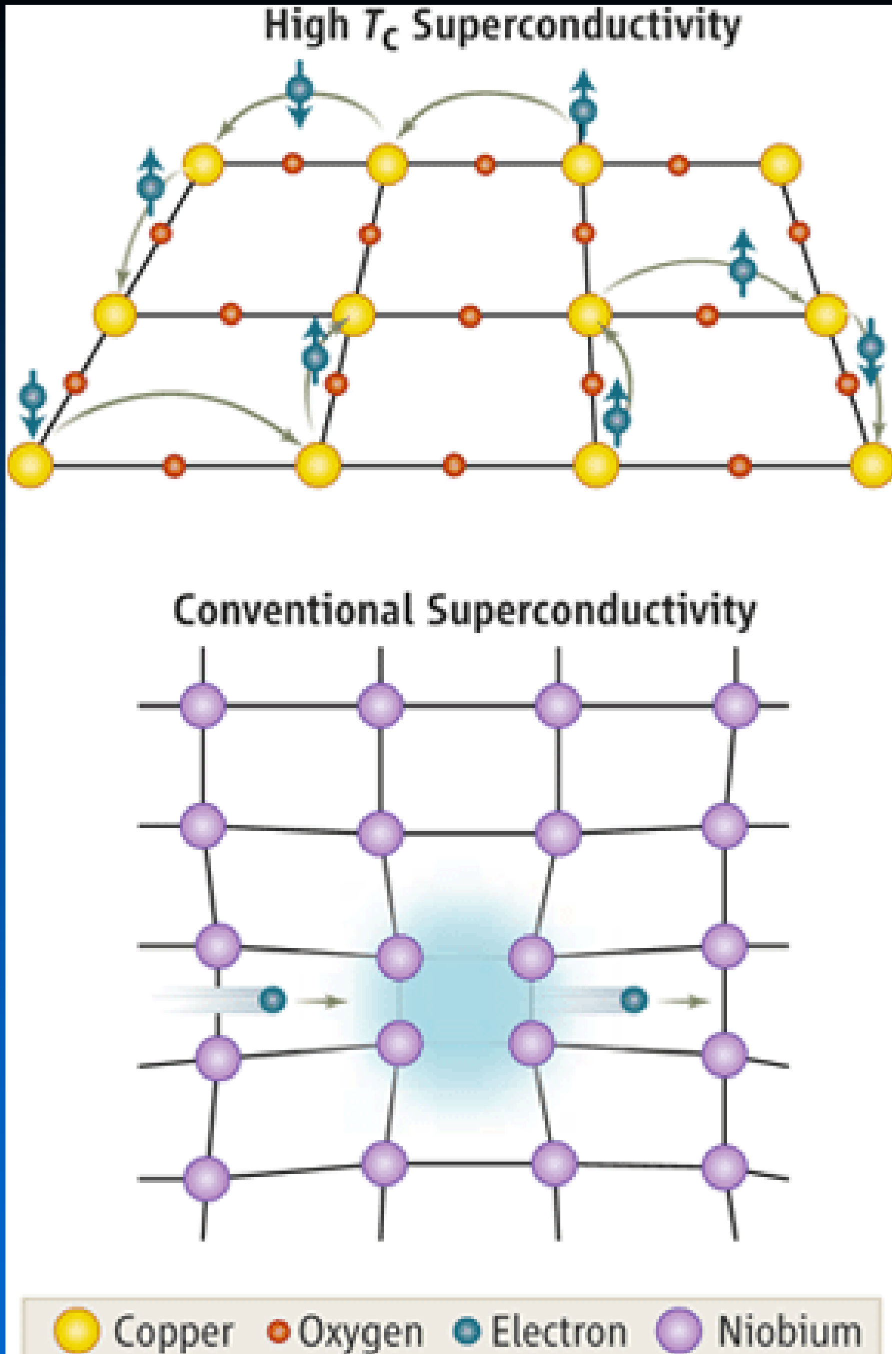


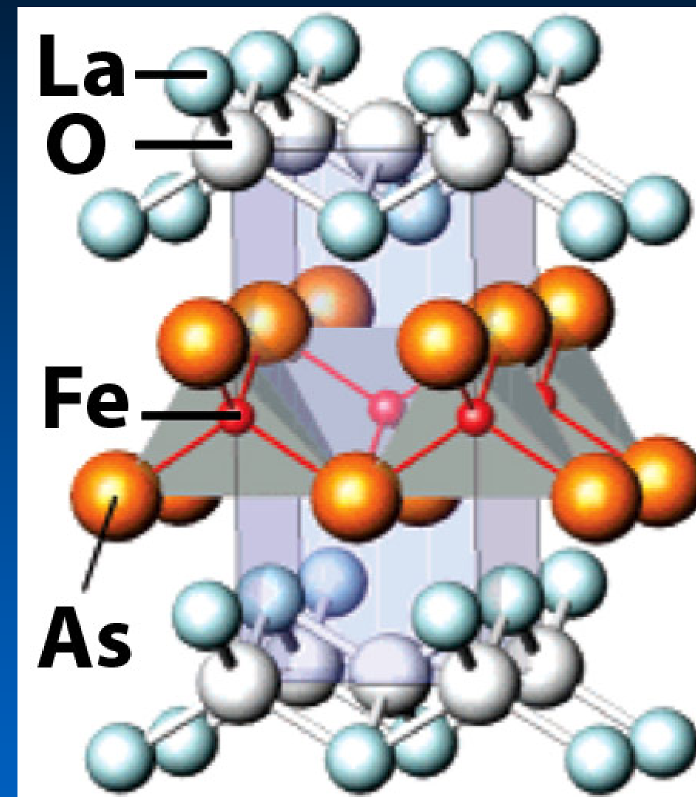
CuO_2 planes are generic ingredient
- superconductivity is quasi-2D
- magnetism associated with Cu spins



Antiferromagnet → **Superconductor**

Hole doping by cation substitution or oxygen doping

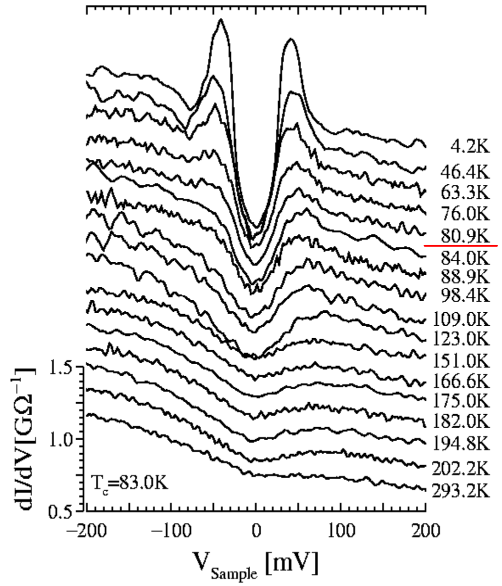




2008 - New high-T_c superconductors

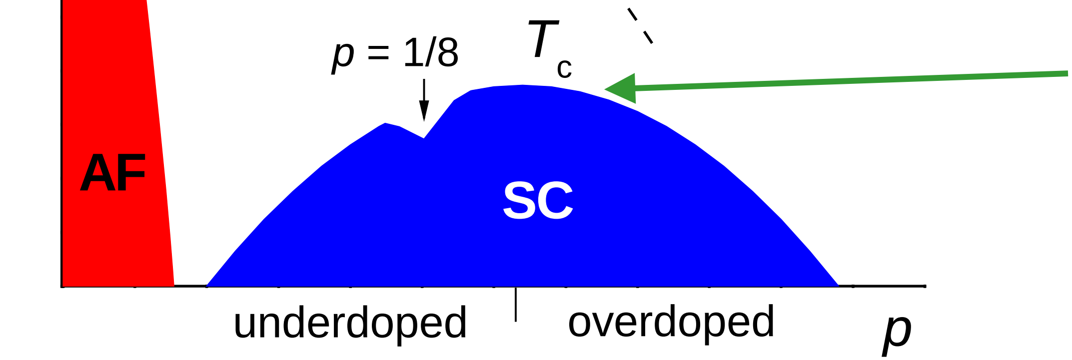
Renner *et al.*, *PRL* **80**, 149 (1998)

$Bi_2Sr_2CaCu_2O_{8+\delta}$ (T_c = 83 K)



Origin of Pseudogap?

- ***Precursor*** of SC gap?
- Some other form of ***competing*** order?



What determines T_c?

$$\Psi(\vec{r}) = |\Psi_0| e^{i\theta(\vec{r})}$$

Macroscopic wave function describing the superconducting state

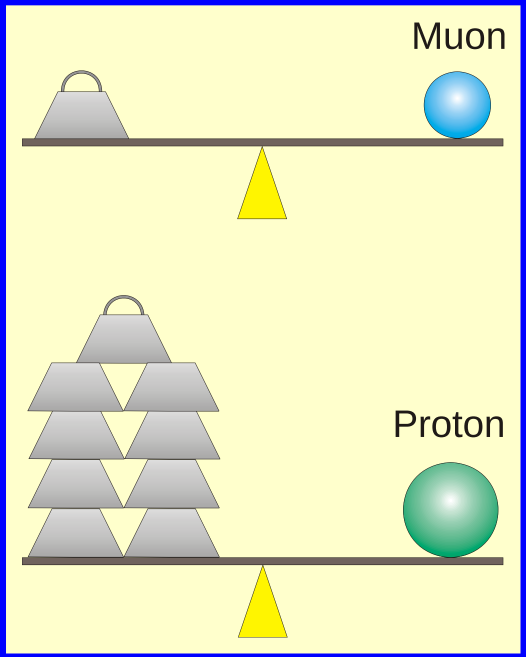
In the superconducting state, the pairing amplitude $|\Psi_0|$ and the phase $\theta(\vec{r})$ are rigid.

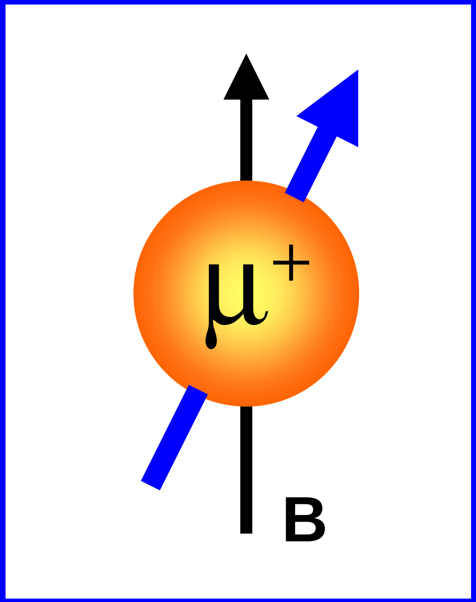
The superconducting state can be destroyed by ***fluctuations*** of the amplitude, phase or both.

- **BCS Superconductor**
  Superconductivity destroyed by amplitude fluctuations
  i.e. destruction of Cooper pairs

- **High-Temperature Superconductor**
  Superconductivity destroyed by phase fluctuations
  i.e. destruction of long-range phase coherence amongst Cooper pairs

Consequently the simple binding of electrons into Cooper pairs and short-range phase coherence may occur at temperatures well above T_c!



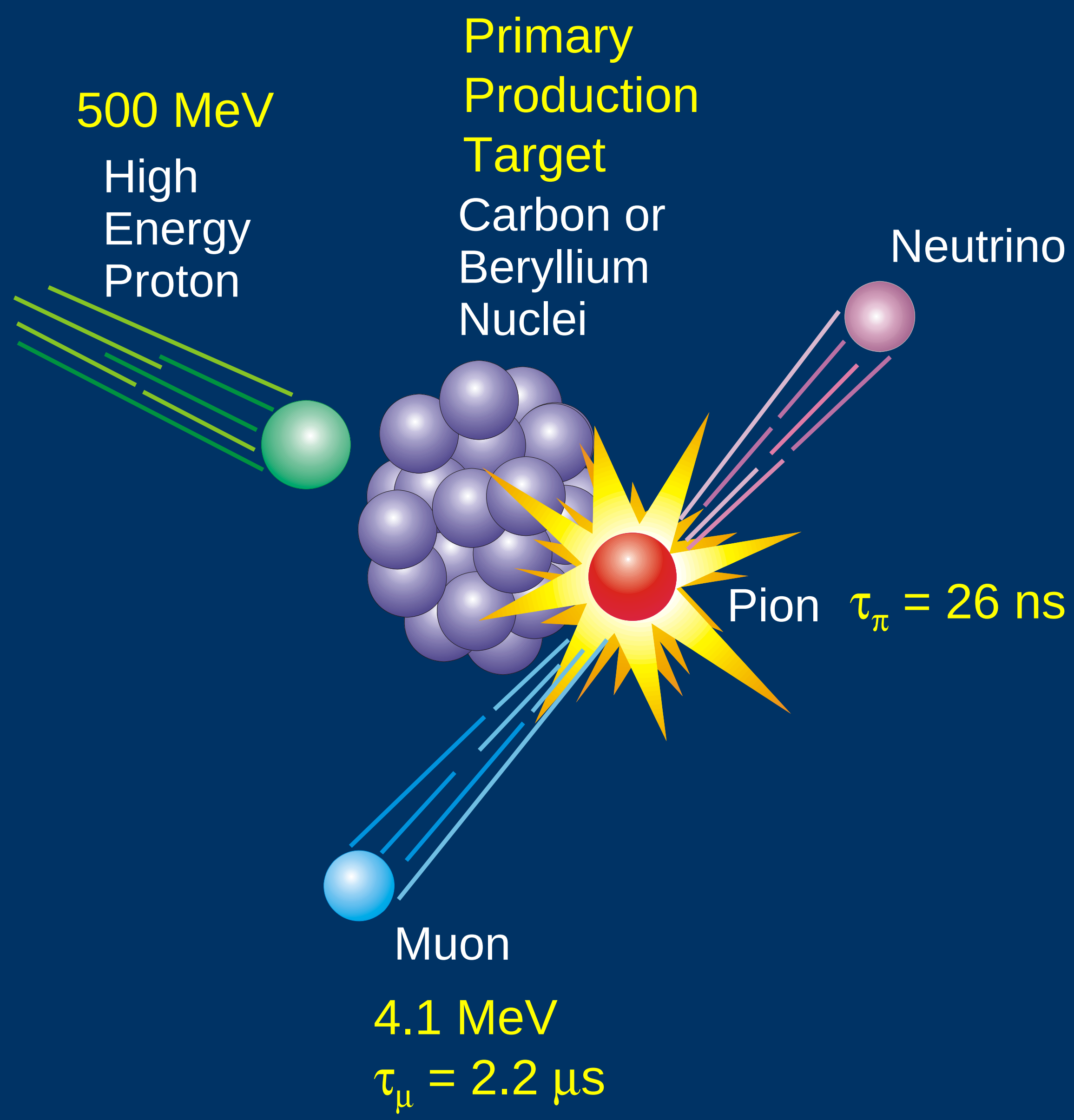


Spin 1/2

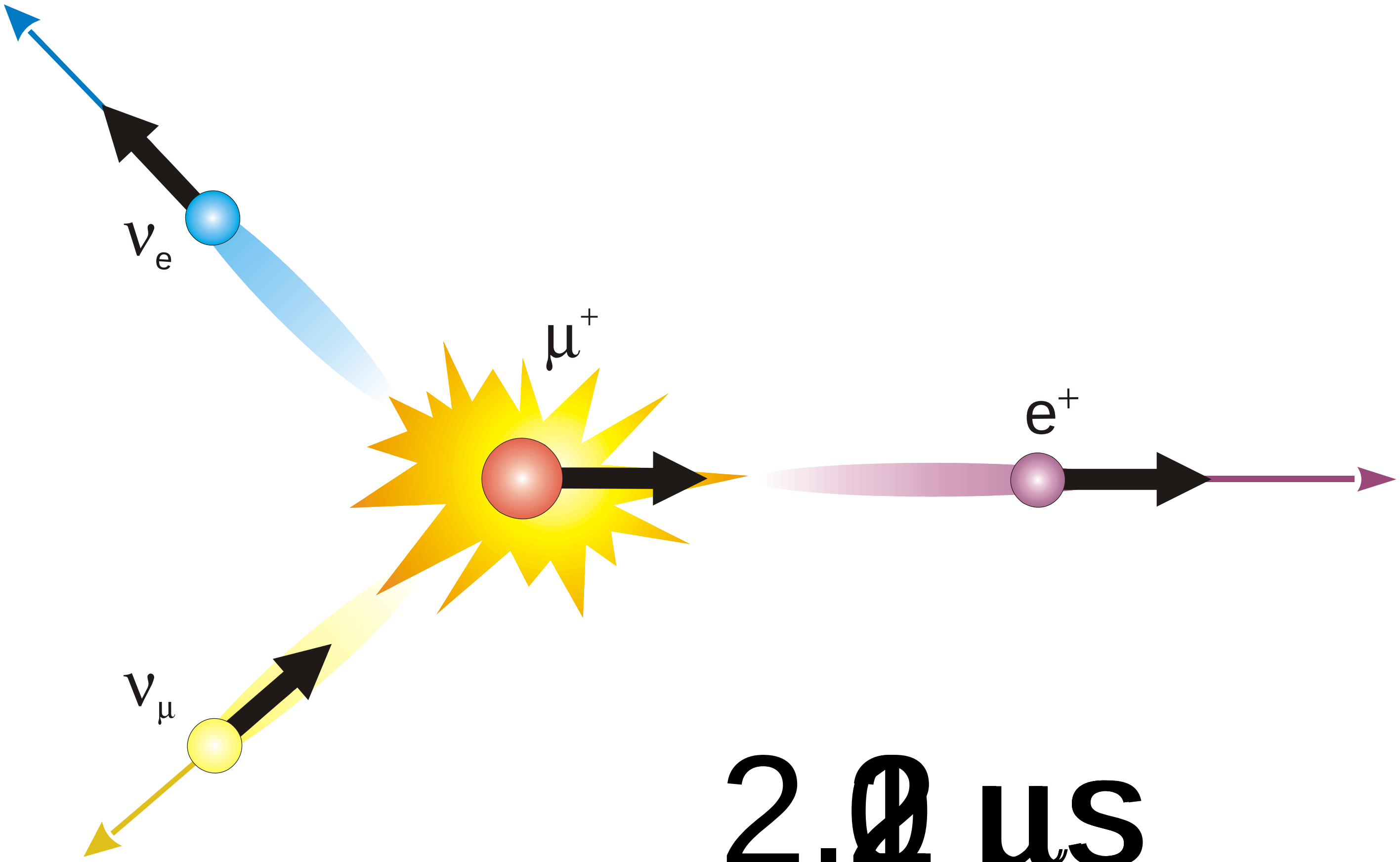
Larmor Precession

$\omega_\mu = \gamma_\mu B$

$\gamma_\mu = 3.17\ \gamma_H$

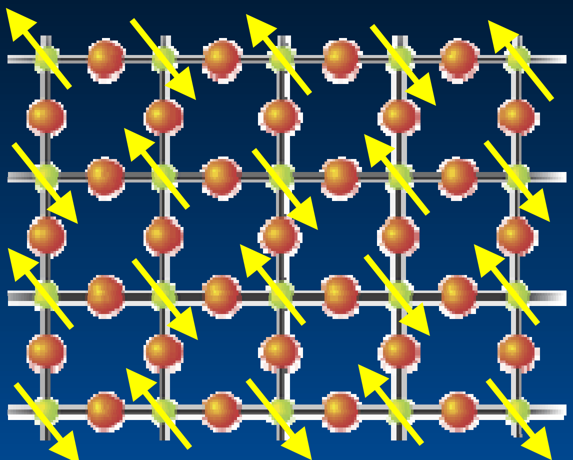


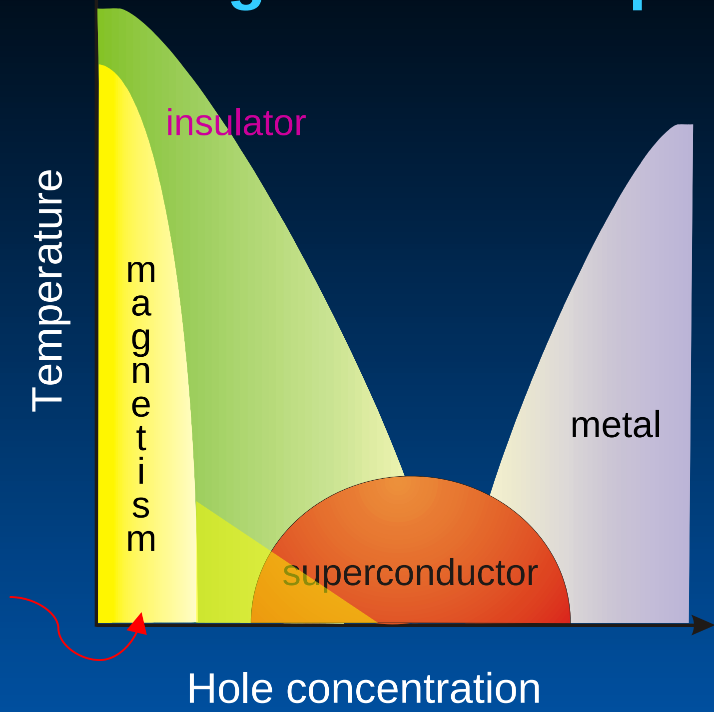
500 MeV
High
Energy
Proton
Primary
Production
Target
Carbon or
Beryllium
Nuclei
Neutrino
Pion τ_π = 26 ns
Muon
4.1 MeV
τ_μ = 2.2 μs

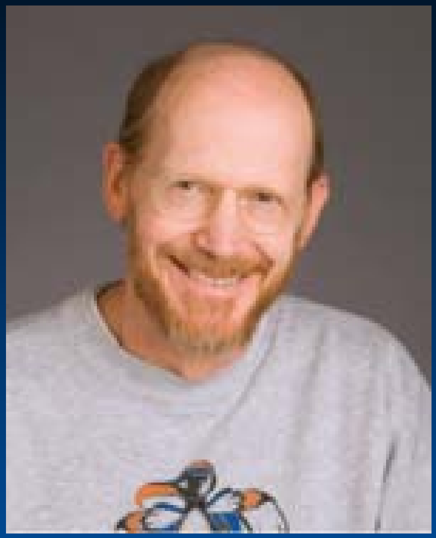


2.0 μs

Coexistence of magnetism & superconductivity

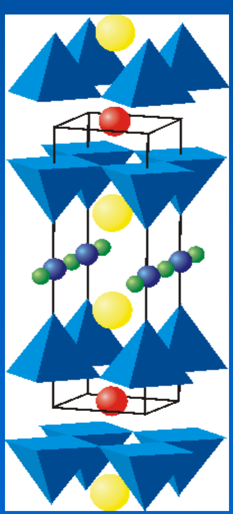


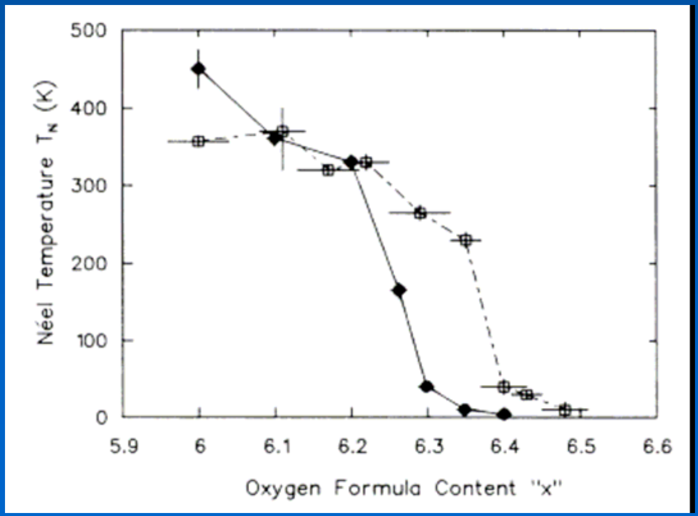




Jess Brewer (UBC)

$YBa_2Cu_3O_x$

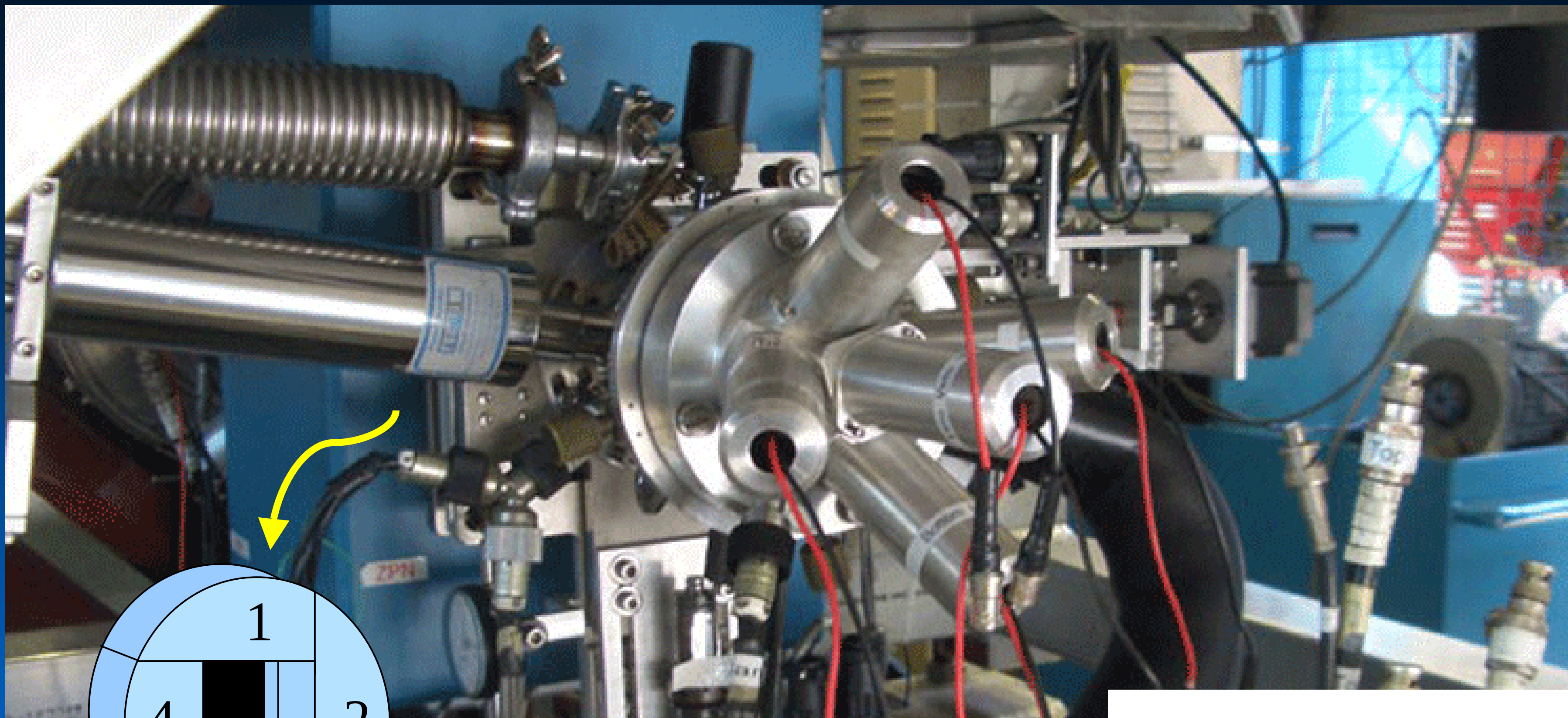


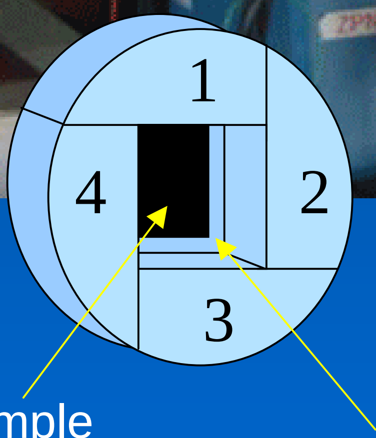


2008 Brockhouse Medal
Canadian Association of Physicists

Physical Review Letters **60**, 1074 (1988)

HiTime: World's only high transverse-field (7 T) μSR spectrometer

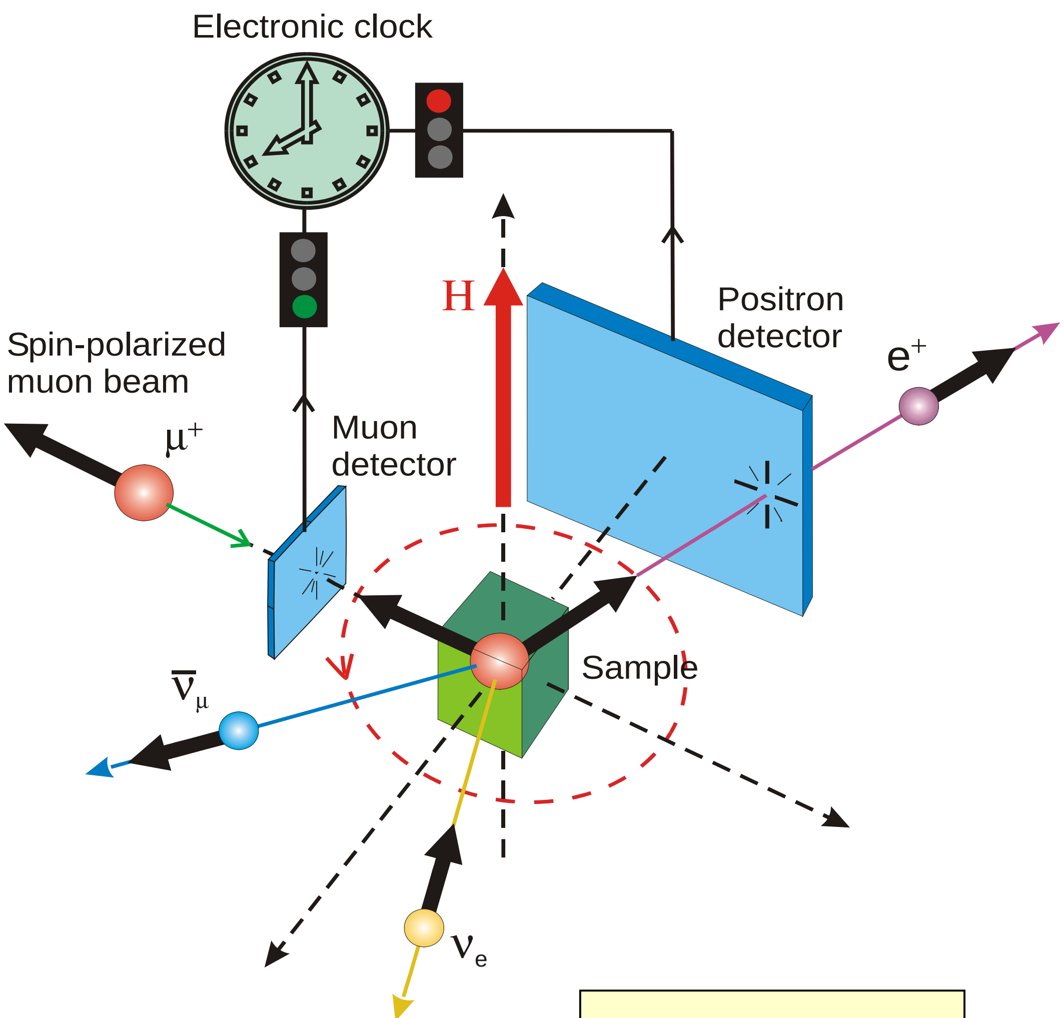




1, 2, 3, 4: e^+ counters

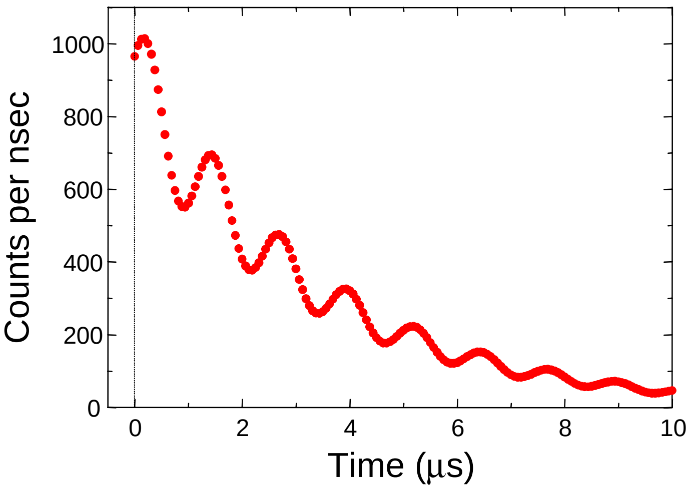
High-field: exclusive to TRIUMF & PSI

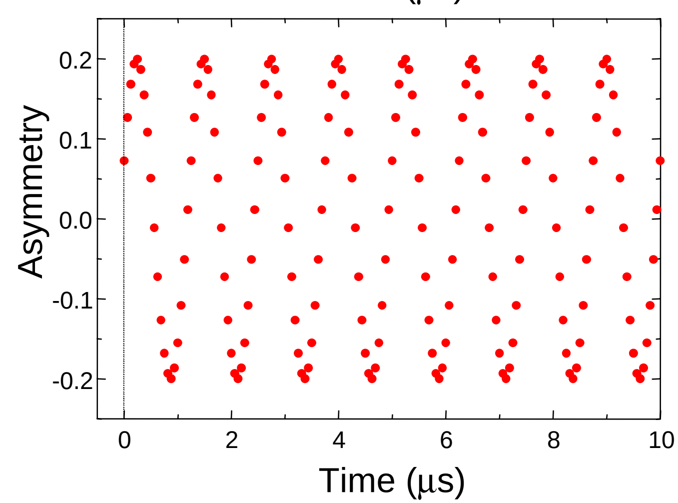
Transverse-Field μSR



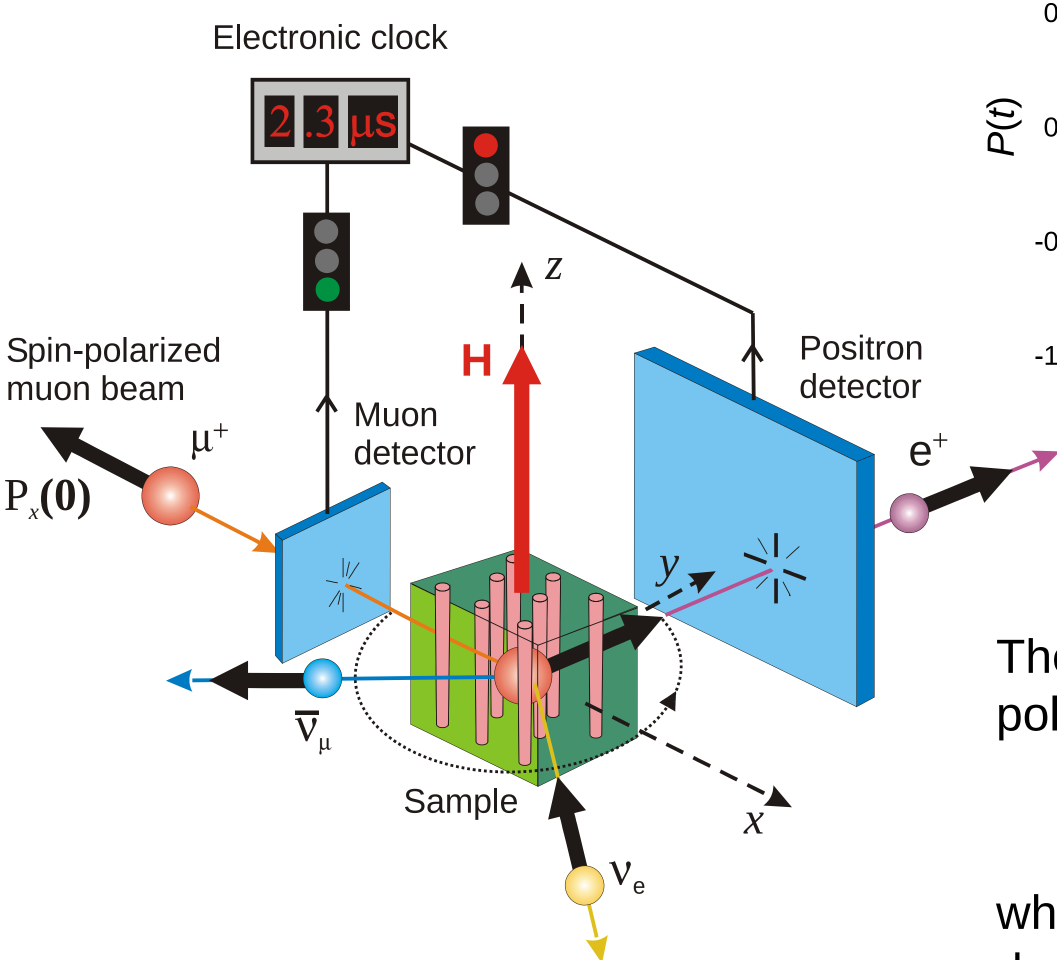
$$\omega = \gamma_\mu B_{local}$$

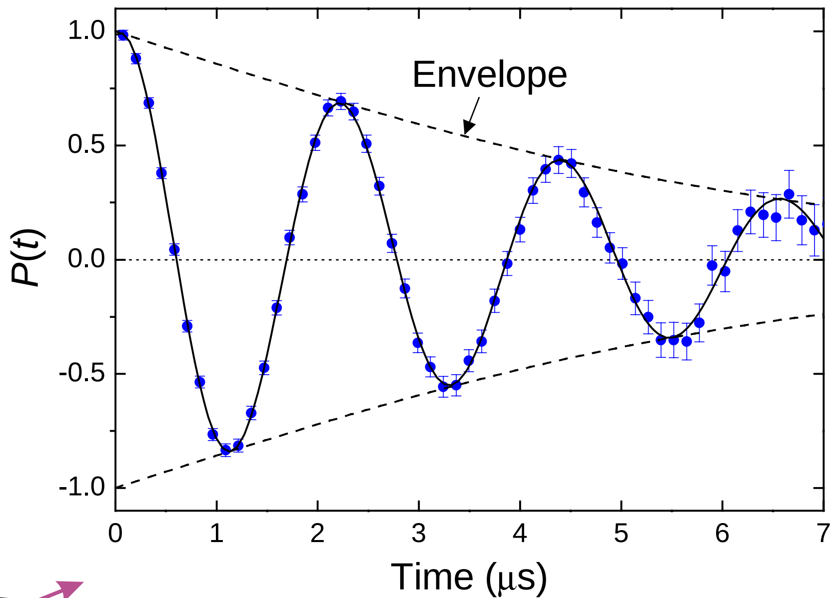
Raw time spectrum





Transverse-Field μSR



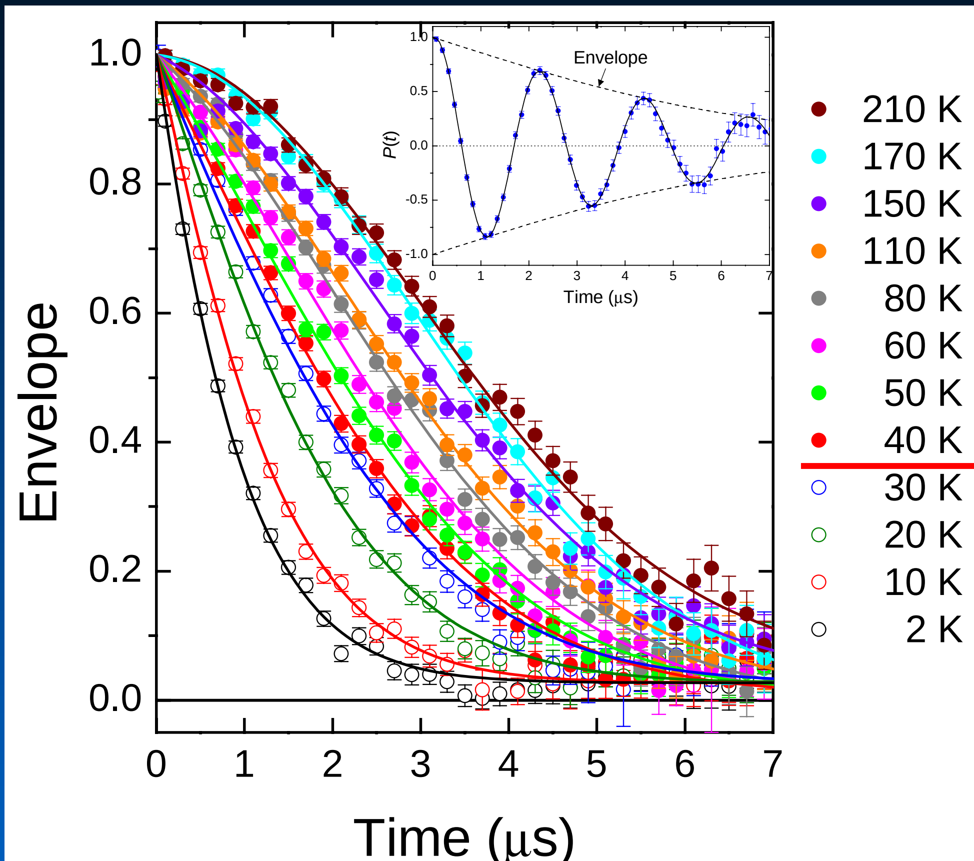


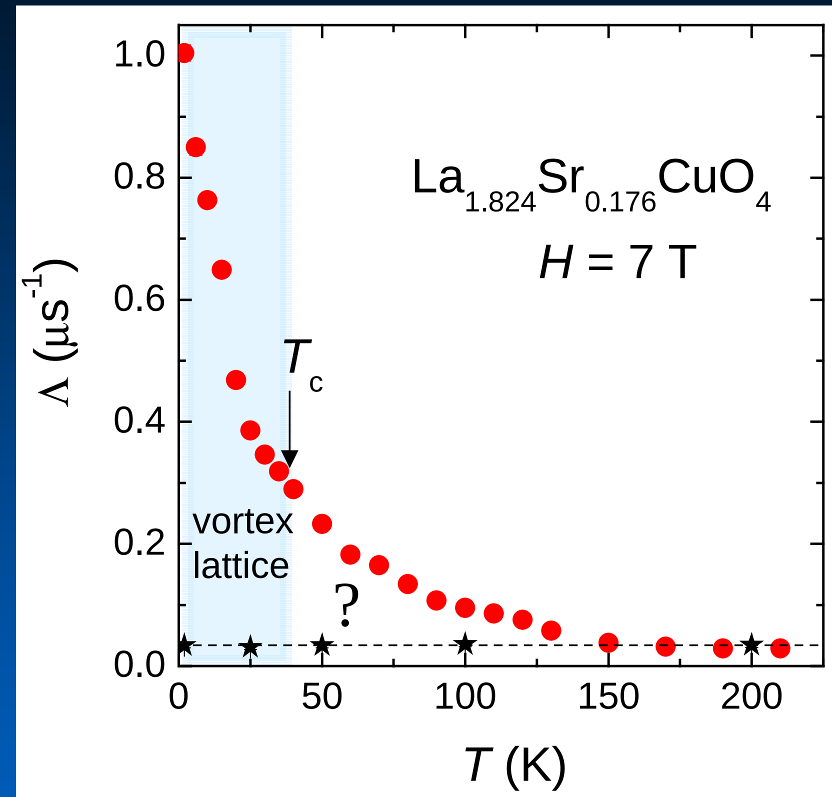
The time evolution of the muon spin polarization is described by:

$$P(t) = G(t)\cos(\gamma_\mu B_\mu t + \phi)$$

where $G(t)$ is a relaxation function describing the ***envelope*** of the TF-μSR signal.

Relaxation of TF-μSR Signal in $La_{1.824}Sr_{0.176}CuO_4$ (T_c = 37.1 K) at H = 7T





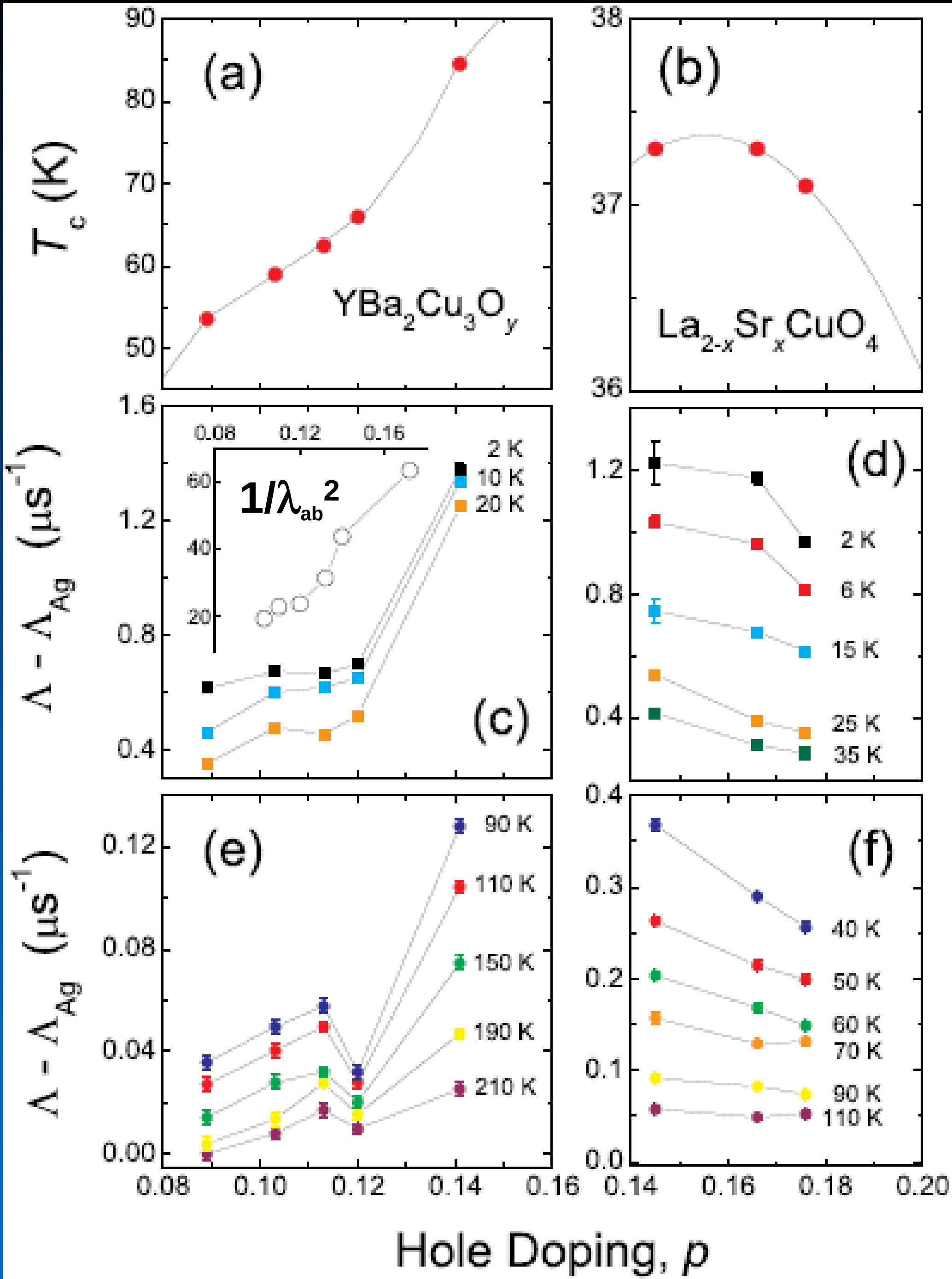
nuclear dipoles

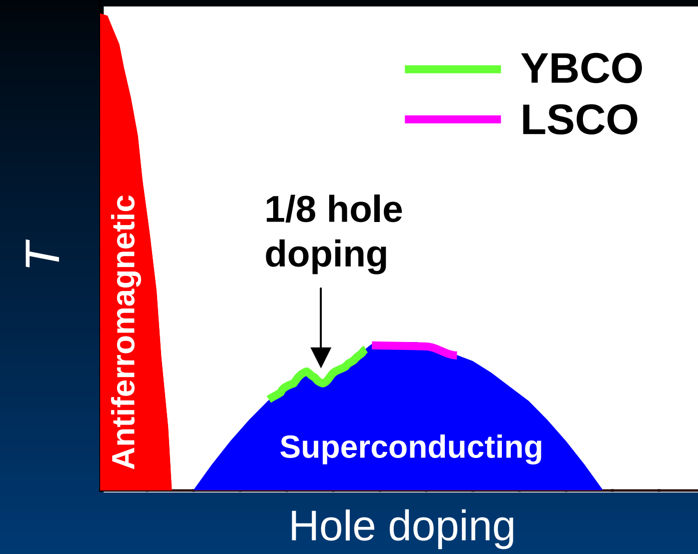
$$G(t) = \underbrace{\exp(-\Lambda t)}_{\text{spatial field inhomogeneity}}\overbrace{\exp(-\Delta^2 t^2)}^{\text{nuclear dipoles}}$$

spatial field inhomogeneity

Inhomogeneous magnetic response above T_c

JES *et al. Phys. Rev. Lett.* **101**, 117001 (2008)
Savici *et al. Phys. Rev. Lett.* **95**, 157001 (2005)





$T < T_c$

Λ tracks T_c and $1/\lambda_{ab}^2$

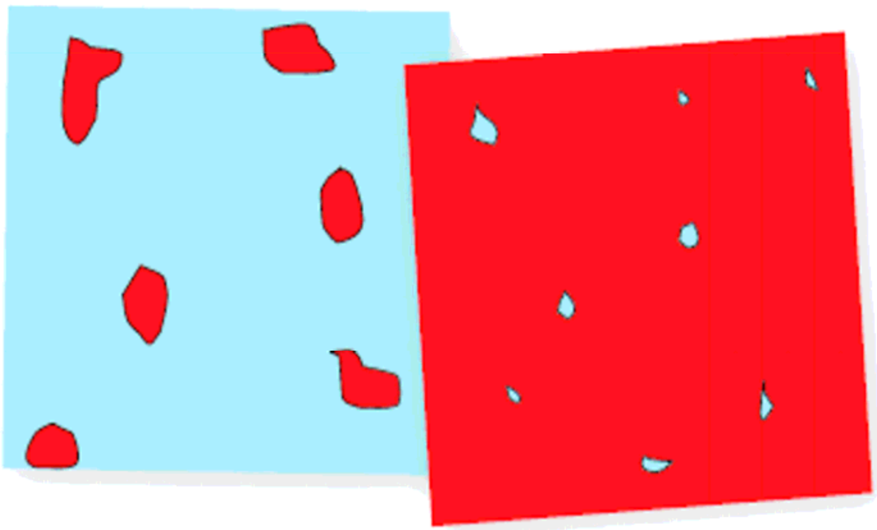
$T > T_c$

Phys. Rev. Lett. **101**, 117001 (2008)

Science **320**, 42-43 (2008)

MEETINGBRIEFS>>

AMERICAN PHYSICAL SOCIETY MEETING | 10–14 MARCH | NEW ORLEANS, LOUISIANA



Patchwork. Islands of superconductivity (red, *left*) may grow and merge as temperature drops.

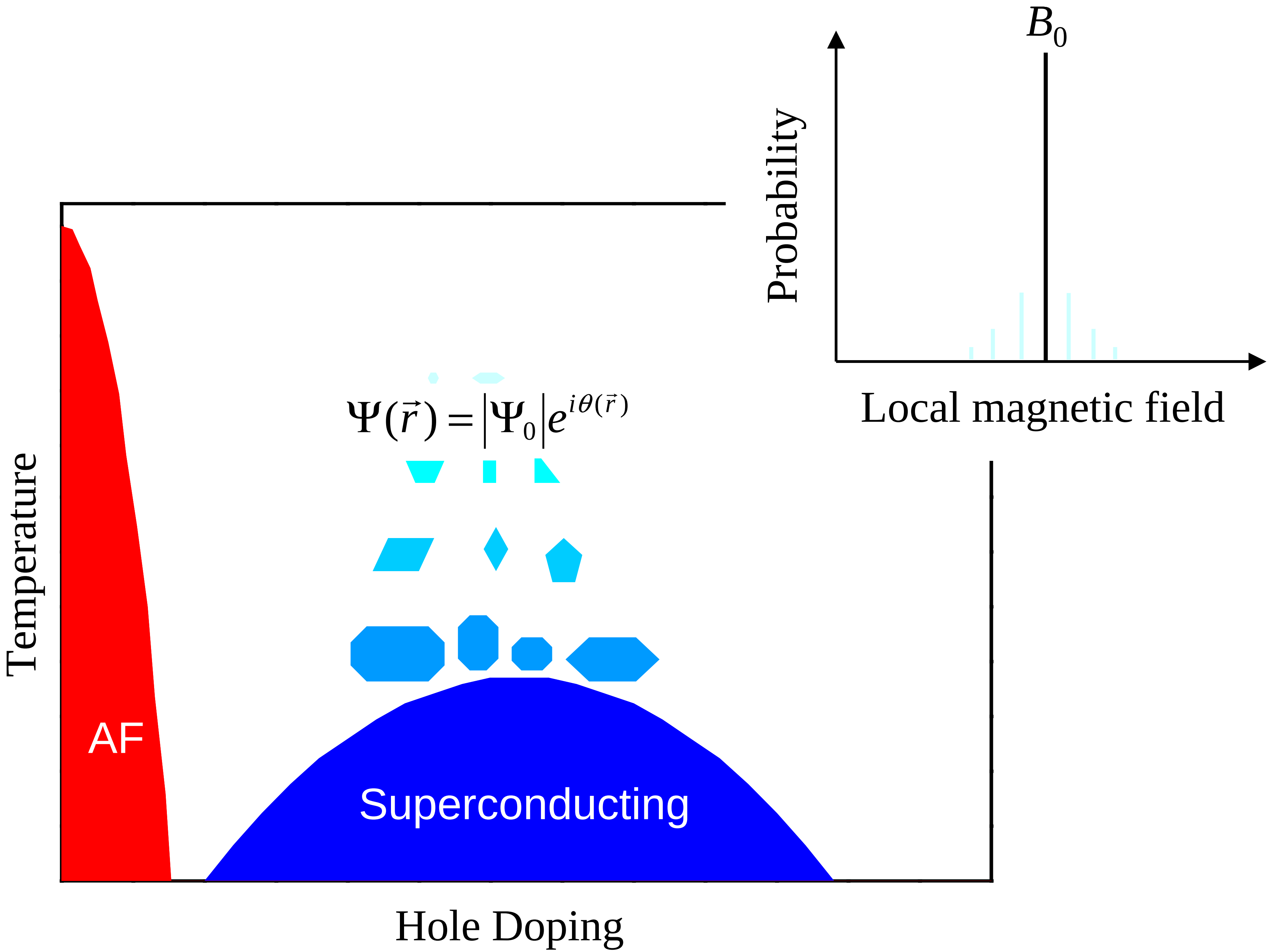
Magnetic Measurements Hint at Toastier Superconductivity

Twenty-two years after the discovery of high-temperature superconductors, theorists continue to disagree about how the complex materials conduct electricity without resistance at temperatures as high as 138 K. Meanwhile, experimenters are cranking out reams of intriguing data. At the meeting, Jeff Sonier of Simon Fraser University in Burnaby, Canada, reported evidence that superconductivity might persist in the materials to even

pairs "condense" into a single quantum wave to flow without resistance. In a conventional superconductor, all this happens simultaneously when the material is cooled below a single "critical temperature." Numerous experiments hint that things are more complicated in high-temperature superconductors. In those materials, electrons appear to pair at temperatures above the superconducting transition. The pairs then condense at the critical temper-

measurements of the magnetic fields within the materials. Sonier and colleagues fired subatomic particles called antimuons into samples of two different high-temperature superconductors—lanthanum strontium copper oxide and yttrium barium copper oxide—while they applied a strong external magnetic field. An antimuon acts like a little gyroscope whose axis sweeps around until the particle decays into a positron, which shoots out of the material in the direction the antimuon was pointing. How far the muon turns depends on the strength of the magnetic field at its position. By measuring the decay of many muons, the researchers found that the field varied dramatically within the materials, even at the highest temperatures they could measure.

Tiny patches of superconductivity could produce just such variations because they would expel the magnetic field, shoving it into the surrounding areas. The researchers performed checks to rule out other possibilities. For example, they "doped" the materials with more oxygen atoms to add electrical charges and found that the variations remained. That indicates that the effect is not produced by the



B_0
Probability
Local magnetic field
$\Psi(\vec{r}) = |\Psi_0| e^{i\theta(\vec{r})}$
Temperature
AF
Superconducting
Hole Doping

Quantum mechanics is absolutely necessary to explain the macroscopic properties of materials.