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The Hunt for High-Tc Superconductivity: from Discovery to Breakthrough

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Los Alamos, NM

LA-UR-23-XXXXX

U.S. DEPARTMENT OF ENERGY

Tulane University, September 18, 2023

National Nuclear Security Administration

THEORETICAL DIVISION Since 1943

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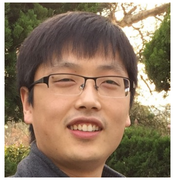
Dr. James Furness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Prof. Bahadur Singh

HIGH PERFORMANCE COMPUTING

NERSC

cost European Cooperation in Science and Technology

LDRD

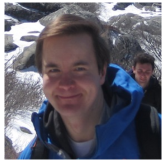
NORTHEASTERN UNIVERSITY 18 98 LVX VERITAS VIRTVS


Prof. Arun Bansil


Prof. Robert Markiewicz


Dr. Matt Matzelle


Prof. Bernardo Barbiellini


Dr. Johannes Nokelainen

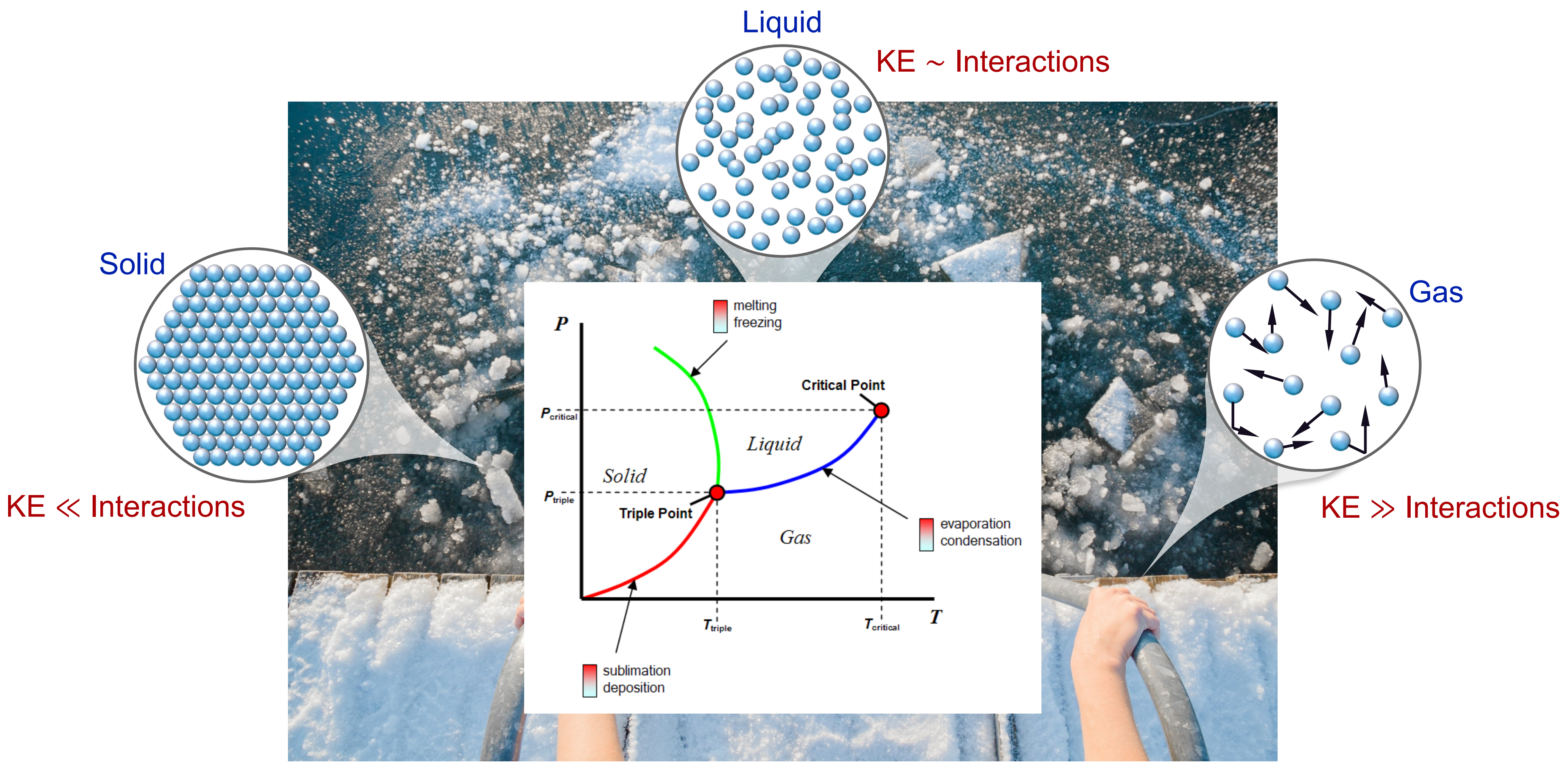
CINT

QUANTUM SCIENCE CENTER

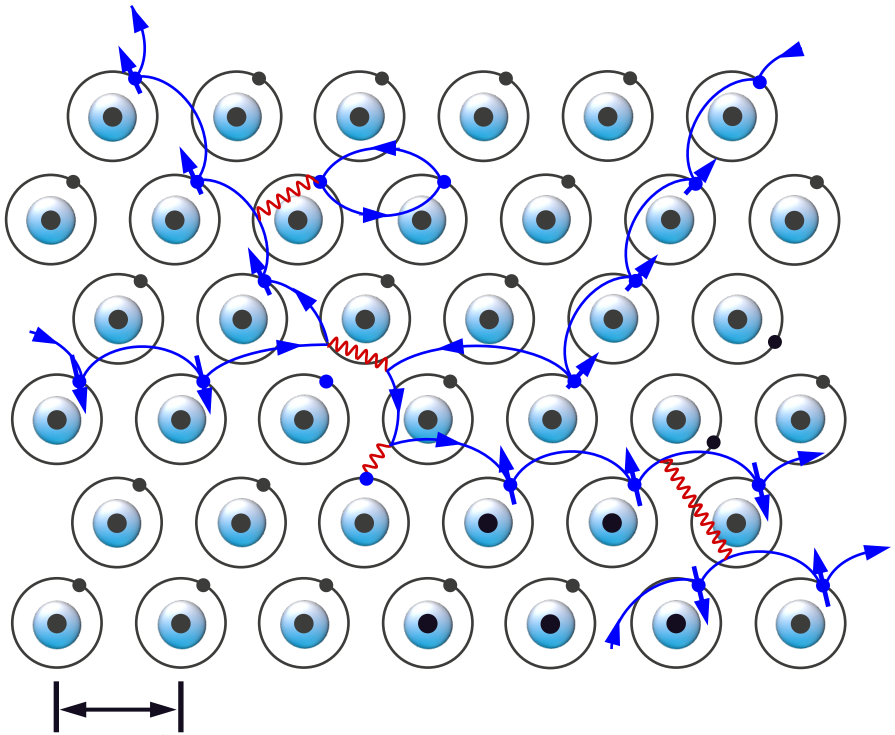
NNSA National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

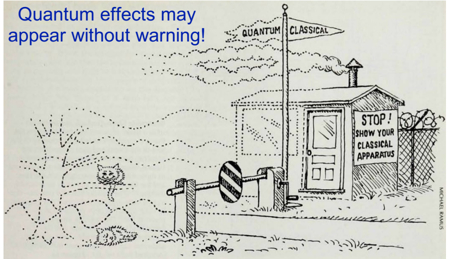
Phases of Matter



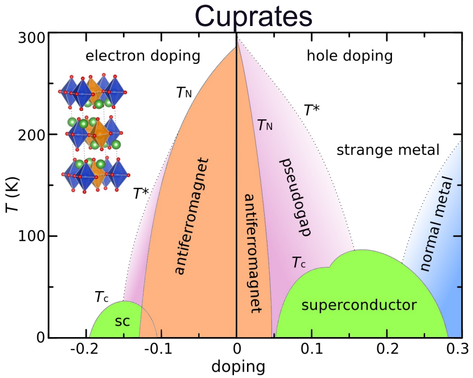
Microscopic View of a Solid

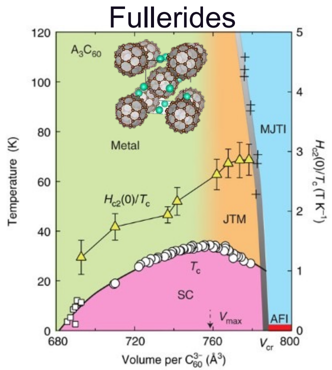


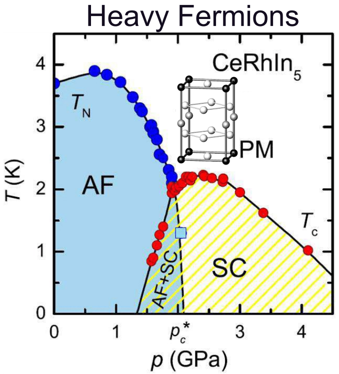
1-10 Å ~ electron de Broglie wavelength

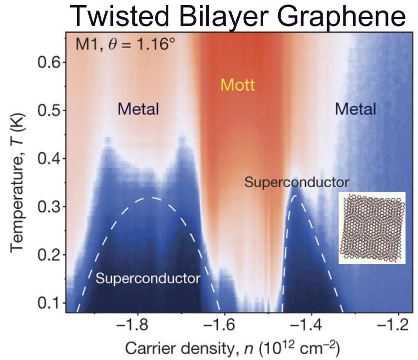


Wojciech H. Zurek.
Physics Today, 44:36-44 (1991)





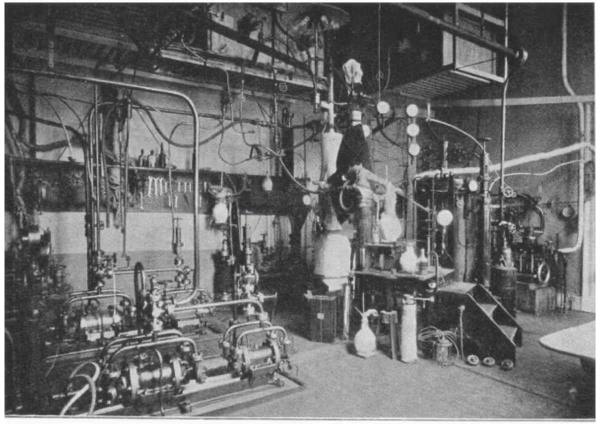




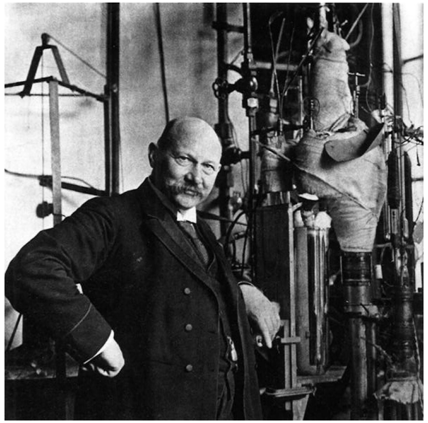
Richness of phases come from the completion from electron kinetic energy and Coulomb interactions, along with electron wave function geometry

Superconductivity

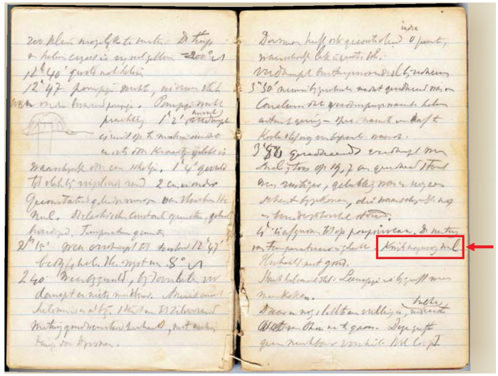
The discovery of superconductivity



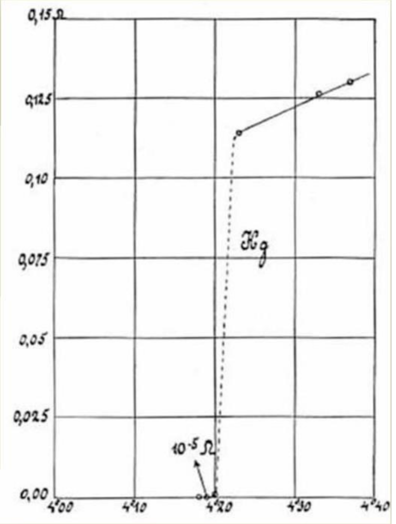
WERKKAMER E.



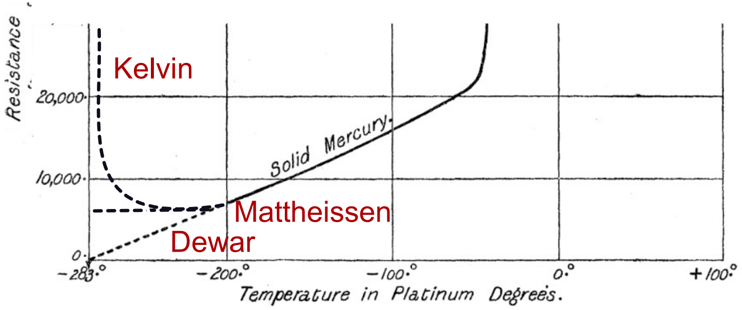
Heike Kamerlingh Onnes



A terse entry for 8 April 1911 in Heike Kamerlingh Onnes's notebook 56 records the first observation of superconductivity, "Mercury['s resistance] practically zero [at 3 K]."



- 1908 Liquification of helium
- 1910 Interest in the low temperature of solids growing



Note: Theories Pre-dates Quantum Mechanics

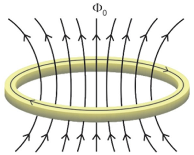
- 1911 "Mercury Practically Zero!",
  The discovery of superconductivity in Hg

When you find a metal cool it and graph it!

K. Gavroglu. Ann. Phys. (Berlin) 524, No. 3–4, A61–A64 (2012)
Comm. Leiden. April 28, 1911; Comm. Leiden. May 27, 1911; Comm. Leiden. November 25, 1911.
Dirk van Delft and Peter Kes. Physics Today 63 (9), 38–43 (2010)

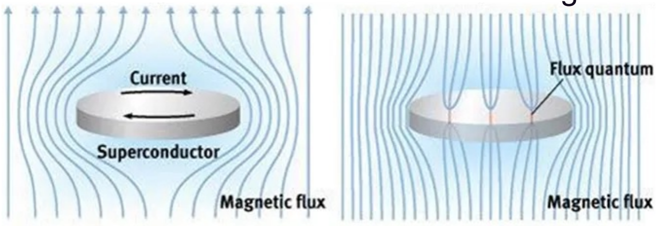
Other superconducting Properties

- 1911 Heike Kamerlingh Onnes discovers superconductivity in Hg.
- 1913 Nobel Prize in Physics 1913 “for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium”
- 1914 Observation of Persistent Currents

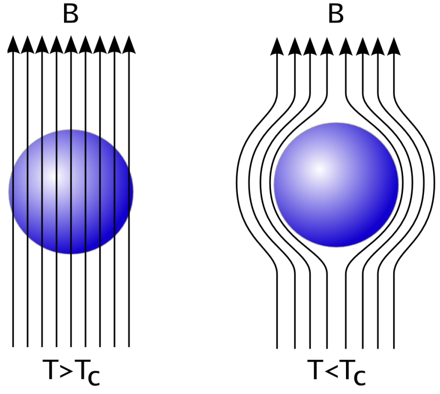


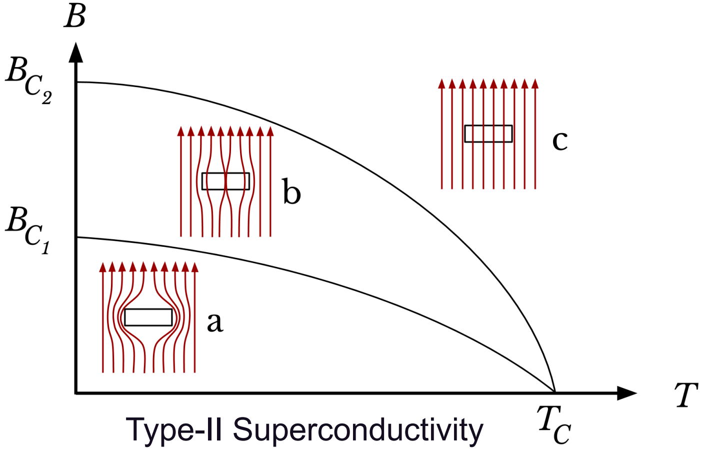
- 1933 Walther Meißner and Robert Ochsenfeld finds a superconductor completely expels magnetic fields (Perfect Diamagnetism)
- 1935 Phenological Model by F. London and H. London
- 1935 Discovery of Partial expulsion at higher fields in alloys J.N. Rjabinin and L. Shubnikov

Meissner Effect   Flux Pinning



Type-I Superconductivity

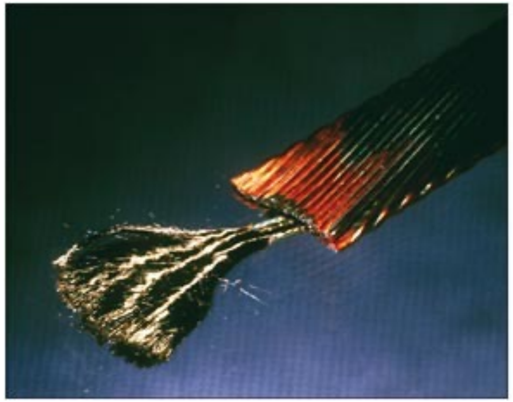




F. London and H. London. Proc. R. Soc. Lond. A14971–88 (1935)
Rjabinin, J. N. and Schubnikow, L.W. Physikalische Zeitschrift der Sowjetunion, 7(1), 122–125 (1935)
Rjabinin, J. N.; Shubnikow, L. W. Nature. 135 (3415): 581 (1935)
A. Shepelev and D. Larbalestier. The discovery of type II superconductors Cern Courier 25 October (2011)

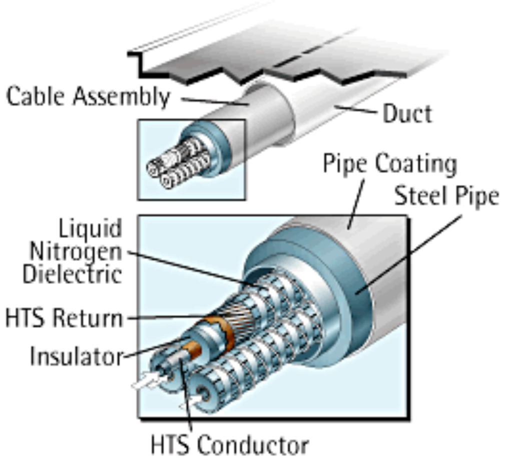
Application of Superconductors

MRI



Superconducting cable (left) the heart of the magnets for the LHC at CERN (right), where experiments found the Higgs boson.

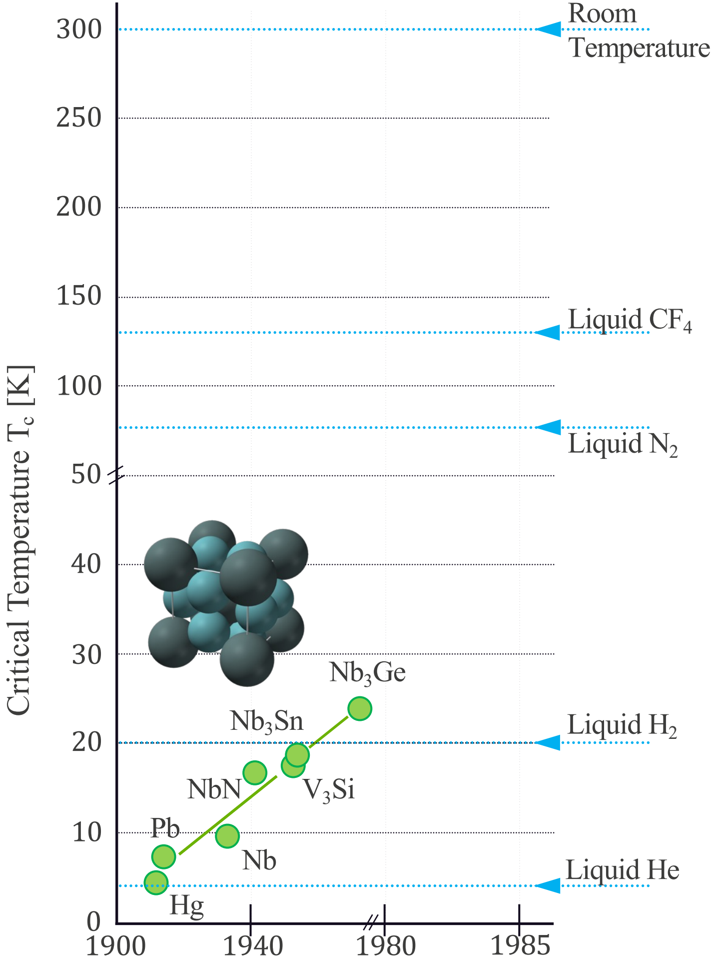
Superconducting Maglev trains



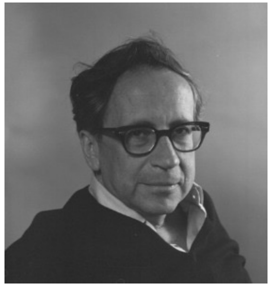
Transmission Lines

Currently used in: Holbrook, Long Island; Essen, Germany; Albany, New York

Finding new Superconducting Materials



John Hulm



Bernd Matthias

__‘Rules’ For High-Tc:__

- Metals. Must have d-electrons (not just s, p, not f)
- High symmetry is good, cubic is best.
- Look for the right filling -- peak in the density of states at the Fermi level
- Stay away from oxides
- Stay away from magnetism
- Stay away from Theorists!

https://en.wikipedia.org/wiki/High-temperature_superconductivity

Failed Theories of Superconductivity

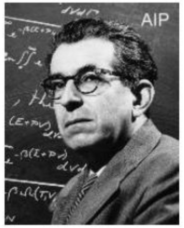

Albert Einstein
(1879-1955)


Niels Bohr
(1885-1962)


Ralph Kronig
(1905-1995)

John Bardeen
(1908-1991)


Werner Heisenberg
(1901-1976)



Fritz London
(1900-1954)


Lev D. Landau
(1908-1968)


Felix Bloch
(1905-1983)

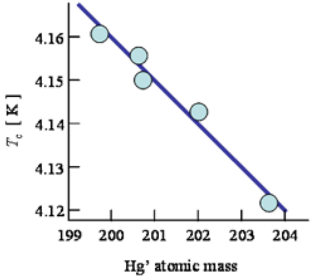
Léon Brillouin
(1889 -1969)


Max Born
(1882-1970)


Herbert Fröhlich
(1905-1991)


Richard Feynman
(1918-1988)

Hints to the problem: Zero Resistance, Perfect Diamagnetism, Isotope Effect



J. Schmalian. Modern Physics Letters B, 24(27), 2679-2691 (2012) [arXiv:1008.0447]
C. A. Reynolds, B. Serin, W. H. Wright, and L. B. Nesbitt, Physical Review 78, 487 (1950)
E. Maxwell, Physical Review 78, 477 (1950); ibid. 79, 173 (1950).

BCS Theory of Superconductivity

PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Theory of Superconductivity*

J. Bardeen, L. N. Cooper,† and J. R. Schrieffer‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_c$ at $T=0°K$ to zero at T_c. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

I. INTRODUCTION

THE main facts which a theory of superconductivity must explain are (1) a second-order phase transition at the critical temperature, T_c, (2) an electronic specific heat varying as $\exp(-T_0/T)$ near $T=0°K$ and other evidence for an energy gap for individual particle-like excitations, (3) the Meissner-Ochsenfeld effect ($\mathbf{B}=0$), (4) effects associated with infinite conductivity ($\mathbf{E}=0$), and (5) the dependence of T_c on isotopic mass, $T_c\sqrt{M}=$const. We present here a theory which accounts for all of these, and in addition gives good quantitative agreement for specific heats and penetration depths and their variation with temperature when evaluated from experimentally determined parameters of the theory.

When superconductivity was discovered by Onnes[1] (1911), and for many years afterwards, it was thought to consist simply of a vanishing of all electrical resistance below the transition temperature. A major advance was the discovery of the Meissner effect[2] (1933), which showed that a superconductor is a perfect diamagnet; magnetic flux is excluded from all but a thin penetration region near the surface. Not very long afterwards (1935), London and London[3] proposed a phenomenological theory of the electromagnetic properties in which the diamagnetic aspects were assumed basic. F. London[4] suggested a quantum-theoretic approach to a theory in which it was assumed that there is somehow a coherence or rigidity in the superconducting state such that the wave functions are not modified very much when a magnetic field is applied. The concept of coherence has been emphasized by Pippard,[5] who, on the basis of experiments on penetration phenomena, proposed a nonlocal modification of the London equations in which a coherence distance, ξ_0, is introduced. One of the authors[6,7] pointed out that an energy-gap model would most likely lead to the Pippard version, and we have found this to be true of the present theory. Our theory of the diamagnetic aspects thus follows along the general lines suggested by London and by Pippard.[7]

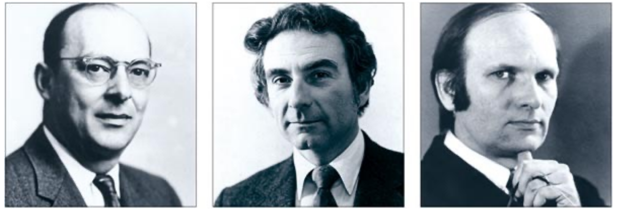
The Sommerfeld-Bloch individual-particle model (1928) gives a fairly good description of normal metals, but fails to account for superconductivity. In this theory, it is assumed that in first approximation one may neglect correlations between the positions of the electrons and assume that each electron moves independently in some sort of self-consistent field determined by the other conduction electrons and the ions. Wave functions of the metal as a whole are designated by occupation of Bloch individual-particle states of energy $\epsilon(\mathbf{k})$ defined by wave vector $\mathbf{k}$ and spin σ; in the ground state all levels with energies below the Fermi energy, $\mathcal{E}_F$, are occupied; those above are unoccupied. Left out of the Bloch model are correlations between electrons brought about by Coulomb forces and interactions between electrons and lattice vibrations (or phonons).

* This work was supported in part by the Office of Ordnance Research, U. S. Army. One of the authors (J. R. Schrieffer) was aided by a Fellowship from the Corning Glass Works Foundation. Parts of the paper are based on a thesis submitted by Dr. Schrieffer in partial fulfillment of the requirements for a Ph.D. degree in Physics, University of Illinois, 1957.
† Present address: Department of Physics and Astronomy, The Ohio State University, Columbus, Ohio.
‡ Present address: Department of Theoretical Physics, University of Birmingham, Birmingham, England.

[1] H. K. Onnes, Comm. Phys. Lab. Univ. Leiden, Nos. 119, 120, 122 (1911).
[2] W. Meissner and R. Ochsenfeld, Naturwiss. 21, 787 (1933).
[3] H. London and F. London, Proc. Roy. Soc. (London) A149, 71 (1935); Physica 2, 341 (1935).
[4] F. London, Proc. Roy. Soc. (London) A152, 24 (1935); Phys. Rev. 74, 562 (1948).
[5] A. B. Pippard, Proc. Roy. Soc. (London) A216, 547 (1953).
[6] J. Bardeen, Phys. Rev. 97, 1724 (1955).
[7] For a recent review of the theory of superconductivity, which includes a discussion of the diamagnetic properties, see J. Bardeen, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1956), Vol. 15, p. 274.

1175

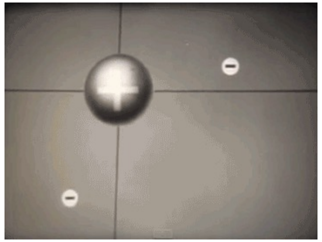
The BCS paper, published in Physical Review on 1 December 1957.

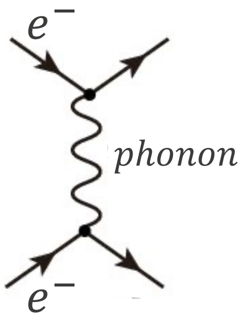


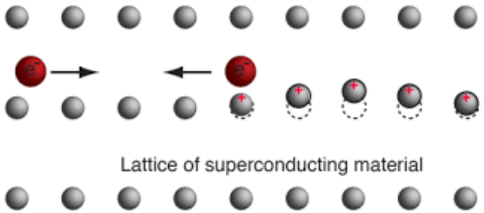
John Bardeen | Leon Cooper | Robert Schrieffer

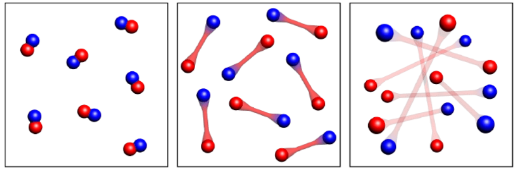
Nobel Prize in Physics 1972

- Theory builds on: Sommerfeld model of electrons in solids. Fermi Surface. Landau Fermi Liquid Theory.
- In spite of the repulsive Coulomb interaction, electrons of opposite momenta bind in pairs, because electrons polarize the crystal lattice







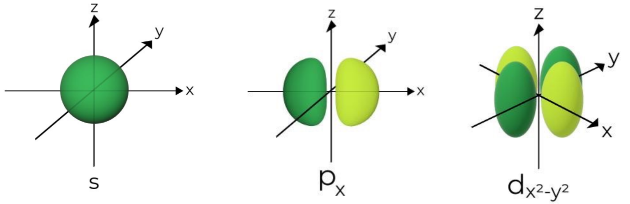


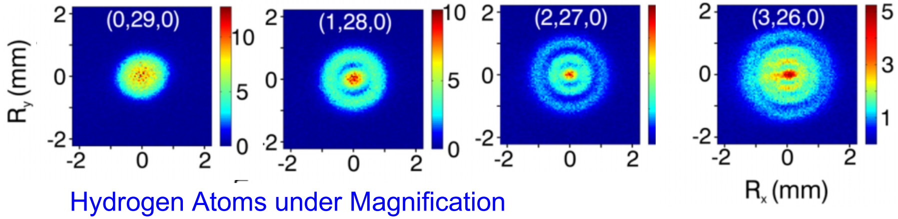
Steven Weinberg From BCS to the LHC Cern Courier 21 January (2008)
J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Phys. Rev. 108, 1175 (1957)
https://www.insidescience.org/news/superconducting-dance-electron-pairs

The Pair Wave Function

Atomic Wave functions

$$\psi(r_e - r_p)|\uparrow\rangle$$





Hydrogen Atoms under Magnification

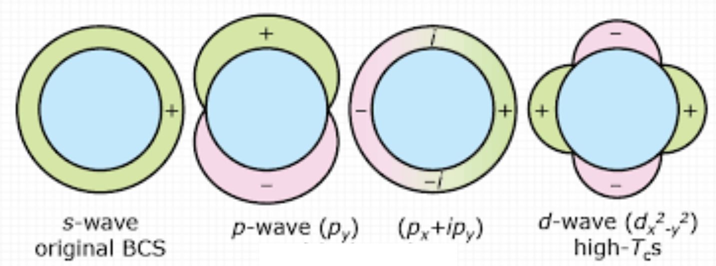
Cooper pair Wave functions

In a superconductor electrons pair and all pairs occupy the same quantum state.

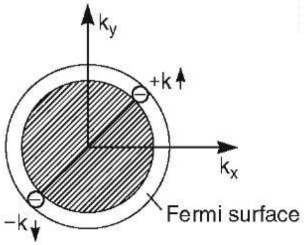
$$\Psi(\boldsymbol{k}, i; -\boldsymbol{k}, j)\frac{(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)}{\sqrt{2}}$$ Singlet

$$\Psi(\boldsymbol{k}, i; -\boldsymbol{k}, j)|\uparrow\rangle|\uparrow\rangle$$ Triplet

Symmetries of the superconducting order parameter



Even Parity | Odd Parity | Even Parity



The relative phase of the wavefunction of two superconductors can be measured!

Josephson Effect

Nobel Prize in Physics 1973

Brian Josephson

H. Kim et al.Science advances, 4(4), eaao4513. (2018)
A. S. Stodolna, et al. Phys. Rev. Lett. 110, 213001 (2013)

Superconducting Gap Function

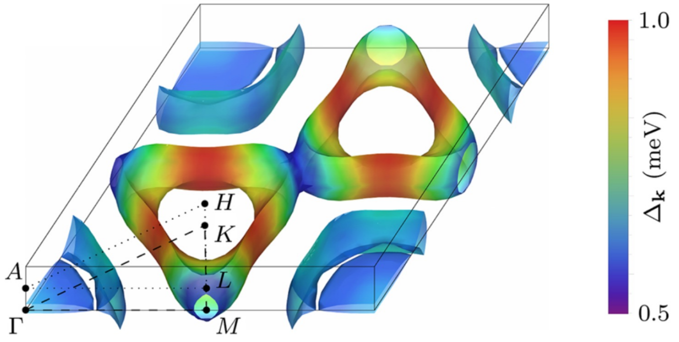
A superconductor has a gap $\Delta_i(\boldsymbol{k})$, which is simple related to the superconducting order parameter

$$\Delta_i(\boldsymbol{k}) = -\sum_{i,\boldsymbol{k}'} V_{i\boldsymbol{k},j\boldsymbol{k}'} \frac{\Delta_j(\boldsymbol{k}')}{2\sqrt{\varepsilon_{j\boldsymbol{k}'}^2 + \Delta_j^2(\boldsymbol{k}')}} \tanh\left[\frac{\sqrt{\varepsilon_{j\boldsymbol{k}'}^2 + \Delta_j^2(\boldsymbol{k}')}}{2k_B T}\right]$$

$$\mathrm{T_c} = 1.13\omega_D e^{-1/N(0)V}$$

DOS at Fermi level

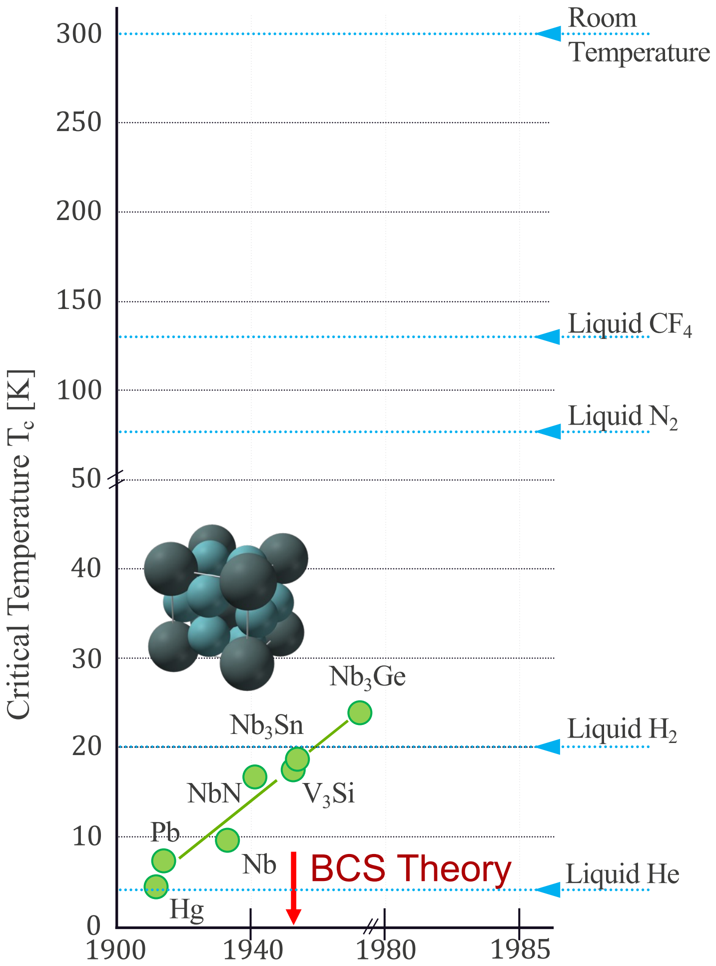
- One band case (one Fermi surface): pairing instability requires effective attractive interaction, i.e. phonons
- Multiple bands (multiple Fermi Sheets): pairing can result from attraction or repulsion among the bands
- Theory was almost universally accepted. Properties that were measured the theory could explain, and it could predict many experiments using only a small set of parameters.
- It is rigorous and builds on top of a successful theory of the normal state.

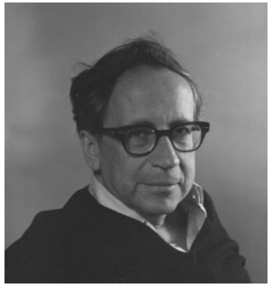


Calculated Gap function in NbS_2

H. Suhl, B. T. Matthias, and L. R. Walker Phys. Rev. Lett. 3, 552 (1959)
Christoph Heil, et al. Phys. Rev. Lett. 119, 087003 (2017)

Slow down in the 70s and early 80s…





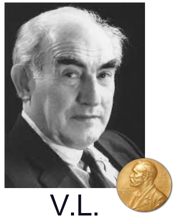
Bernd Matthias

"BCS tells us everything but finds us nothing"

V.L. Ginzburg and D.A. Kirzhnits, On the problem of high temperature superconductivity 345

1. Introduction

The critical temperature T_c of known superconductors does not exceed 20–21°K. Using traditional ways for choosing new alloys one can hope to raise this temperature by 5–10°. This, however, does not solve the problem of a radical increase of T_c up to liquid air temperature (about 80–100°K) or, even more radically, up to room temperatures (about 300°K). The importance of this problem and also the scepticism expressed sometimes with respect to the possibility of its solution (see, particularly below) induced us to consider it once again.



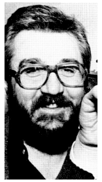
V.L. Ginzburg

Nobel Prize in Physics 2003

21. Is There a Maximum T_c?

As of January 1982, there has been a maximum T_c of ~23°K for the last 8 years.[184] This represents a normal fluctuation in the steady trend of the 3°K increase of T_c per decade[185] that has occurred since 1911. However, the investment of manpower and money in the last decade has been large and the results disappointing. Nevertheless, it is clearly dangerous to assert[186] that T_c is saturating at a maximum. Two different sensible arguments were advanced in the past[15,187] to set a limit for T_c, and each was later shown to be wrong.[76,188] Meanwhile the maximum T_c jumped 3°K.

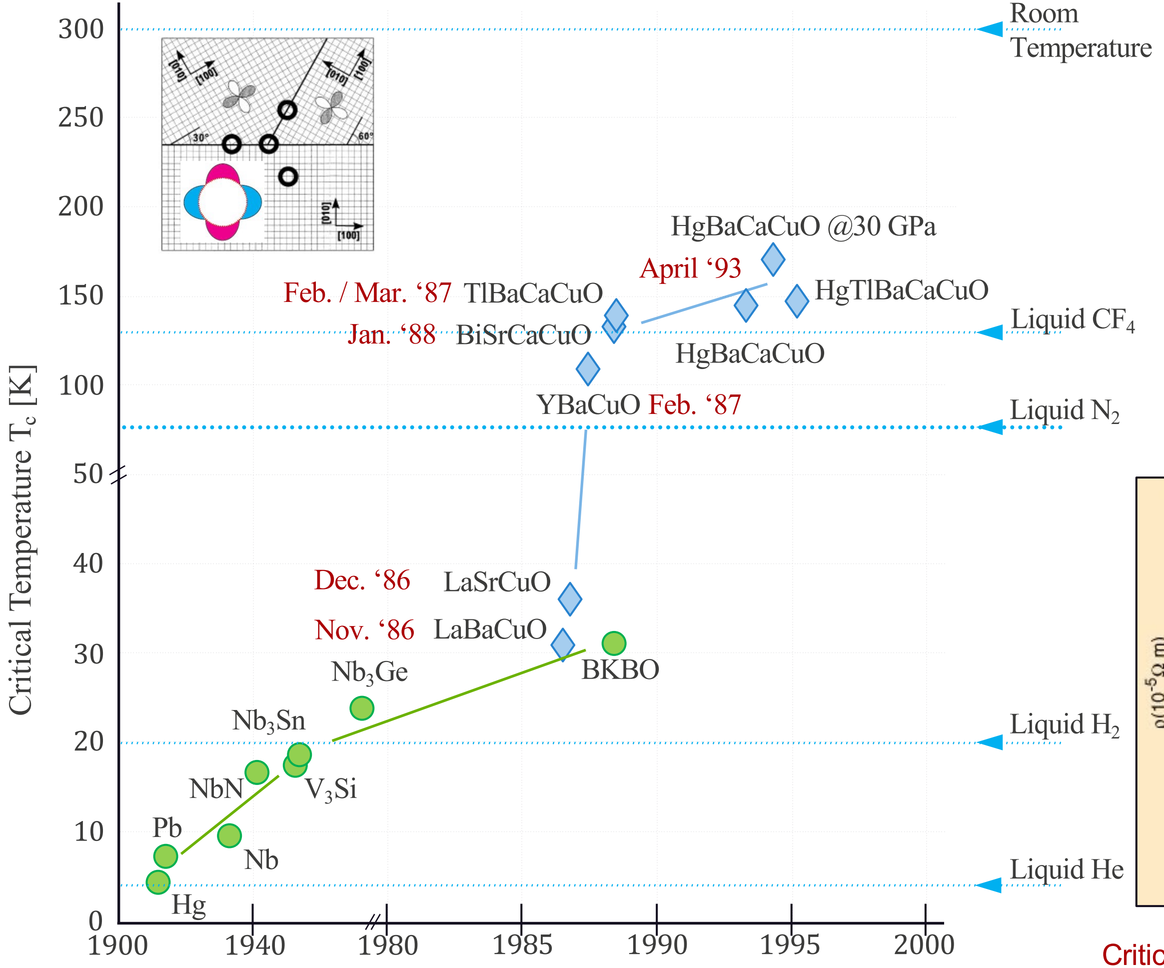
P.B. Allen

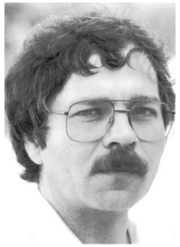


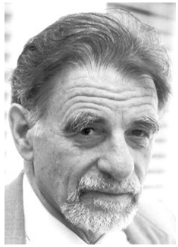
B. Mitrović

V.L. Ginzburg and D.A. Kirzhnits Physics Reports 4 (7), 343-356 (1972)
P.B. Allen and B. Mitrović Solid State Physics 37, 1-92 (1983)

A Sudden Breakthrough…





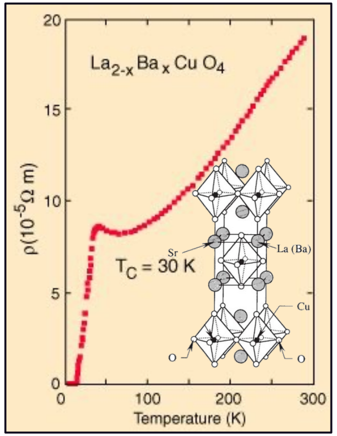


J. Georg Bednorz

K. Alexander Müller

Nobel Prize in Physics 1987

One of the fastest awards on record!



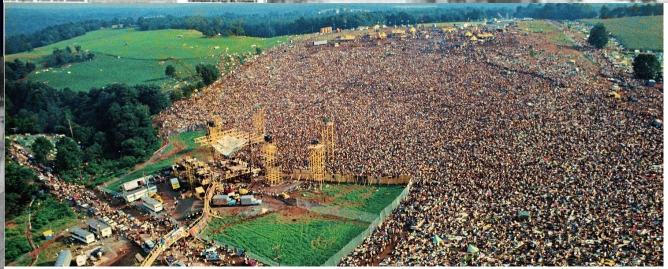
'Violates all of Matthias' Rules:

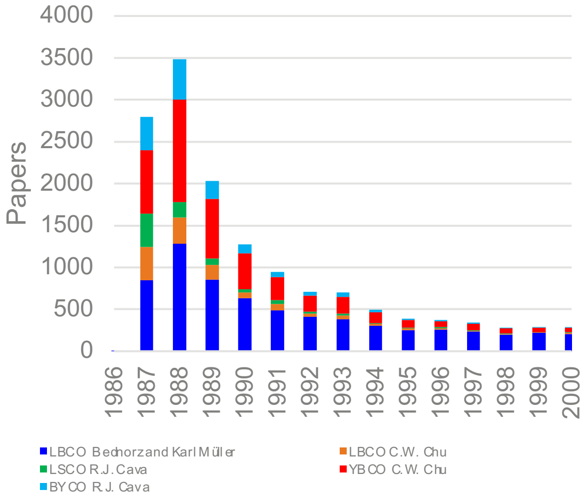
- Near a (Mott) insulator
- Layered Perovskite Structure
- Is an oxide
- Near an AFM magnet

Critically: These materials do not fall within the BCS framework.

J.G. Bednorz and K.A. Muller Z. Phys. B 64, 189-193 (1986)
C. C. Tsuei and J. R. Kirtley. Rev. Mod. Phys. 72, 969 (2000)

March 18, 1987: Woodstock of Physics





- The discoveries were so recent that no papers on them had been submitted by the deadline. However, a last-minute session was added to discuss the new research.
- Session started at 7:30pm with lines forming at 5:30pm and finished at 3:30am
- Nearly 2,000 scientists tried to squeeze into the ballroom, with more watching outside the room on television monitors.
- The session consisted of a marathon of talks, given by about 50 speakers

Complete Historic Session Available on YouTube!

https://www.aps.org/publications/apsnews/updates/woodstock.cfm

Possible Ingredients of High-Tc in the Cuprates

Spin-Fluctuations

- d-wave pairing near a spin-density-wave instability D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch. Phys. Rev. B 34, 8190(R) (1986)
- Spin-fluctuation-induced superconductivity in the copper oxides: A strong coupling calculation. P. Monthoux and D. Pines. Phys. Rev. Lett. 69, 961 (1992)

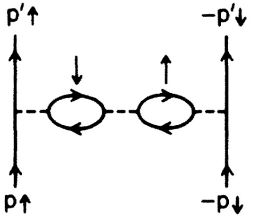
Plasmons / Excitons

- A Cu d-d excitation model for the pairing in the high-T c cuprates. W. Weber Zeitschrift für Physik B Cond. Matt. 70, 323–329 (1988)
- Landscape of coexisting excitonic states in the insulating single-layer cuprates and nickelates. C. Lane and J.-X. Zhu. Physical Review B 101, 155135 (2020)
- Acoustic plasmons and conducting carriers in hole-doped cuprate superconductors. A. Singh, H. Y. Huang, C. Lane, J. H. Li, J. Okamoto, S. Komiya, R.S. Markiewicz, A. Bansil, T. K. Lee, A. Fujimori, C. T. Chen, and D. J. Huang. Phys. Rev. B 105, 235105 (2022)

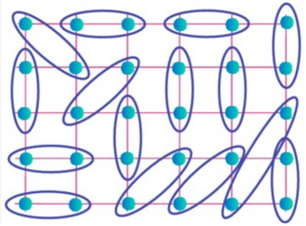
Resonating Valence Bond State

- The Resonating Valence Bond State in La_2CuO_4 and Superconductivity. P. W. Anderson Science 235, 1196-1198 (1987)
- A renormalised Hamiltonian approach to a resonant valence bond wavefunction. F C Zhang, C Gros, T M Rice and H Shiba. Supercond. Sci. Technol. 1, 36 (1988)
- A Unified Theory Based on SO(5) Symmetry of Superconductivity and Antiferromagnetism. S.-C. Zhang. Science 275, 1089 (1997)

Glue



vs.



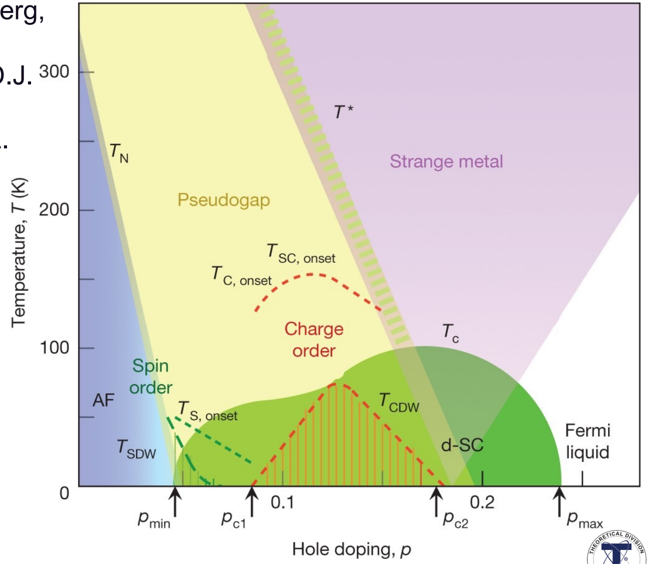
Fabric

CDW / Phonon Softening

- CDW and SDW mediated pairing interactions. N.E. Bickers, D.J. Scalapino and R.T. Scalettar. Int. J. Mod. Phys. B 1, 687-695 (1987)
- Vibronic mechanism of high-Tc superconductivity. M. Tachiki, M. Machida, and T. Egami. Phys. Rev. B 67, 174506 (2003)
- Competing stripe and magnetic phases in the cuprates from first-principles. Y. Zhang, C. Lane, J.W. Furness, B. Barbiellini, J.P. Perdew, R.S. Markiewicz, A. Bansil, and J. Sun. PNAS, 117, 68 (2020)

Stripes and Intertwined orders

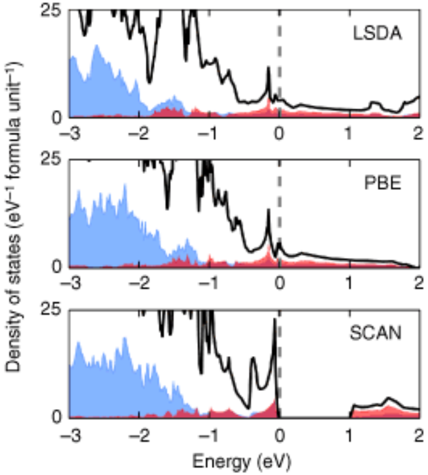
- Are Stripes a Universal Feature of High-Tc Superconductors? Barbara Goss Levi Physics Today 51 (6), 19–22 (1998)
- Colloquium: Theory of intertwined orders in high temperature superconductors. Eduardo Fradkin, Steven A. Kivelson, and John M. Tranquada. Rev. Mod. Phys. 87, 457 (2015)
- The Physics of Pair-Density Waves: Cuprate Superconductors and Beyond. D.F. Agterberg, J.C.S. Davis, S.D. Edkins, E. Fradkin, D.J. Van Harlingen, S.A. Kivelson, P.A. Lee, L. Radzihovsky, J.M. Tranquada, and Y. Wang.



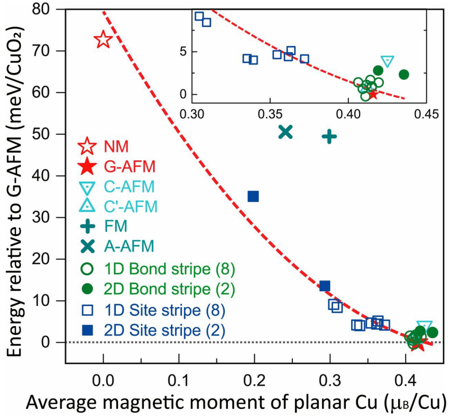
Still many open Questions!

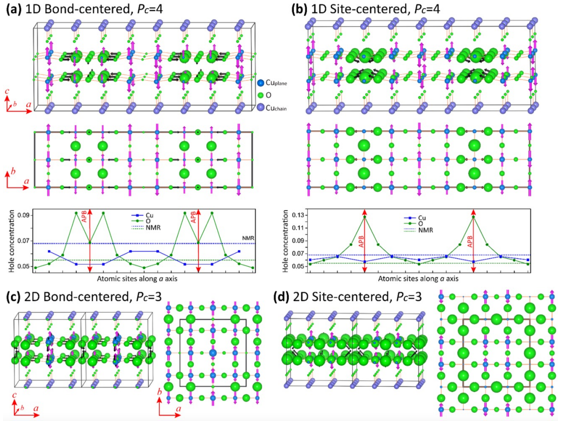
First-principles Ground State and Excitation Properties

La_2CuO_4: AFM Phase and Band Gap



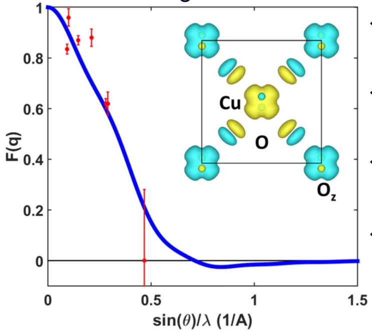
- LSDA and PBE: Metal
- SCAN: AFM Insulator (no U)
- Band Gap
  - Theory: 0.98 eV
  - Expt. (Optics): ~ 1.0 eV
- Generalize Kohn-Sham gives fundamental gap (no excitonic effects)



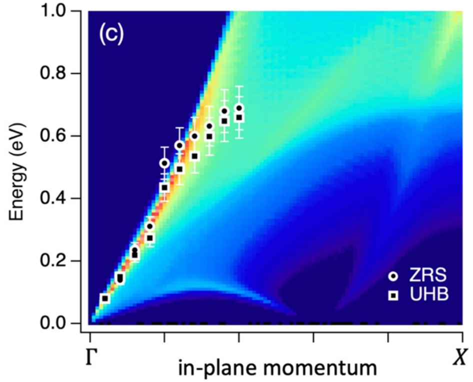


- Ground state has many competing phases; role in superconducting glue, models of pseudogap, nematicity, temperature effects, etc.

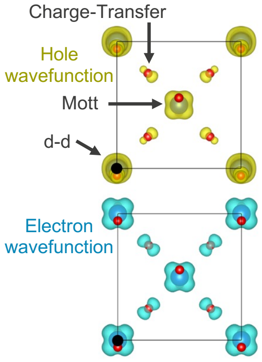
La_2CuO_4: Magnetic Form Factor

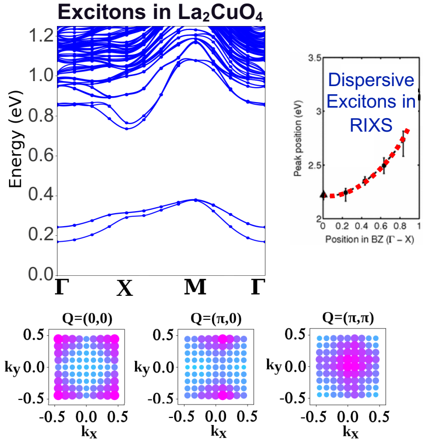


- AFM state yields moments on Cu and O_z sites.
- The predicted moment on Cu: 0.495 μB [Exp. 0.48±0.15 μB]
- Cu-O hybridization effects intrinsically included.
- In-plane magnetization has quadropole form.



- Agreement between theoretical loss function for LSCO and RIXS spectra

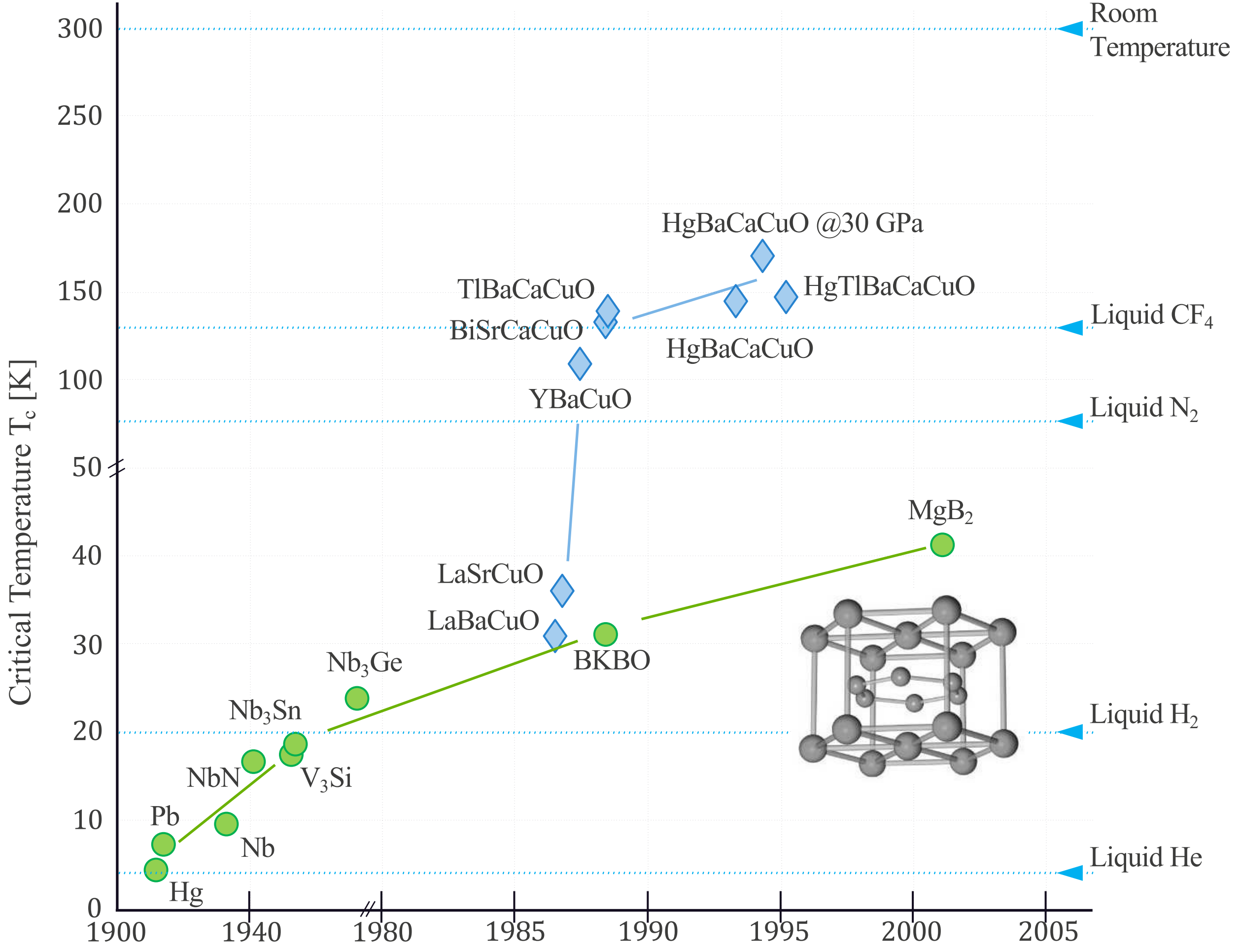


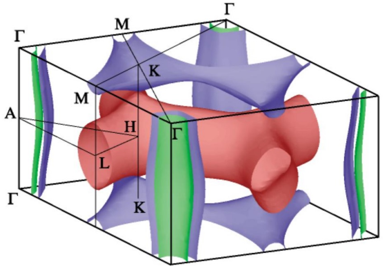


- Excitons in LCO are composed of Mott-Hubbard, d−d, and charge-transfer types.

Y. Zhang, C. Lane, et al. PNAS, 117, 68 (2020)
C. Lane, et al. Physical Review B 98, 125140 (2018)
J.W. Furness,et al. Communications Physics 1, 11 (2018)
C. Lane and J.-X. Zhu Physical Review B 101, 155135 (2020)
A. Singh, H. Y. Huang, C. Lane, et al. Physical Review B 105, 235105 (2022)

A conventional Surprise





- Quasi-two-dimensional layered system, violate all of Matthias' Rules
- Discovered by accident (searching for Ferromagnets)
- Conventional, phonon mediated superconductor
- Violates Tc < 23 K
- Multicomponent order parameter, multiple active Fermi sheets
- Workhorse material for MRIs and the LHC

Low Temperature Heat Capacities of Magnesium Diboride (MgB_2) and Magnesium Tetraboride (MgB_4)

By Robinson M. Swift and David White[1]

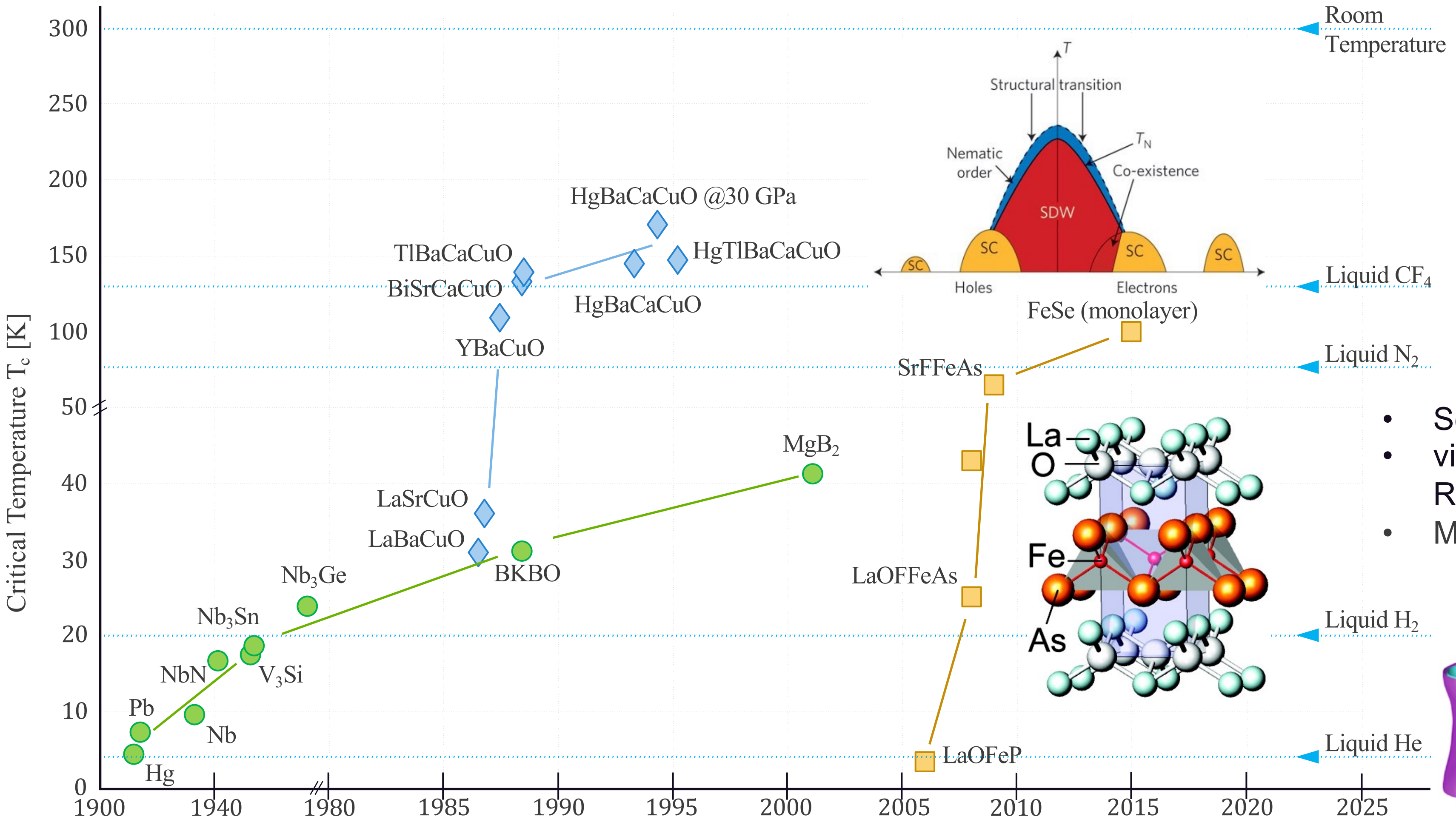
Received February 14, 1957

The heat capacities of magnesium diboride (MgB_2) and magnesium tetraboride (MgB_4) were measured in the temperature range 18 to 305°K. The values of heat capacity, entropy, enthalpy and free energy function have been tabulated at integral values of temperature. The entropy at 298.16°K. of MgB_2 is 8.60 ± 0.04 cal. deg.$^{-1}$ mole^{-1}, that of MgB_4 is 12.41 ± 0.06 cal. deg.$^{-1}$ mole^{-1}. The heat capacity of these compounds at the lowest temperatures measured do not exhibit at T^2 relationship characteristic of some substances having a layer structure.

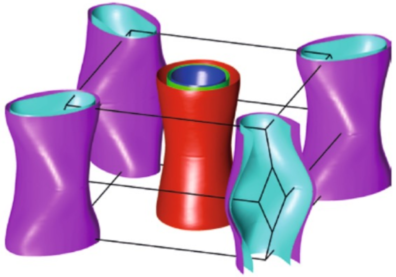
Should have been discovered in 1957!

Jun Nagamatsu, Norimasa Nakagawa, Takahiro Muranaka, Yuji Zenitani & Jun Akimitsu Nature 410, 63–64 (2001)
P.C. Canfield and G.W. Crabtree. Physics Today 56 (3), 34–40 (2003)

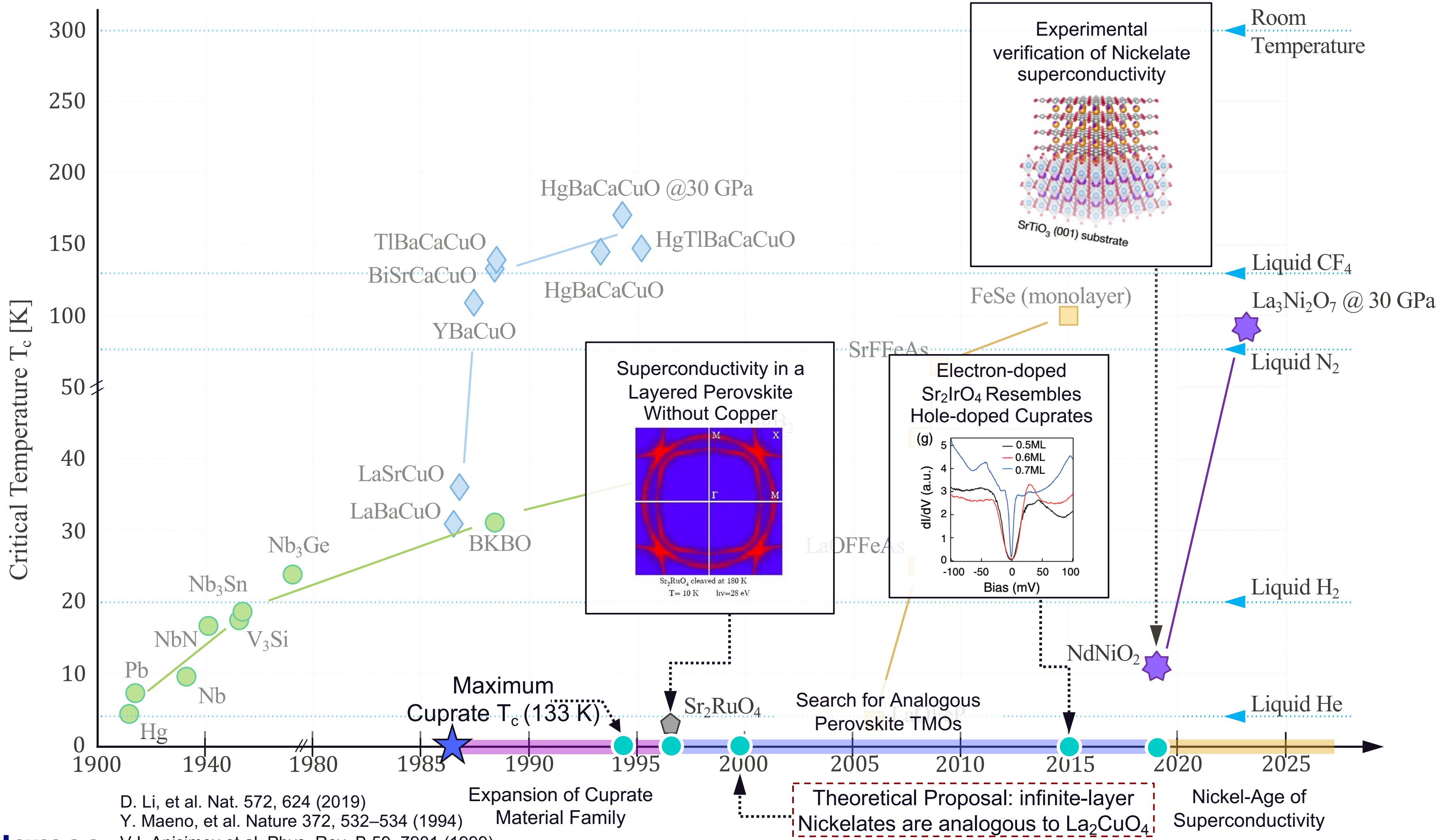
Iron Age of Superconductivity



- Serendipitous Discovery
- violate all of Matthias' Rules (2D, near mag)
- Multiband system



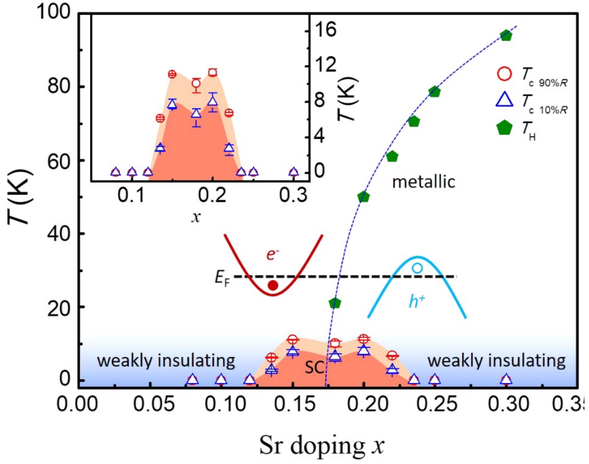
Birth of a New Age…

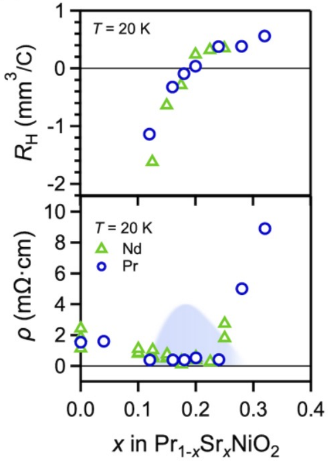


D. Li, et al. Nat. 572, 624 (2019)
Y. Maeno, et al. Nature 372, 532–534 (1994)
V.I. Anisimov et al. Phys. Rev. B 59, 7901 (1999)
Y. J. Yan, et al. Phys. Rev. X 5, 041018 (2015)

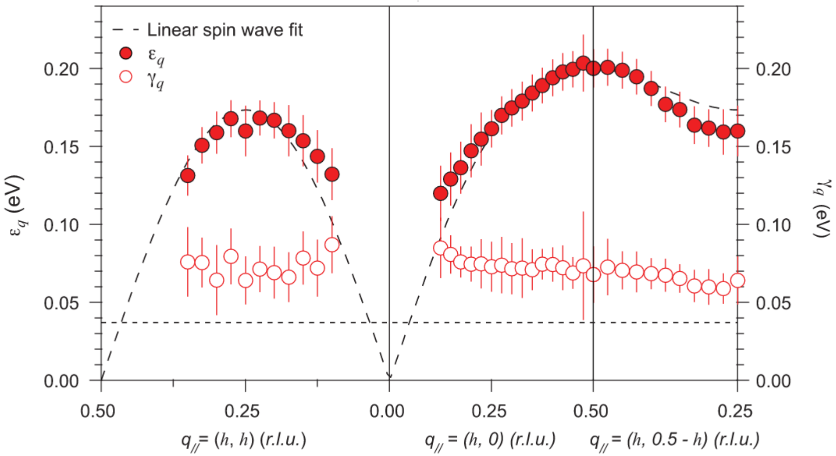
Electronic and magnetic properties of the Infinite-Layer Nickelates

Superconductivity and Character of doped Carriers





Magnetic Correlations and Excitations



Transport

- SC in (La,Nd,Pr)NiO_2, $T_c \sim 12 - 14$ K
- Dip in SC dome of (La,Nd)NiO_2, indicates possible stripes
- Under- and over-doped regime weakly insulating
- R_H crosses changes sign at optimal doping

XAS / RIXS

- Hole resides on Ni-$d_{x^2-y^2}$
- *dd* transition distinct from Cuprates
- Hole might be forming singlets
- Possible minor 5*d* doping

RE Substitution

- Role of *f*-electron probably minimal
- 5*d*/3*d* hybridization might be important

Neutron Scattering

- No AFM order, but strong non-local correlations

μSR / χ(H,T)

- Intrinsic magnetism
- Strong non-local magnetic correlations
- Glassy short-range behavior
- Weak to intermediate spin-cluster interactions

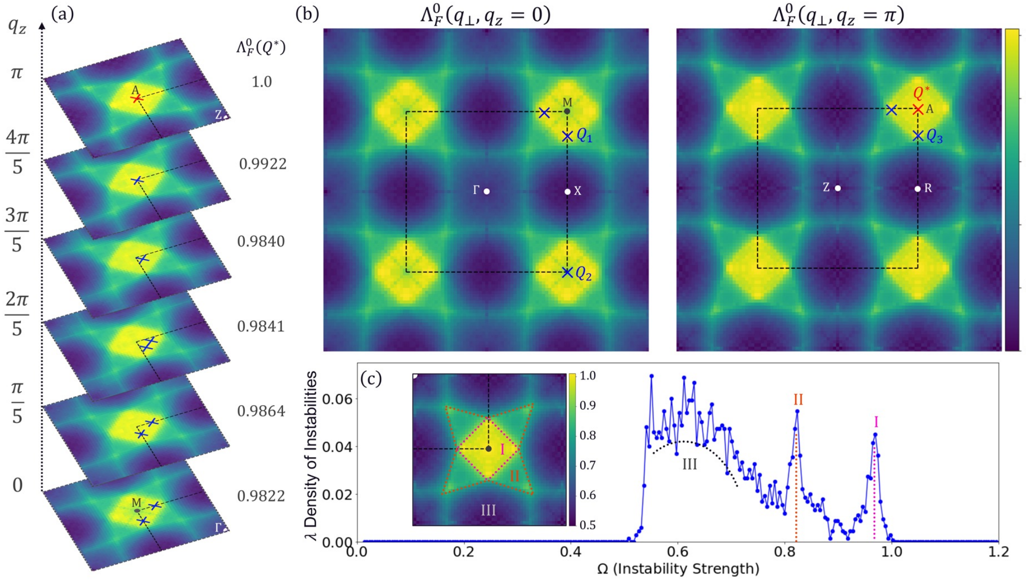
RIXS

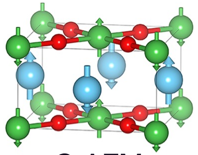
- 2D AFM spin wave dispersion
- $J_{ex} = 63.6 \pm 3.3$ meV ~ cuprates
- Damping appears to be constant in zone

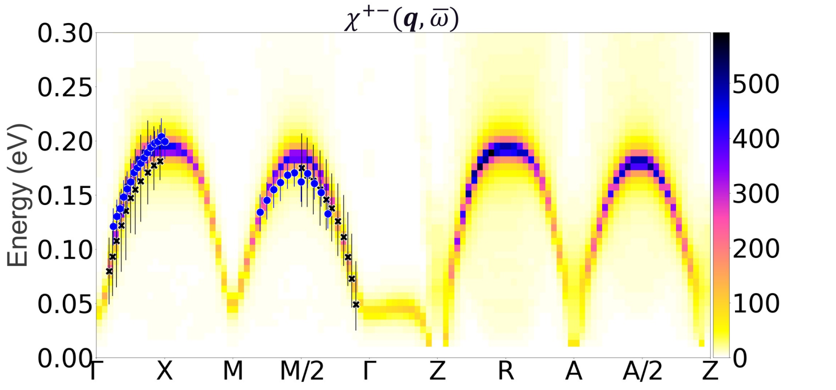
S. Zeng, et al. Phys. Rev. Lett. 125, 147003 (2020)
M. Osada et al. Nano Lett. 20, 8, 5735–5740 (2020)
M. Osada et al. Phys. Rev Materials 4, 121801 (2020)
M. Hepting, Nat. Mater. 19, 381–385 (2020)
D. Li, et al. Nat. 572, 624–627 (2019)
M. Hayward, et al. Solid state sciences 5(6) 839-850 (2003)
M. Hayward, et al. JACS, 121(38), 8843-8854 (1999)

K. Lee et al. arXiv:2203.02580
J. Fowlie, et al. Nature Physics (in press) (2022) arXiv:2201.11943
R. A. Ortiz, et al. Phys. Rev. Research 4, 023093 (2022)
S. Zeng et al. Sci. Adv. 8, eabl9927 (2022)
H. Lu et al. Science 373, 213–216 (2021)
M. Osada et al. Adv. Mater. 33, 2104083 (2021)
M. Rossi, et al. Phys Rev B 104, L220505 (2021)

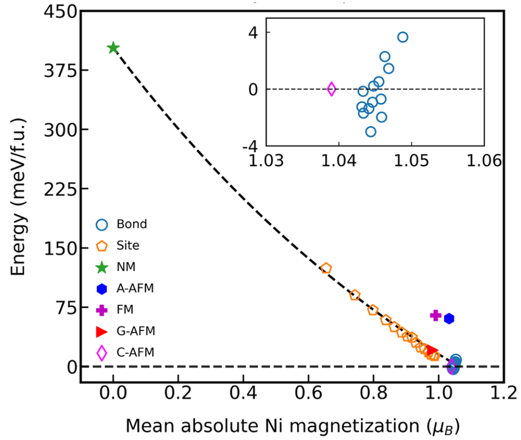
Magnetic instabilities and excitations in $LaNiO_2$





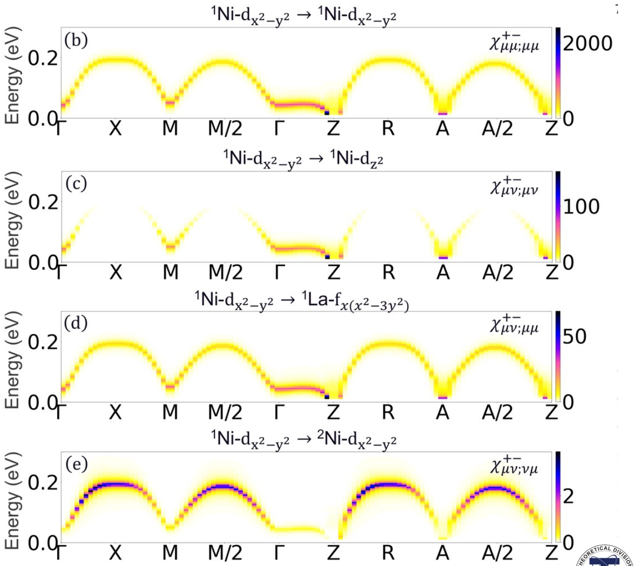


- χ^{+-} exhibits highly dispersive magnetic excitations following the spin-1/2 AFM magnons on a square lattice in agreement with experimental spectra.



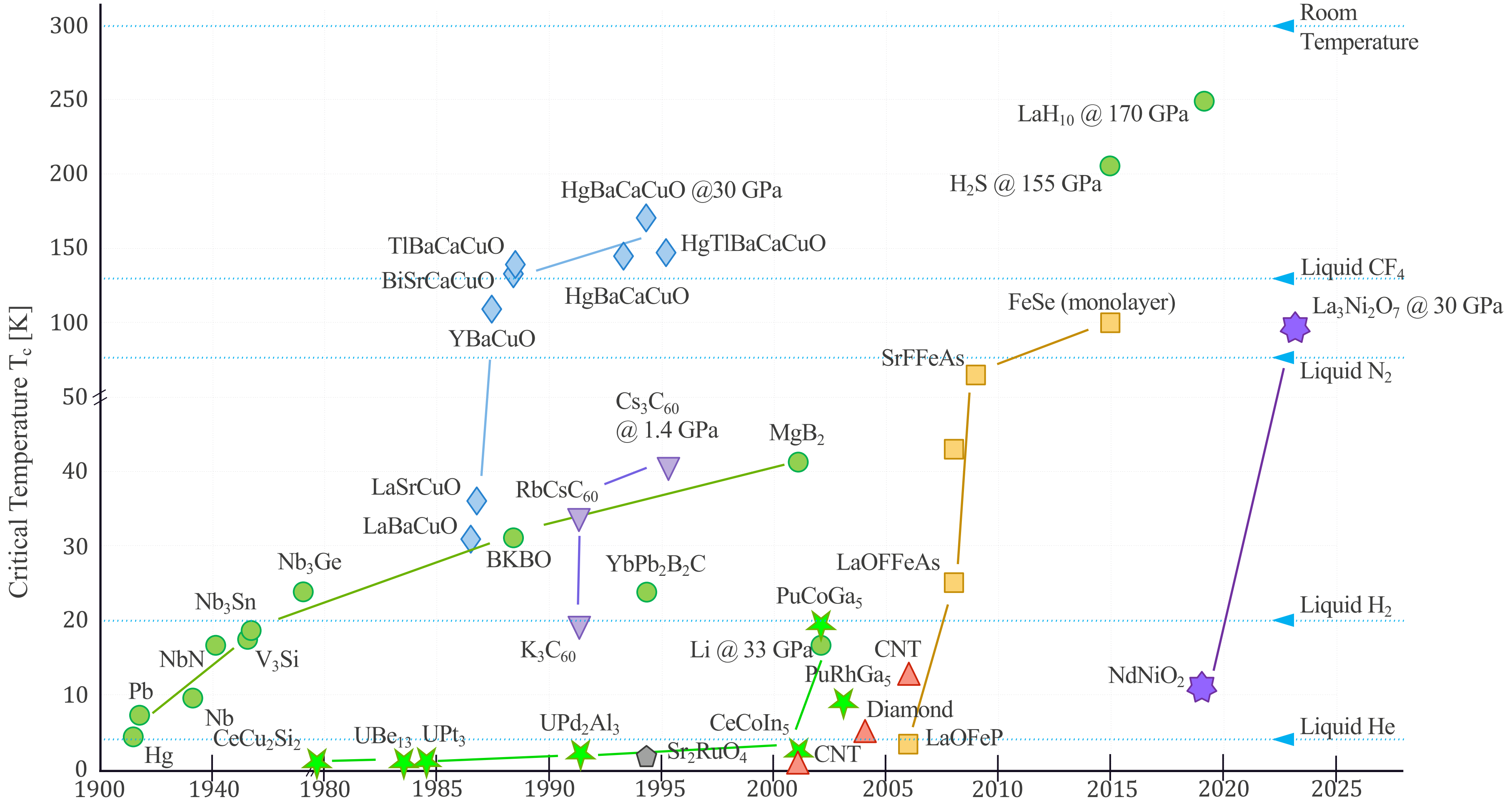
- Predicts a leading G-AFM instability is virtually degenerate with a dense manifold of 2D and 3D incommensurate magnetic stripe orders (indicated by the Van Hove-like singularities).
- Our analysis indicates that the magnetic properties of the infinite-layer nickelates are closer to those of the doped cuprates

- non-trivial Ni–La hybridization could contribute to the long-range behavior of the Heisenberg exchange parameters
- To reproduce both the charge and magnetic fluctuations, a minimum of two orbitals is required.



C. Lane, et al. Communications Physics 6, 90 (2023)
R. Zhang, C. Lane, et al. Under Review Nature Communications
R. Zhang, C. Lane, et al. Communications Physics 4, 118 (2021)

Present State of Superconducting Materials



Concluding Remarks

Summary/Outlook

- BCS pairing theory of superconductivity is a prototypical example of a condensed matter physics problem. It has inspired the Weinberg Salam model for Electroweak interactions.
- So far there is no quantitative theory of superconductivity in strongly correlated materials. The limits on Tc are still unknown
- Almost all known superconducting materials were found without theoretical guidance.
- The next-generation of first-principles approaches is beginning to captures a more holistic picture of correlated materials, giving way to a more quantitative theory of materials.

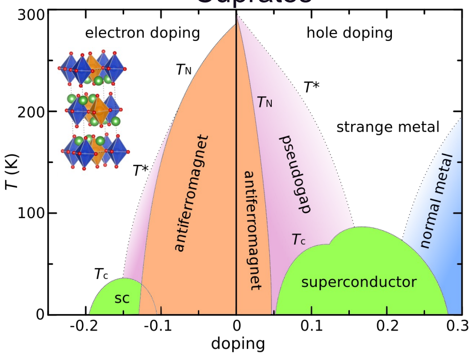
Superconductivity Illustrates the Process of Scientific Discovery

- Non-linear, convoluted, different from the linearity to courses and books
- Knowledge builds overtime on top of previous discoveries – "There are decades where nothing happens; and there are weeks where decades happen".
- Interplay of technical advances and scientific discovery

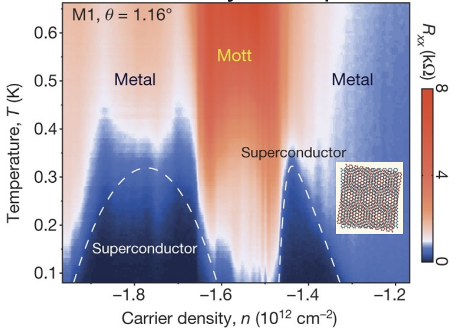
Open Challenges:

- What is the origin of these phases of matter?
- Why and and how does the transition temperature depend on specific material properties?
- Can we predict/find new materials with even higher transition temperatures?
- How can we move from serendipitous discovery to theoretical design of materials?

Cuprates



Twisted Bilayer Graphene



From BCS to the LHC. Steven Weinberg Int.J.Mod.Phys.A 23 1627-1635 (2008)