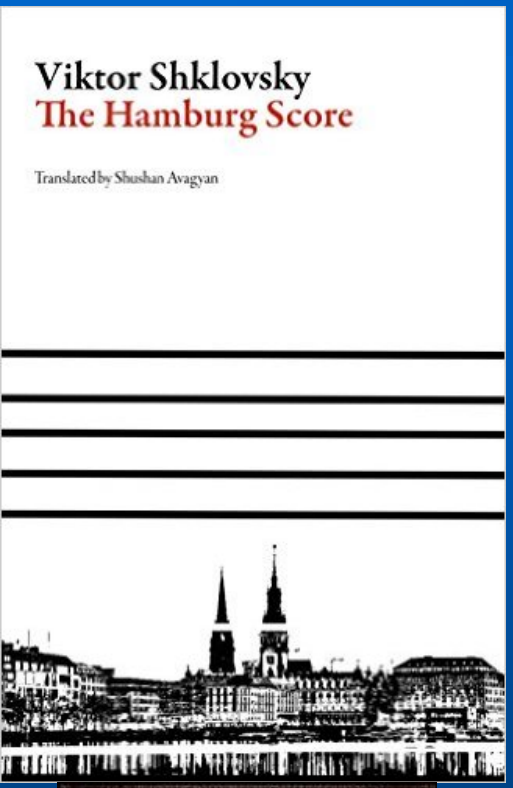
Radboud Universiteit

Quantum theory of real materials: From graphene to high-temperature superconductors

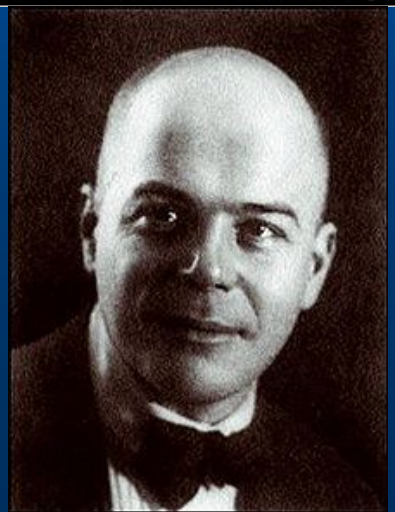
Mikhail Katsnelson

Hamburg Prize for Theoretical Physics



In Russian: a methaphor of honest, true rating

Legend invented by writer and literary theorist Viktor Shklovsky (1893-1984)
on secret matches of circus wrestlers in one of Hamburg innes (not confirmed historically)
to establish a true hierarchy



The Hamburg Score

Hamburg Prize for Theoretical Physics

There is no theoretical physics in this country East of Utrecht
(conventional wisdom)

Ship me somewhere East of Suez, where the best is like the worst
(R. Kipling)

OK... I am a materials scientist... But Nijmegen is beautiful

How materials scientist can receive a prize in theoretical physics?

Theory of condensed matter group

http://www.ru.nl/tcm/

What is “true” theory? Should it be “fundamental”?

Knowledge begins, so to speak, in the middle, and leads into the unknown - both when moving upward, and when there is a downward movement. Our goal is to gradually dissipate the darkness in both directions, and the absolute foundation - this huge elephant carrying on his mighty back the tower of truth - it exists only in a fairy tales (Hermann Weyl)

What does it mean for condensed matter physics and materials science?

Everything follows from quantum mechanics plus electrodynamics; QED is enough to explain all properties of matter around us

$$\begin{aligned} \gamma^\alpha(\partial_\alpha - ieA_\alpha)\psi + im\psi &= 0 \quad \text{where} \quad \alpha = 0, \ldots, 3 \\ F_{\alpha\beta} &= A_{\beta,\alpha} - A_{\alpha,\beta} \\ \partial^\alpha F_{\alpha\beta} &= -4\pi e j_\beta \\ \text{where} \quad j_\alpha &= \overline{\psi}\gamma_\alpha\psi. \end{aligned}$$

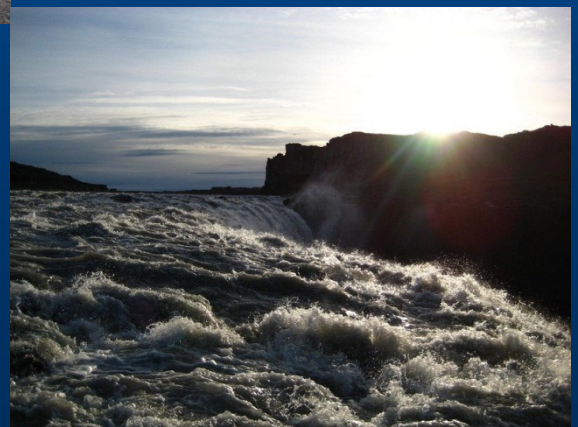
That is all. Please tell me why iridium is brittle and platinum is ductile, copper is red and silver is white, iron is ferromagnetic and vanadium is not... Not talking on biochemistry and biophysics!

Does it help?

$$\nabla \cdot u = 0$$

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = f + \mu \nabla^2 u - \nabla p$$

Navier-Stocks equations:
Turbulence is here!
Can you explain this?



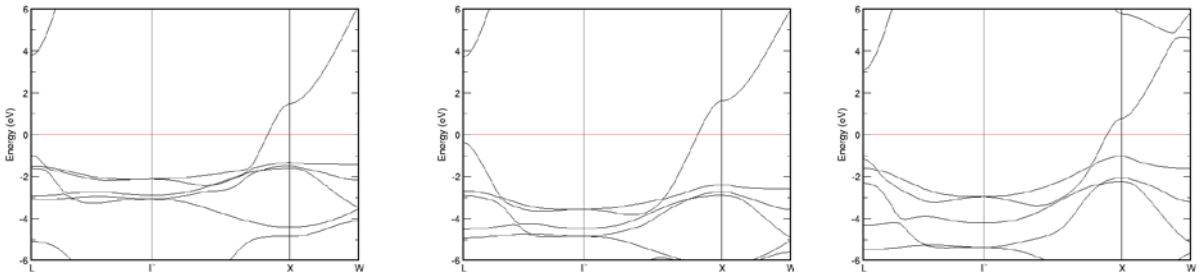
Scylla and Charybdis

Understanding “in general”

Everything is from water/fire/earth/gauge fields/quantum space-time foam/strings... and the rest is your problem.

But why silver is white, copper is red an gold is yellow?

Density functional calculations



Cu Ag Au

Taken from C. Ortiz, O. Eriksson and M. Klintenberg Comput. Mater. Sci. **44**, 1042 (2009).

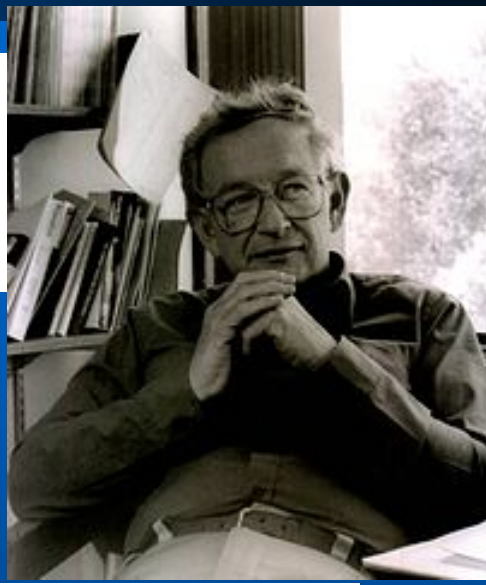
Scylla and Charybdis II

Local moments and localized states

P. W. Anderson

Reviews of Modern Physics, Vol. 50, No. 2, April 1978

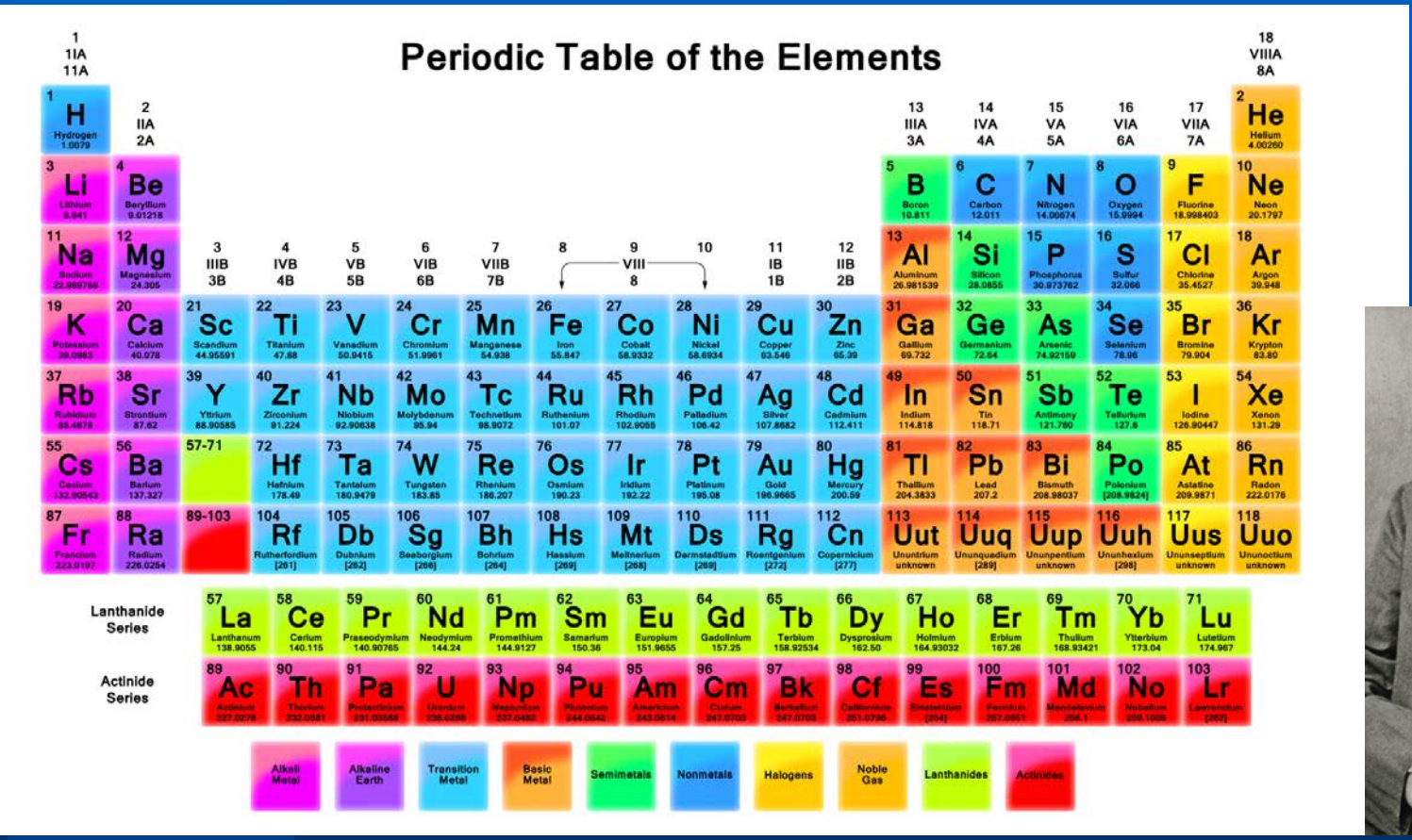
(Nobel lecture)

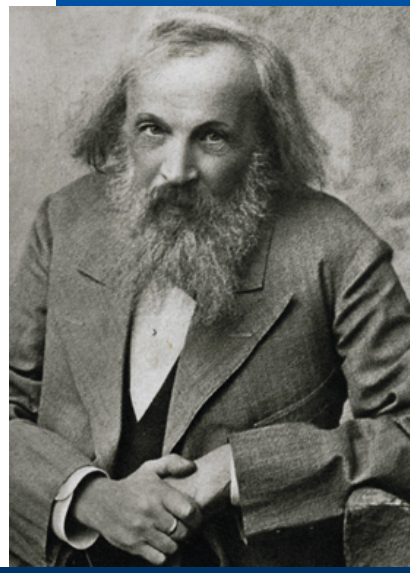


shall soon discuss. Very often such a simplified model throws more light on the real workings of nature than any number of *ab initio* calculations of individual situations, which even where correct often contain so much detail as to conceal rather than reveal reality. It can be a disadvantage rather than an advantage to be able to compute or to measure too accurately, since often what one measures or computes is irrelevant in terms of mechanism. After all, the perfect computation simply reproduces Nature, it does not explain her.

Periodic Table

Can we understand something elementary?



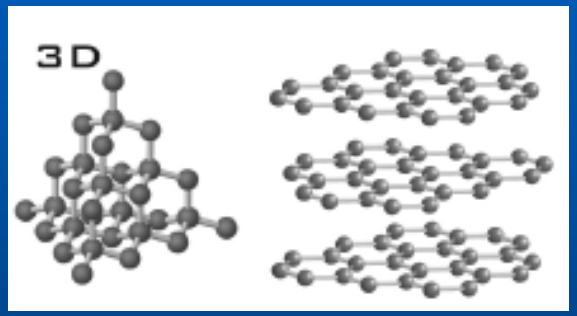


D. I. Mendeleev

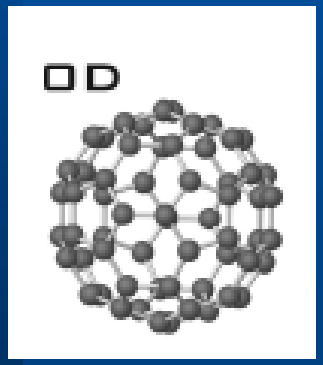
Carbon, an elemental solid

Diamond

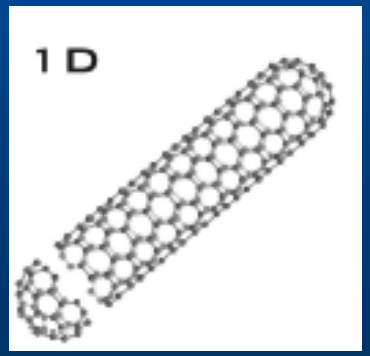
Graphite



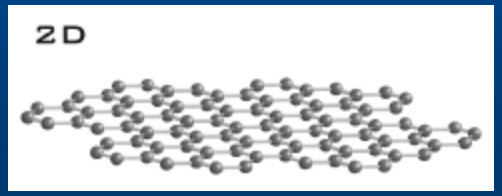
Crystal lattices



Fullerenes



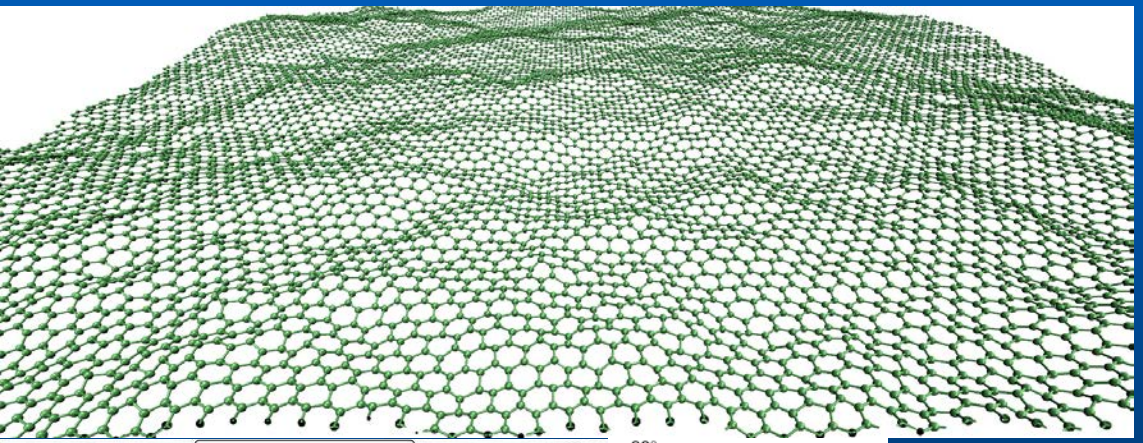
Nanotubes



Graphene

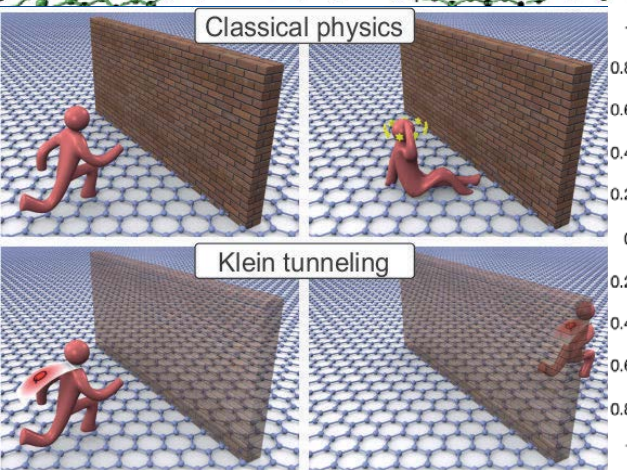
Why graphene is interesting?

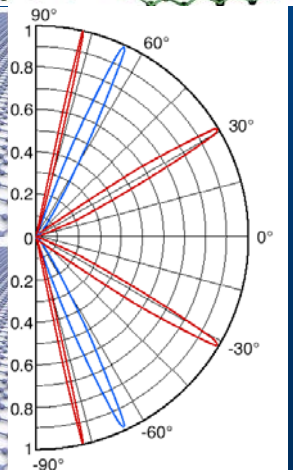
1. *Applications (modern electronics is 2D, bulk is ballast)*
2. *Prototype membrane (new drosophila for 2D statistical mechanics)*
3. *CERN on the desk (mimic high energy physics)*



Ripples

Fasolino, Los & MIK,
Nature Mater. 6, 858 (2007)

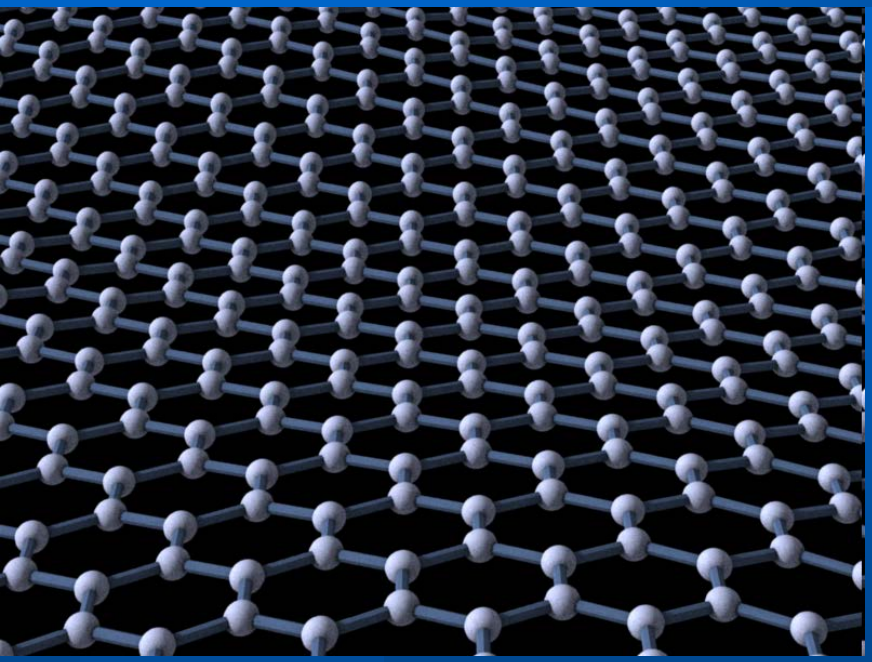


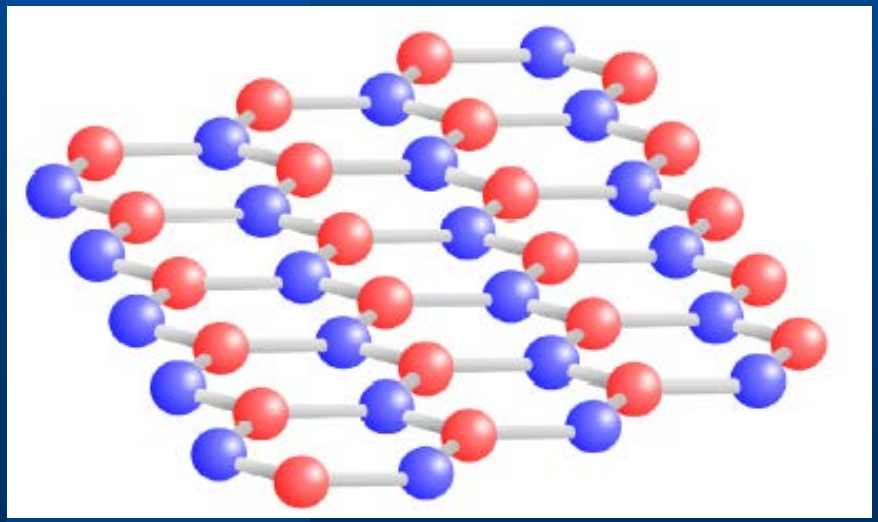


Klein tunneling

MIK, Novoselov, Geim, Nature Phys.
2, 620 (2006)

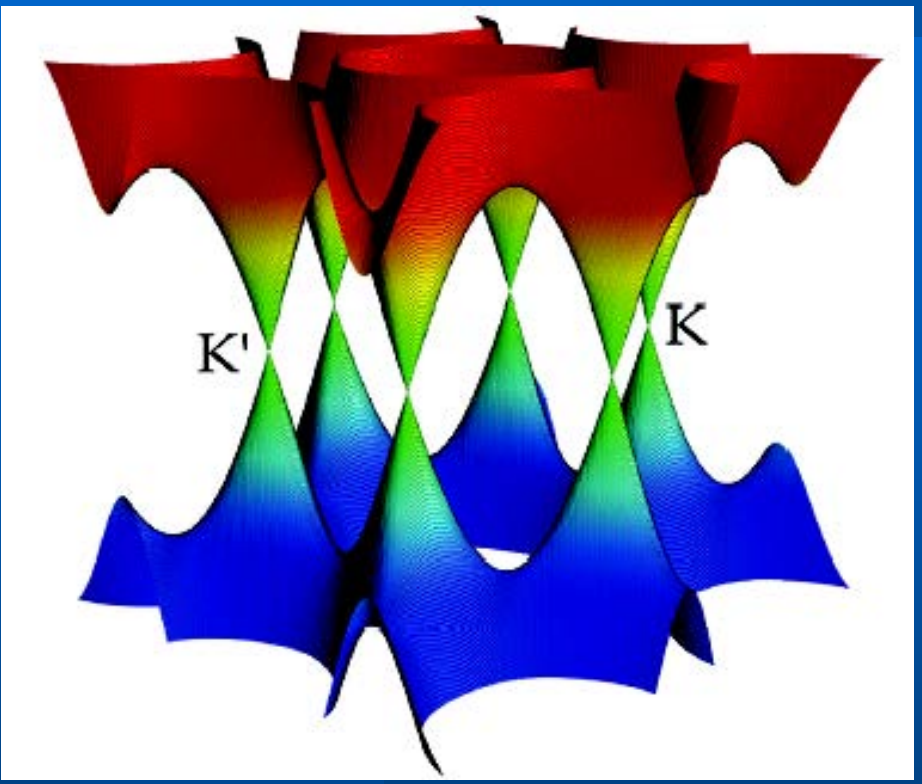
Honeycomb lattice





Two equivalent sublattices, A and B (pseudospin)

Massless Dirac fermions



sp^2 hybridization, π bands crossing the neutrality point

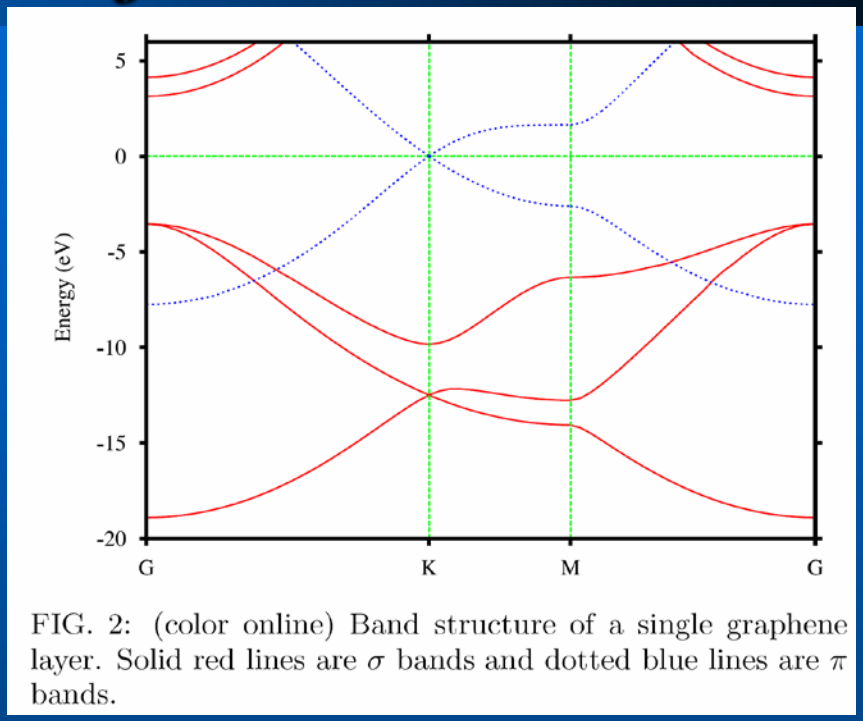
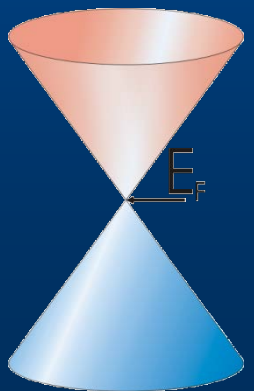


FIG. 2: (color online) Band structure of a single graphene layer. Solid red lines are σ bands and dotted blue lines are π bands.

Neglecting intervalley scattering: massless Dirac fermions

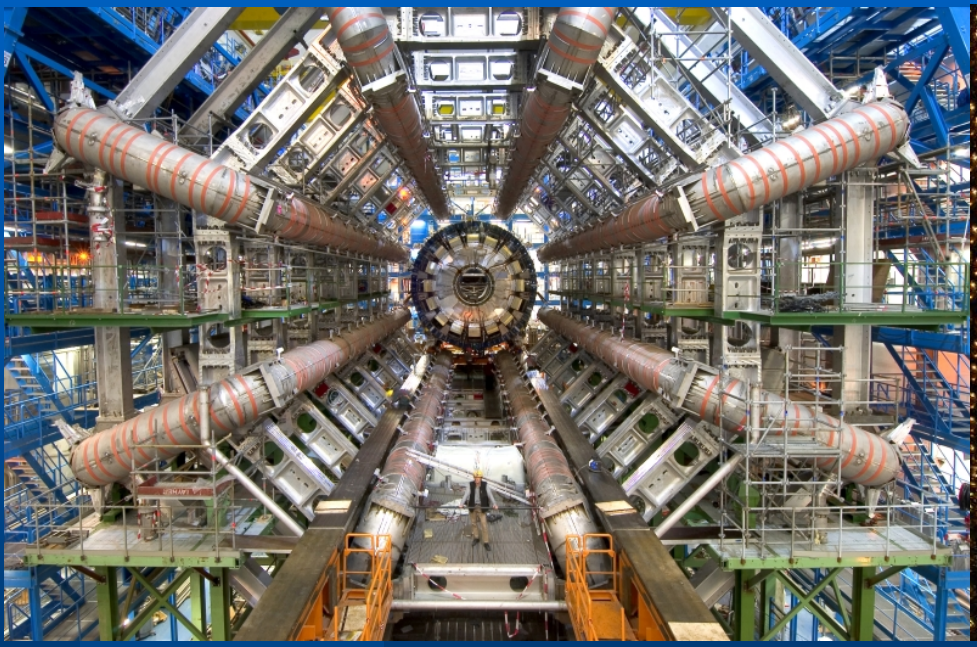
Massless relativistic particles (light cones)

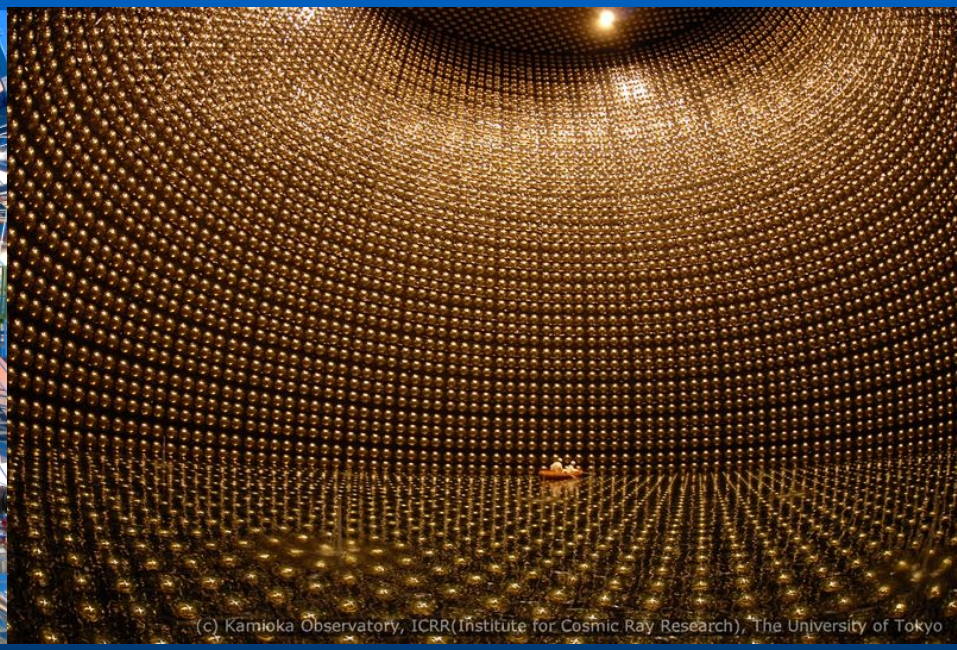


Symmetry protected (*T* and *I*)

Massless Dirac fermions in "real life"

Any particle can be considered as practically massless if it is ultrarelativitic, that is accelerated almost to velocity of light





Building accelerators and colliders, detectors of cosmic rays...
Neutrinos are always massless

Can solid-state realization be useful and instructive? Yes!!!

Theoretical physics as a variety of mistique experience

Beloved, believe not every spirit, but try the spirits whether they are of God (1 John 4:1)

Ye shall know them by their fruits. Do men gather grapes of thorns, or figs of thistles? (Matthew 7:16)

Fruits: to predict something correctly (like Maxwell electromagnetic waves, and then – applications)

Top pleasure and top dream for a theoretician

Graphene

1. Klein tunneling
2. Pseudomagnetic fields due to deformations
3. Relativistic collapse at a supercritical charge

Predicted and confirmed

Chiral tunnelling and the Klein paradox in graphene

M. I. KATSNELSON[1]*, K. S. NOVOSELOV[2] AND A. K. GEIM[2]*

nature physics | VOL 2 | SEPTEMBER 2006

nature physics
LETTERS
PUBLISHED ONLINE: 1 FEBRUARY 2009 | DOI: 10.1038/NPHYS1198

Quantum interference and Klein tunnelling in graphene heterojunctions

Andrea F. Young and Philip Kim*

LETTERS
PUBLISHED ONLINE: 27 SEPTEMBER 2009 | DOI: 10.1038/NPHYS1420
nature physics

Energy gaps and a zero-field quantum Hall effect in graphene by strain engineering

F. Guinea[1]*, M. I. Katsnelson[2] and A. K. Geim[3]*

Strain-Induced Pseudo–Magnetic Fields Greater Than 300 Tesla in Graphene Nanobubbles

N. Levy,[1,2]*† S. A. Burke,[1]*‡ K. L. Meaker,[1] M. Panlasigui,[1] A. Zettl,[1,2] F. Guinea,[3] A. H. Castro Neto,[4] M. F. Crommie[1,2]§

30 JULY 2010 VOL 329 SCIENCE

PRL 99, 236801 (2007) PHYSICAL REVIEW LETTERS week ending 7 DECEMBER 2007

Vacuum Polarization and Screening of Supercritical Impurities in Graphene

A. V. Shytov,[1] M. I. Katsnelson,[2] and L. S. Levitov[3]

PRL 99, 246802 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Atomic Collapse and Quasi–Rydberg States in Graphene

A. V. Shytov,[1] M. I. Katsnelson,[2] and L. S. Levitov[3]

Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene

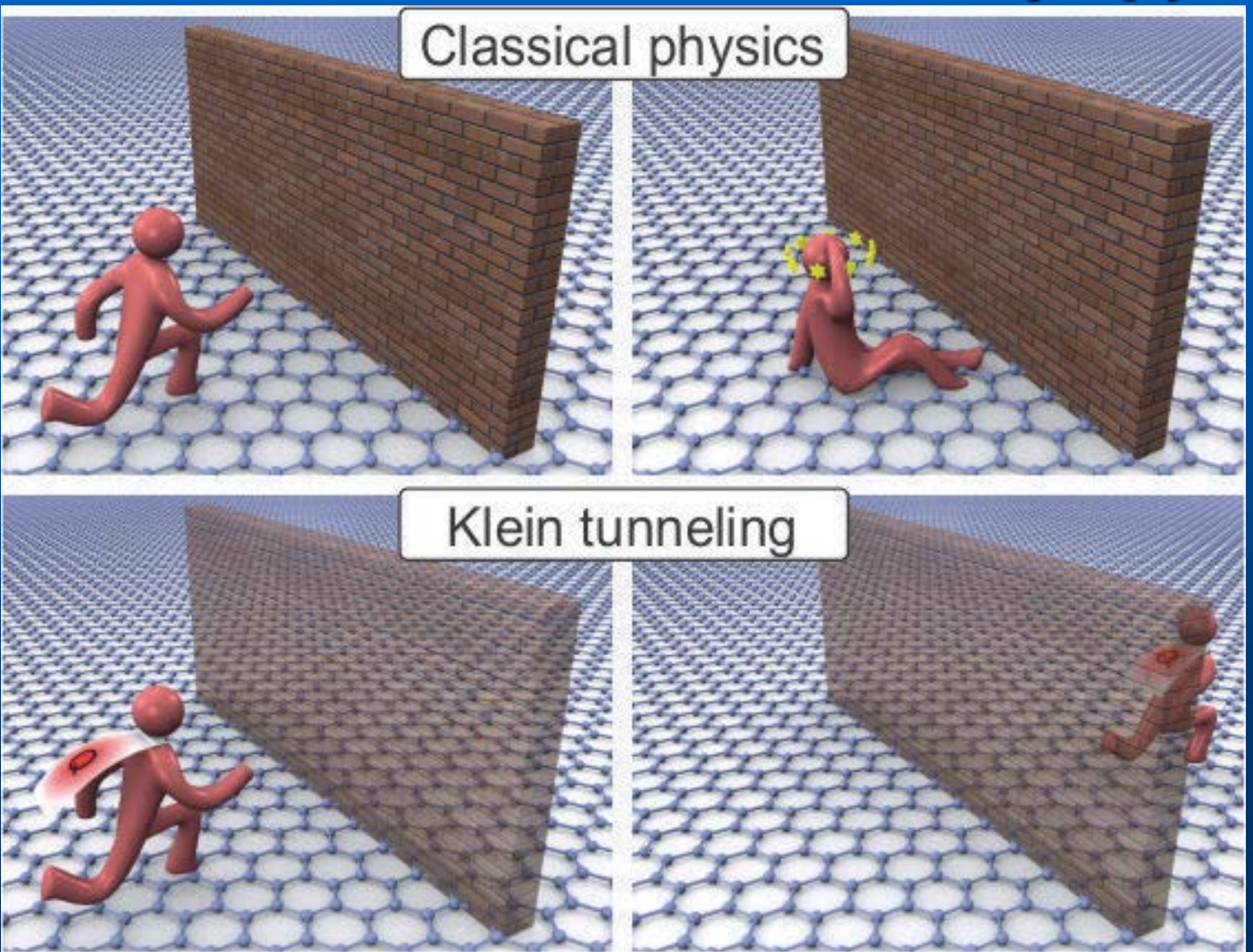
Yang Wang,[1,2]* Dillon Wong,[1,2]* Andrey V. Shytov,[3] Victor W. Brar,[1,2] Sangkook Choi,[1] Qiong Wu,[1,2] Hsin-Zon Tsai,[1] William Regan,[1,2] Alex Zettl,[1,2] Roland K. Kawakami,[5] Steven G. Louie,[1,2] Leonid S. Levitov,[4] Michael F. Crommie[1,2]†

10 MAY 2013 VOL 340 SCIENCE

Chiral tunneling and Klein paradox

MIK, Novoselov, Geim, Nat. Phys. 2, 620 (2006)

Electronics: heterostructures (*p-n-p* junctions etc.)

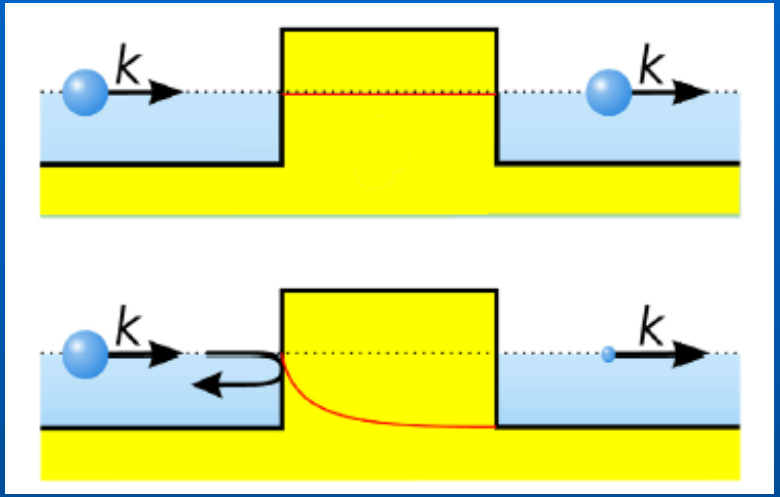


(C) Florian Sterl

Klein paradox II

Ultrarelativisic

Nonrelativistic



Tunnel effect: momentum and coordinate are complementary variables, kinetic and potential energy are not measurable simultaneously

Relativistic case: even the *coordinate itself* is not measurable, particle-antiparticle pair creation

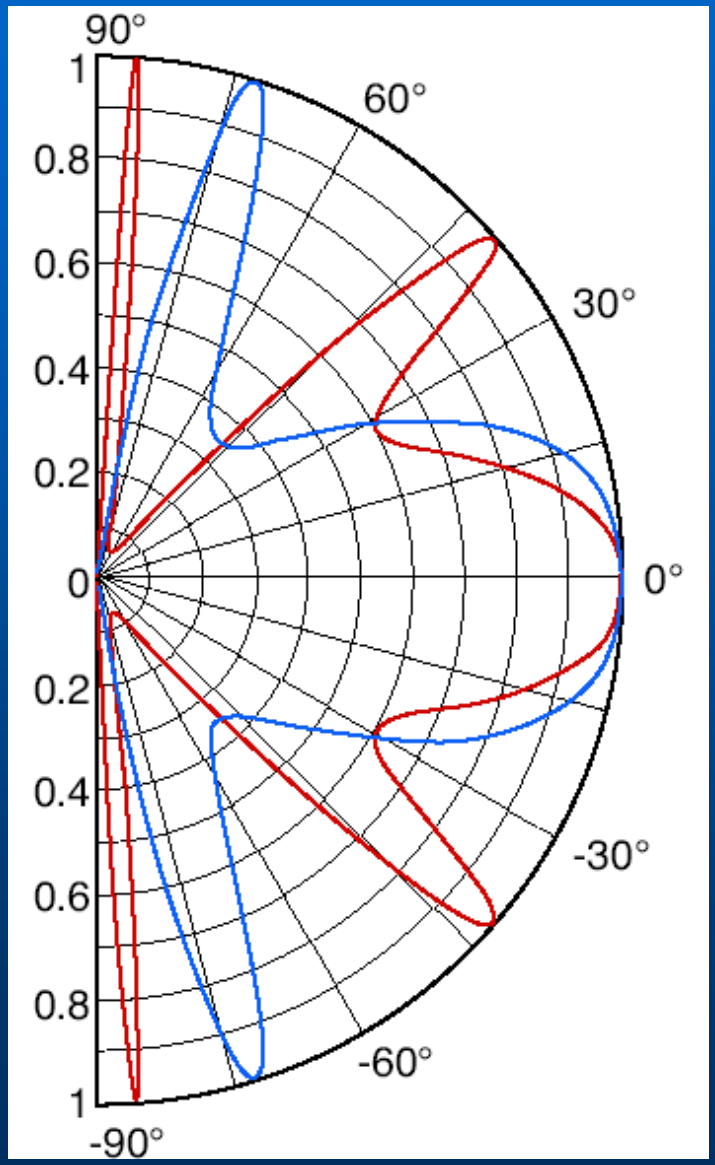
Klein paradox III

Transmission probability

Barrier width 100 *nm*

Electron concentration outside barrier 0.5×10^{12} cm^{-2}

Hole concentration inside barrier 1×10^{12} cm^{-2} (red) and 3×10^{12} cm^{-2} (blue)



Klein tunneling: Experimental confirmation

PRL **102,** 026807 (2009) PHYSICAL REVIEW LETTERS week ending 16 JANUARY 2009

Evidence for Klein Tunneling in Graphene *p-n* Junctions

N. Stander, B. Huard, and D. Goldhaber-Gordon*

Department of Physics, Stanford University, Stanford, California 94305, USA

(Received 13 June 2008; published 16 January 2009)

Transport through potential barriers in graphene is investigated using a set of metallic gates capacitively coupled to graphene to modulate the potential landscape. When a gate-induced potential step is steep enough, disorder becomes less important and the resistance across the step is in quantitative agreement with predictions of Klein tunneling of Dirac fermions up to a small correction. We also perform magnetoresistance measurements at low magnetic fields and compare them to recent predictions.

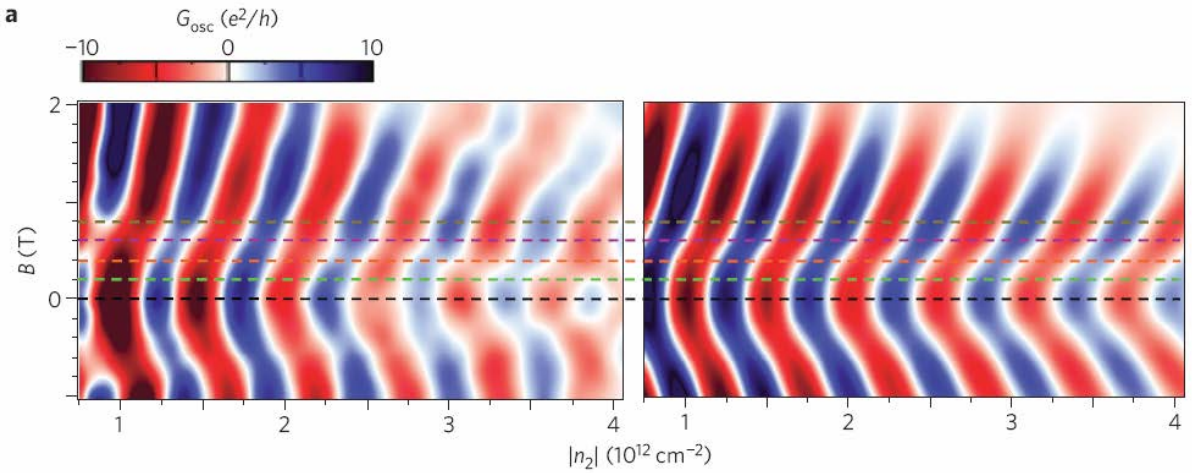
nature physics

LETTERS

PUBLISHED ONLINE: 1 FEBRUARY 2009 | DOI: 10.1038/NPHYS1198

Quantum interference and Klein tunnelling in graphene heterojunctions

Andrea F. Young and Philip Kim*



Relativistic collapse for supercritical charges

Coulomb potential

$$V_0(\mathbf{r}) = \frac{Ze^2}{\epsilon r}$$

following Shytov, MIK & Levitov, PRL 99, 236801; 246803 (2007)

Naive arguments: Radius of atom *R*, momentum *ħ/R*. Nonrelativistic case:

E(R) ~ ħ² /mR² – Ze²/R

Minimum gives a size of atom.

Relativistic case: *E(R) ~ ħc*/R – Ze²/R*

Either no bound state or fall on the center.

Vacuum reconstruction at *Z* > 170

Supercritical charges II

Superheavy nuclei

I. Pomeranchuk and Y. Smorodinsky, J. Phys. USSR **9**, 97 (1945)

Graphene:
$v \approx c/300$,
$\alpha_{eff} \approx 1$

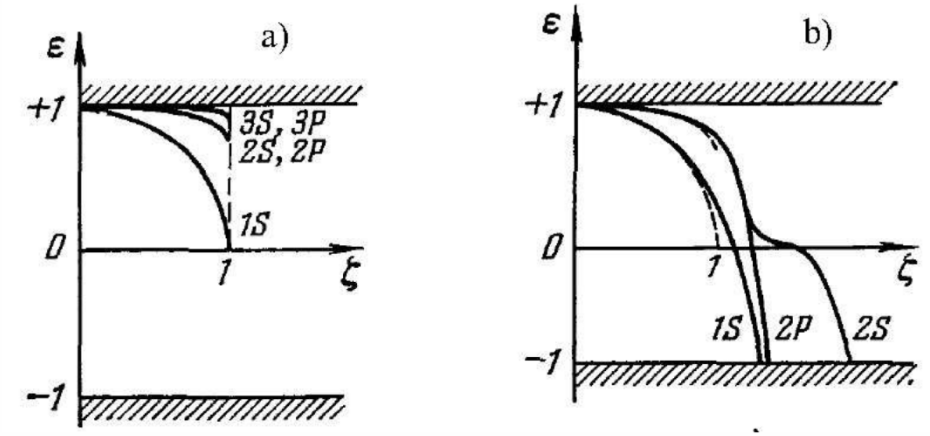
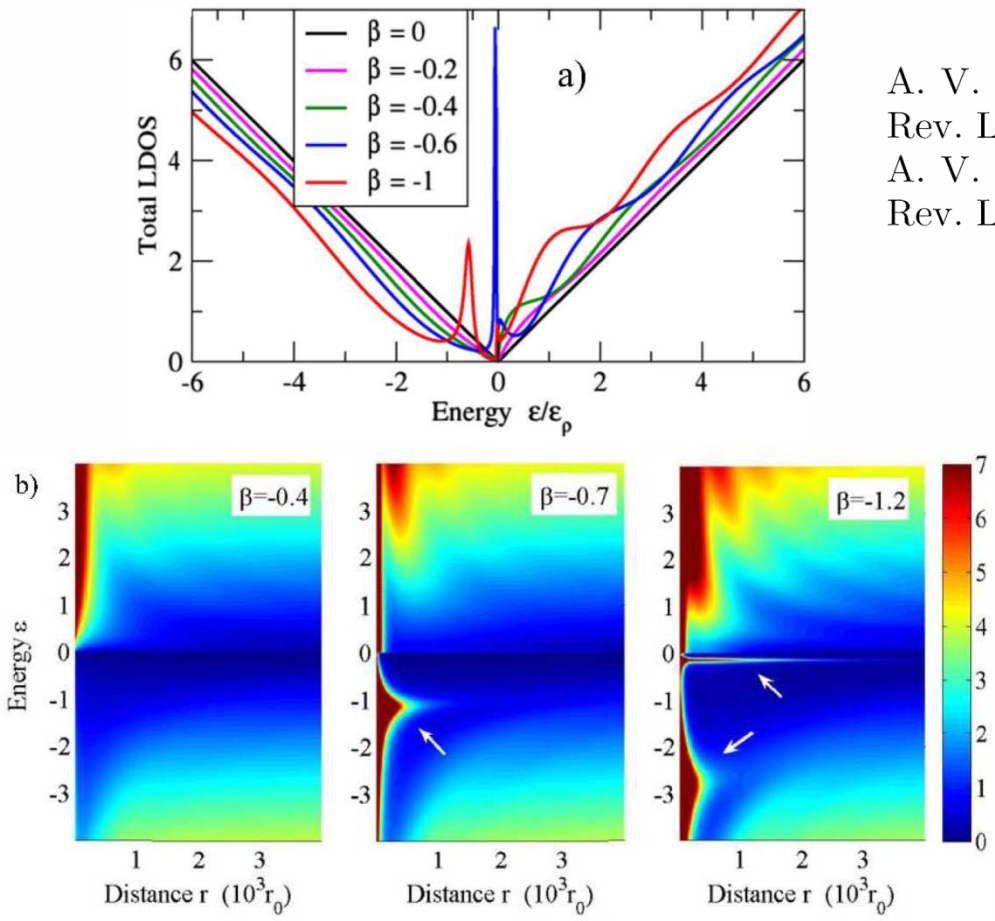


FIG. 1: a) Energy levels of superheavy atoms obtained from Dirac equation for Coulomb potential $-Ze^2/r$, plotted as a function of $\zeta = Z\alpha$, where Z is nuclear charge, and $\alpha = e^2/\hbar c$ is the fine structure constant. Energy is in the units of mc^2. (b) Energy levels for Coulomb potential regularized on the nuclear radius. As Z increases, the discrete levels approach the continuum of negative-energy states and dive into it one by one at supercritical $Z > 170$ (from Ref.[23]).

[23] Y. B. Zeldovich and V. S. Popov, Usp. Fiz. Nauk **105**, 403

Supercritical charge III

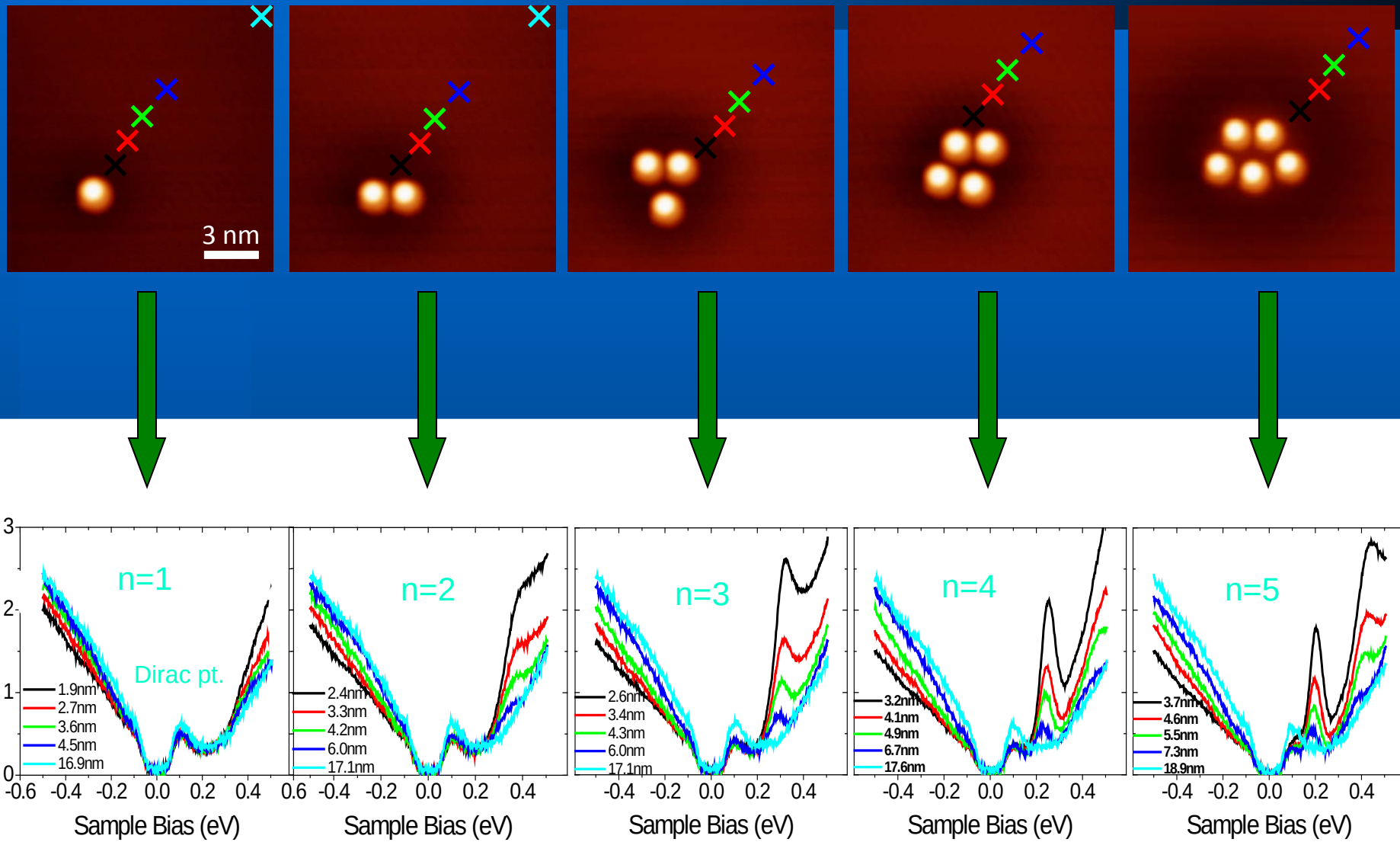


A. V. Shytov, M. I. Katsnelson, and L. S. Levitov, Phys. Rev. Lett. **99**, 236801 (2007), arXiv:0705.4663

A. V. Shytov, M. I. Katsnelson, and L. S. Levitov, Phys. Rev. Lett. **99**, 246802 (2007), arxiv.org:0708.0837

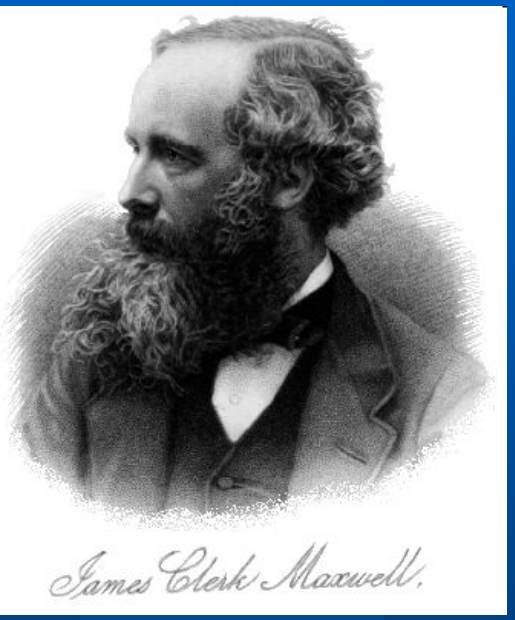
FIG. 3: (a) Local density of states (12) calculated at a fixed distance $\rho = 10^3 r_0$ from the charged impurity, where r_0 is a short-distance parameter of the order of carbon lattice spacing (from Ref.[10]). Peaks in the LDOS, which appear at supercritical β and move to more negative energies at increasing $|\beta|$, correspond to the resonant states. (b) Spatial map of the density of states, shown for several values of β, with resonances marked by white arrows (from Ref.[11]). Note that the spatial width of the resonances decreases at they move to lower energies, $\Delta\rho \propto 1/|\varepsilon|$, while the linewidth increases, $\gamma \propto |\varepsilon|$. The oscillatory structure at positive energies represents standing waves with maxima at $k\rho \approx (n + \frac{1}{2})\pi$, similar to those studied in carbon nanotubes [26]. Energy is given in the units of $\varepsilon_0 = 10^{-3}\hbar v/r_0 \approx 30\,\mathrm{mV}$ for $r_0 = 0.2\,\mathrm{nm}$.

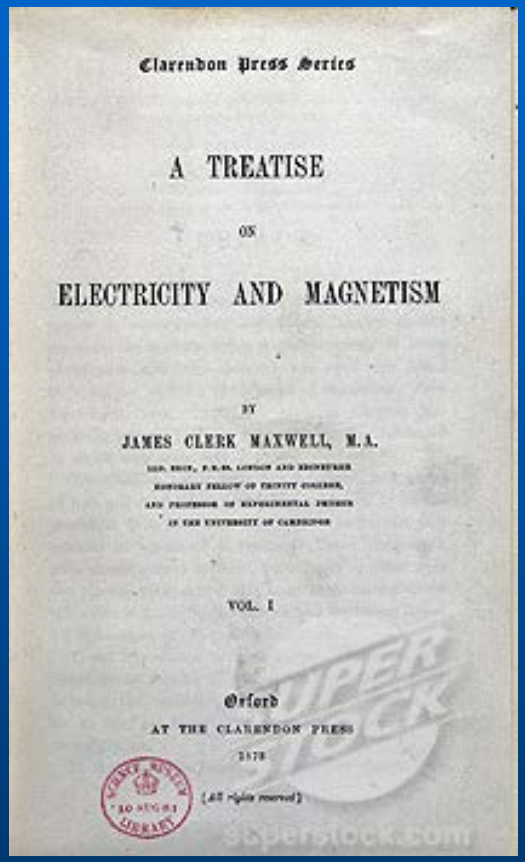
Exper.: Tuning Z by Building Artificial Nuclei from Ca Dimers



Y. Wang et al, Science 340, 734 (2013)

Gauge fields from mechanics: back to Maxwell




Clarendon Press Series

A TREATISE

ON

ELECTRICITY AND MAGNETISM

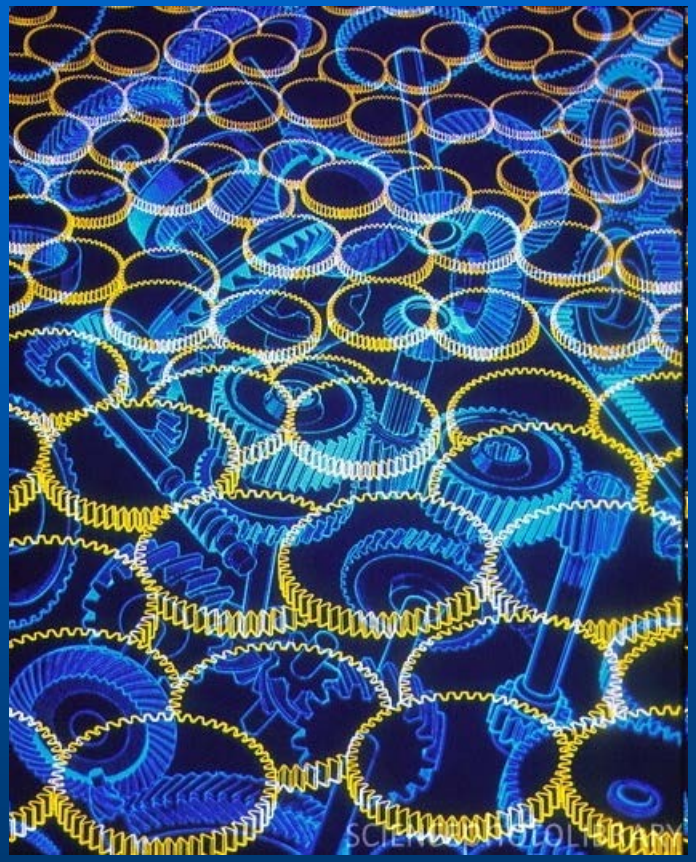
BY

JAMES CLERK MAXWELL, M.A.

VOL. I

Oxford

AT THE CLARENDON PRESS



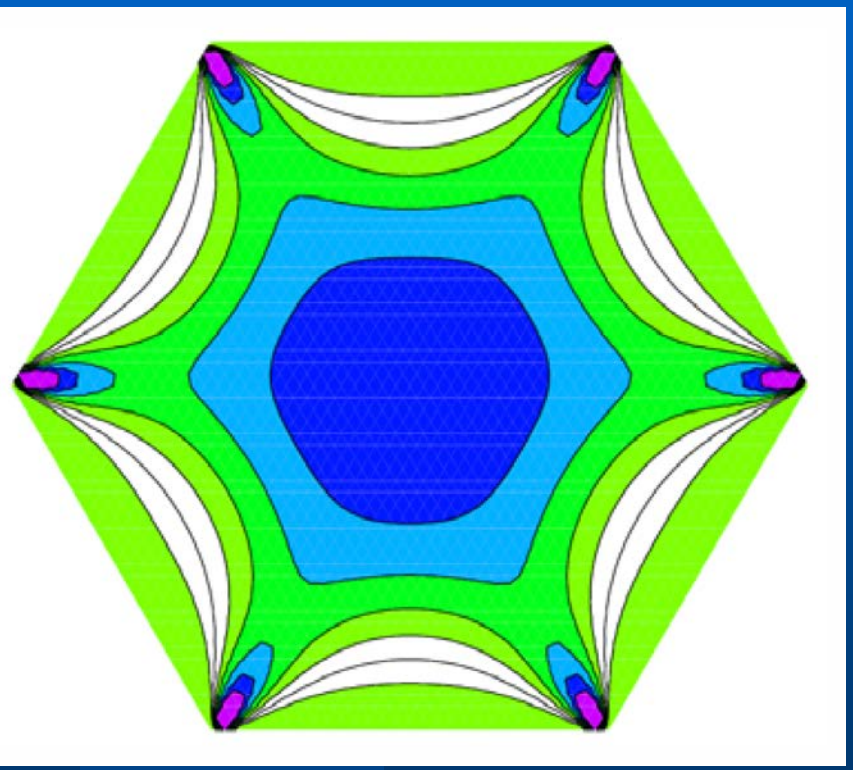
Electromagnetic fields as deformations in ether; gears and wheels

Review: Vozmediano, MIK & Guinea, Phys. Rep. 496, 109 (2010)

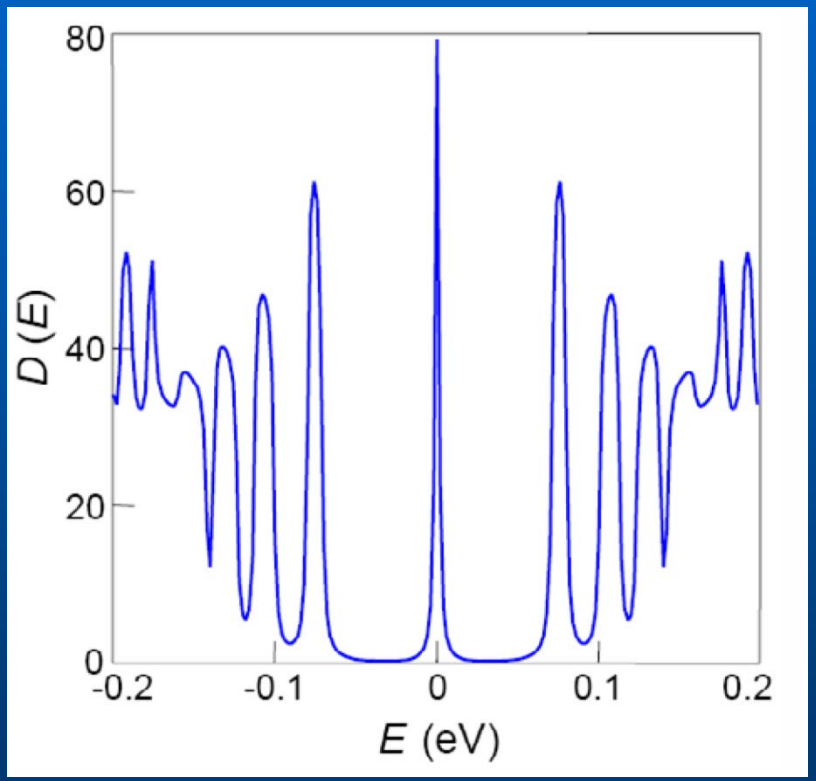
Zero-field QHE by strain engineering

F. Guinea, MIK & A. Geim, Nature Phys. 6, 30 (2010)

Can we create uniform (or almost uniform) pseudomagnetic field?



If you keep trigonal symmetry, quasi-uniform pseudomagnetic field can be easily created



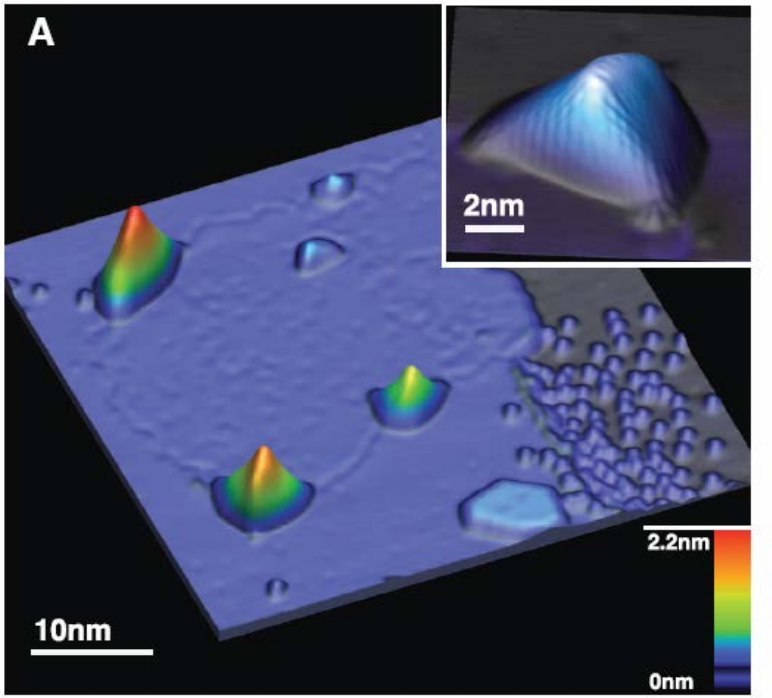
Normal stress applied to three edges size 1.4 μm, DOS in the center (0.5 μm)

Experimental confirmation

Strain-Induced Pseudo–Magnetic Fields Greater Than 300 Tesla in Graphene Nanobubbles

N. Levy,[1,2]*† S. A. Burke,[1]*‡ K. L. Meaker,[1] M. Panlasigui,[1] A. Zettl,[1,2] F. Guinea,[3] A. H. Castro Neto,[4] M. F. Crommie[1,2]§

30 JULY 2010 VOL 329 SCIENCE



Graphene on Pt(111)

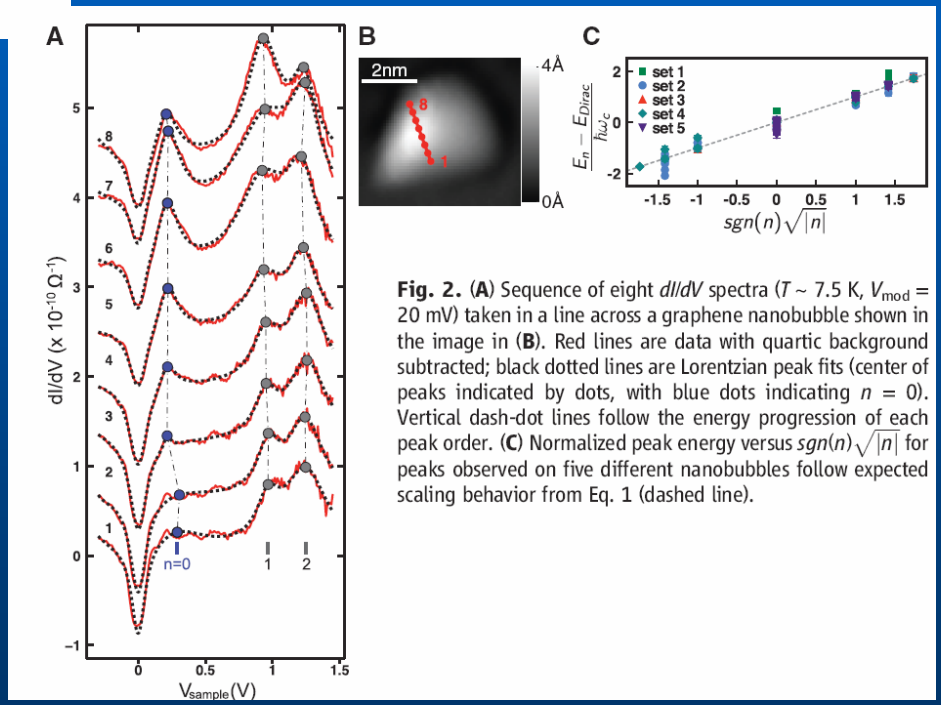


Fig. 2. (**A**) Sequence of eight *dI*/*dV* spectra (T ~ 7.5 K, V_{mod} = 20 mV) taken in a line across a graphene nanobubble shown in the image in (**B**). Red lines are data with quartic background subtracted; black dotted lines are Lorentzian peak fits (center of peaks indicated by dots, with blue dots indicating n = 0). Vertical dash-dot lines follow the energy progression of each peak order. (**C**) Normalized peak energy versus $sgn(n)\sqrt{|n|}$ for peaks observed on five different nanobubbles follow expected scaling behavior from Eq. 1 (dashed line).

STM observation of pseudo-Landau levels

From atoms to solids

Atoms:

Electron-electron interaction plays crucial role

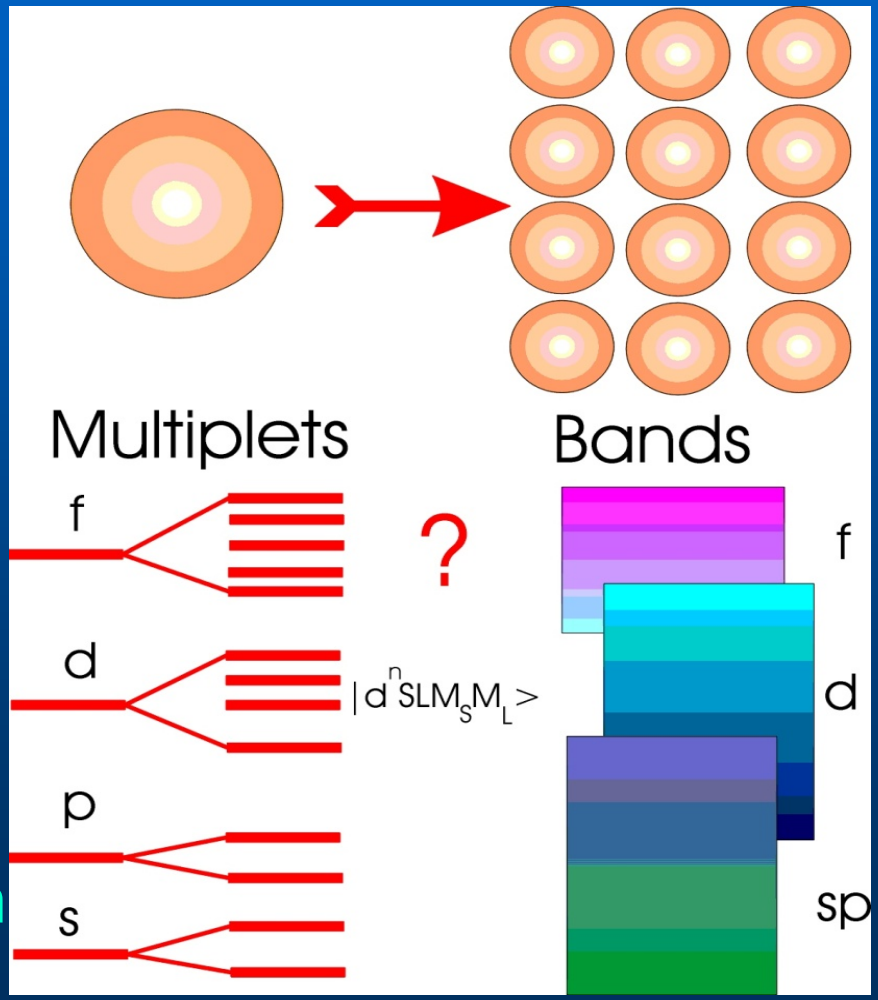
Optimal filling

Terms, multiplets

Hund's rules

Making solids from atoms: electrons at given site

How to combine?!



Crystals:

Bloch waves propagating through the crystal

Dispersion law

Fermi surface

Electron-electron Interaction just renormalizes parameters (Fermi liquid)...

The beginning: “Polar model”

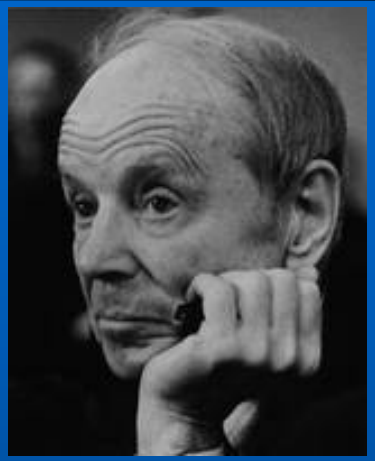
On the Electron Theory of Metals.

By S. Schubin and S. Wonsowsky.

Sverdlovsk Physical Technical Institute.

(Communicated by R. H. Fowler, F.R.S.—Received December 29, 1933.)

Proc. R. Soc. Lond. A 1934 **145**, published 2 June 1934



S. P. Shubin (1908-1938) S. V. Vonsovsky (1910-1998)

$$\int \frac{e^2}{|x-x'|}\,\phi_\alpha{}^2(x)\,\phi_\alpha{}^2(x')\,dx\,dx' = \mathrm{A}$$

$$\int \sum_{\gamma\neq\beta}\left[\mathrm{G}_\gamma(x)\,\phi_\alpha{}^2(x') + \frac{e^2}{|x-x'|}\,\phi_\gamma{}^2(x')\right]\phi_\alpha(x)\,\phi_\beta(x)\,dx\,dx' = \mathrm{L}_{\alpha\beta}$$

$$\int \frac{e^2}{|x-x'|}\,\phi_\alpha{}^2(x)\,\phi_\beta{}^2(x')\,dx\,dx' = \mathrm{B}_{\alpha\beta}$$

$$\int \frac{e^2}{|x-x'|}\,\phi_\alpha(x)\,\phi_\beta(x)\,\phi_\alpha(x')\,\phi_\beta(x')\,dx\,dx' = \mathrm{J}_{\alpha\beta}$$

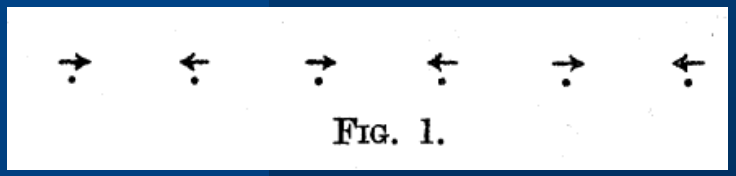


Fig. 1.

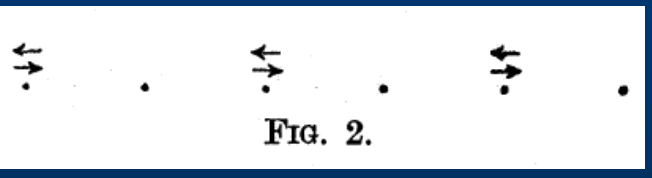


Fig. 2.

The beginning: "Polar model" II

Schrödinger equation in "atomic representation" (double *f*, hole *g*, spin right *k*, spin left *h*)

$$\{\varepsilon - s(A+D) - [\sum_{f<f'}(B_{ff'} - J_{ff'}) + \sum_{g<g'}(B_{gg'} - J_{gg'}) - \sum_{f,g}(B_{fg} + J_{fg})]\}C(fgh)$$
$$+ \sum_{h,k} J_{hk}[C(T_{hk}|fgh) - C(fgh)] + \sum_{f,g} J_{fg}[C(T_{fg}|fgh) - C(fgh)]$$
$$+ \sum_{f,p} L_{fp} C(T_{fp}|fgh) - \sum_{g,p} L_{gp} C(T_{gp}|fgh) = 0, \qquad (9)$$

Metal-insulator transition and Mott insulators

(II). The minimum energy corresponds to a certain $s = s_0$, where $0 < s_0 < n$. This case we have, for instance, when

$$A + 6(J - B) > 0, \quad A + 6J - 12L < 0.$$

Then, so long as s remains small, the lowest energy level *diminishes* as s increases; for a certain $s = s_0$ it attains a minimum and then again begins to increase. For such metals—at not very high temperatures—the number of "free" electrons approximates to twice this s_0 (electrons + holes !) and is therefore *smaller* than the number of atoms. In order to calculate s_0 in terms of our integrals, the energy must be evaluated up to the second approximation in powers of s/n; we shall not, however, make these rather cumbersome calculations here.

Metal

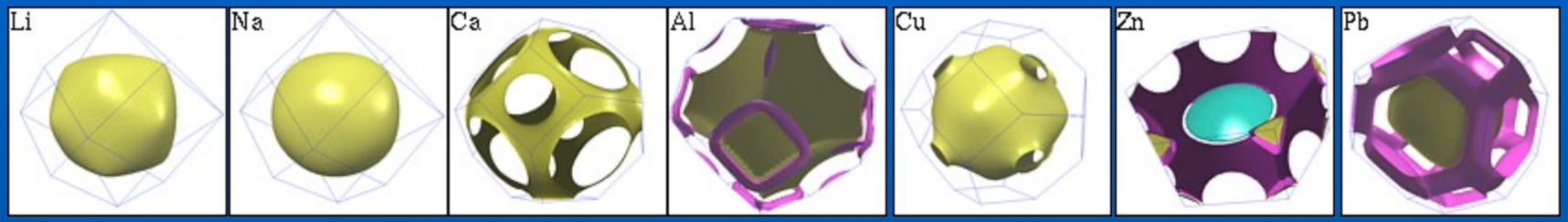
Insulator

(III). The minimum energy corresponds to $s = 0$. This is the case when

$$A + 6(J - B) > 0, \quad A + 6J - 12L > 0.$$

When do we have a problem?

sp metals (empty or completely filled df shells): purely itinerant behavior



http://www.phys.ufl.edu/fermisurface/periodic_table.html

4f (rare earth) metals: *f* electrons are atomic like, *spd* electrons are itinerant

PHYSICAL REVIEW B **74**, 045114 (2006)

Multiplet effects in the electronic structure of light rare-earth metals

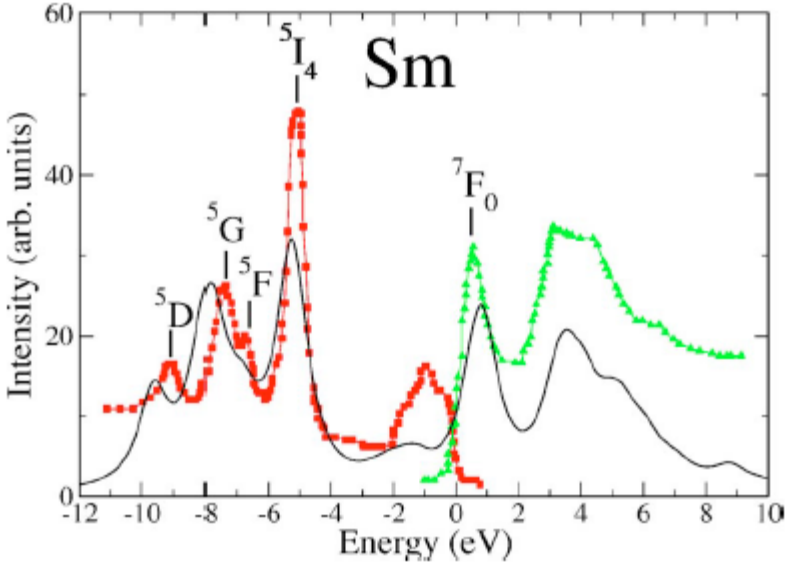
S. Lebègue,[1,2] A. Svane,[3] M. I. Katsnelson,[4] A. I. Lichtenstein,[5] and O. Eriksson[1]

Photoemission (red) and inverse photoemissin (green)

PES

$f^5 \rightarrow f^4$

$^5I_4$, ^5F, ^5G, and ^5D final states

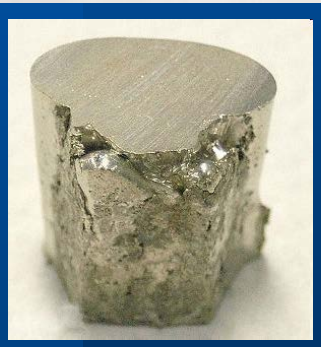


Itinerant-electron magnets: coexistence

Fe

Co

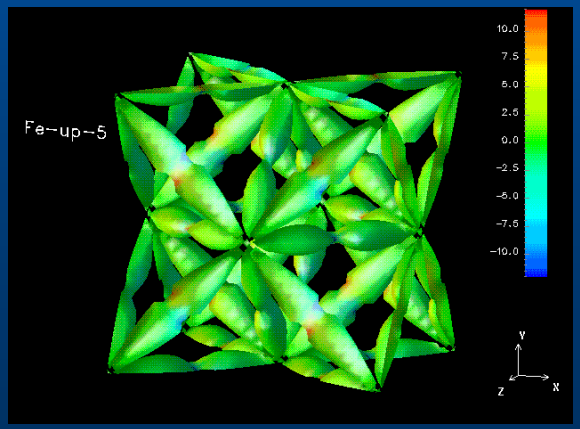
Ni

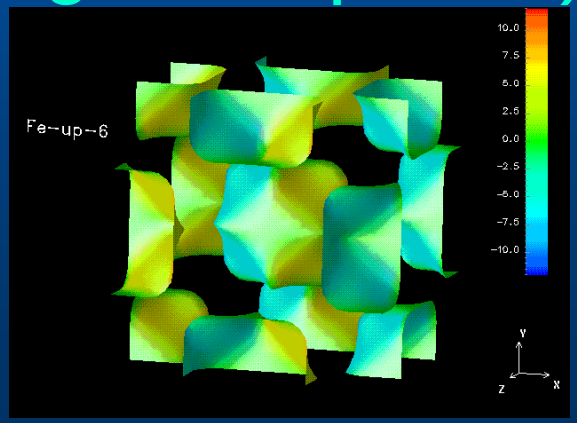


Iron, majority spin FS

Local magnetic moments do exist above T_C (Curie-Weiss law, spectroscopy, neutrons…)

d electrons are itinerant (FS, chemical bonding, transport…)





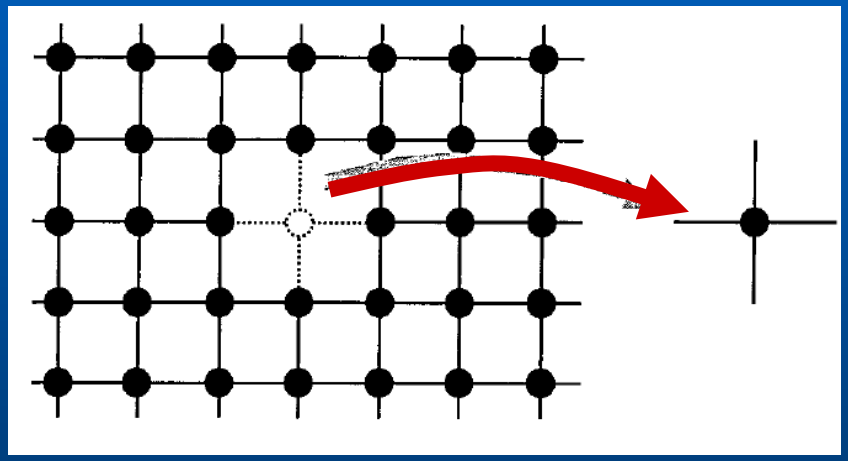
4f electrons are normally pure localized but not 3d

Dynamical Mean Field Theory

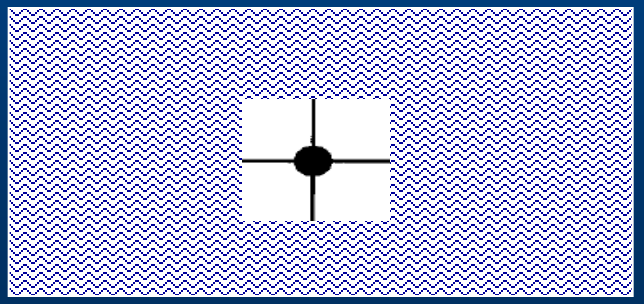
A.Georges, G.Kotliar, W.Krauth and M.Rozenberg, Rev. Mod. Phys. '96

A natural generalization of the familiar MFT
to the problem of electrons in a lattice

Key idea: take one site out of a lattice and embed it in a self-consistent bath = mapping to an effective impurity problem



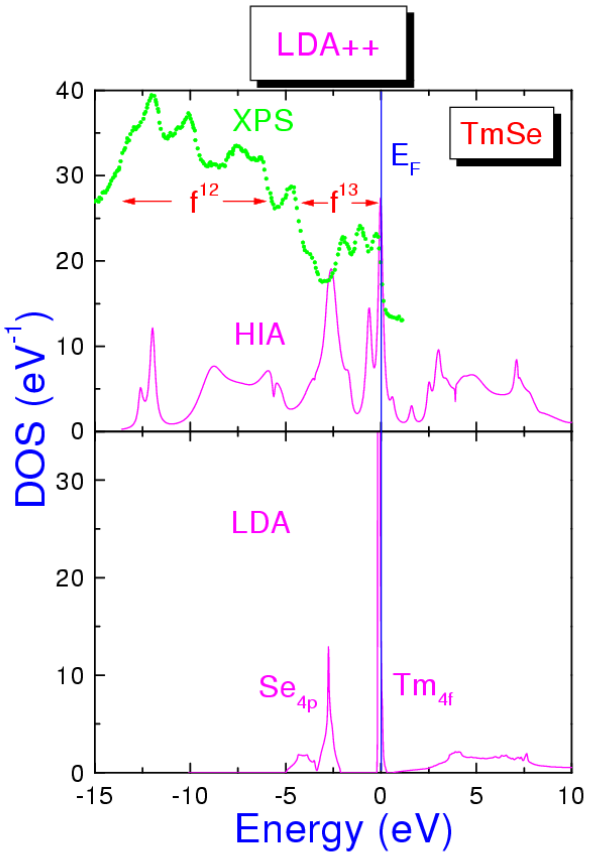
Effective impurity: atomic-like features, many-body problem



Putting into crystal: itinerant features, single-body problem

Combination with realistic calculations

A.Lichtenstein and MIK, PRB 57, 6884 (1998); JPCM 11, 1037 (1999)
V.Anisimov et al, JPCM 9, 7339 (1997)



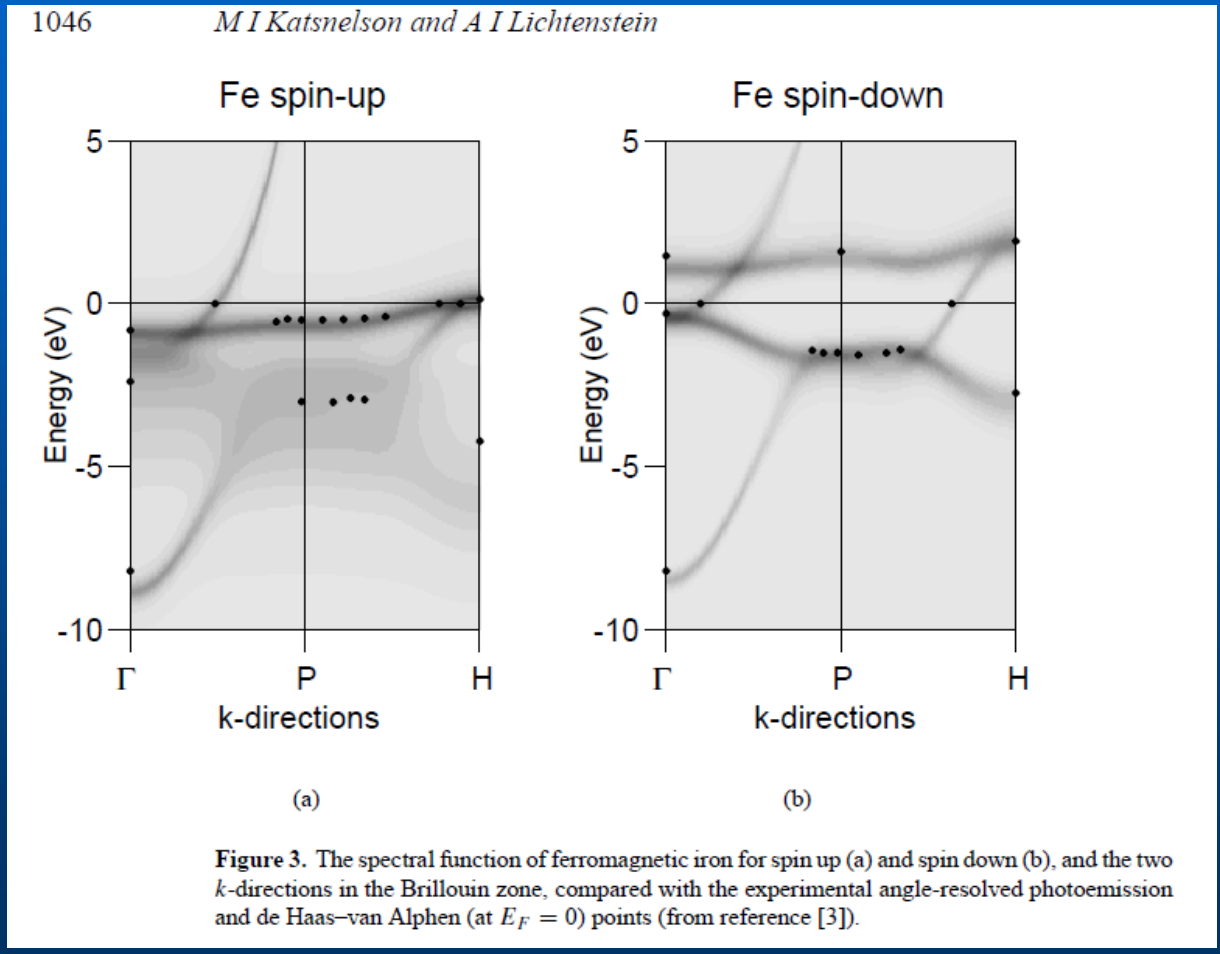


Figure 3. The spectral function of ferromagnetic iron for spin up (a) and spin down (b), and the two k-directions in the Brillouin zone, compared with the experimental angle-resolved photoemission and de Haas–van Alphen (at $E_F = 0$) points (from reference [3]).

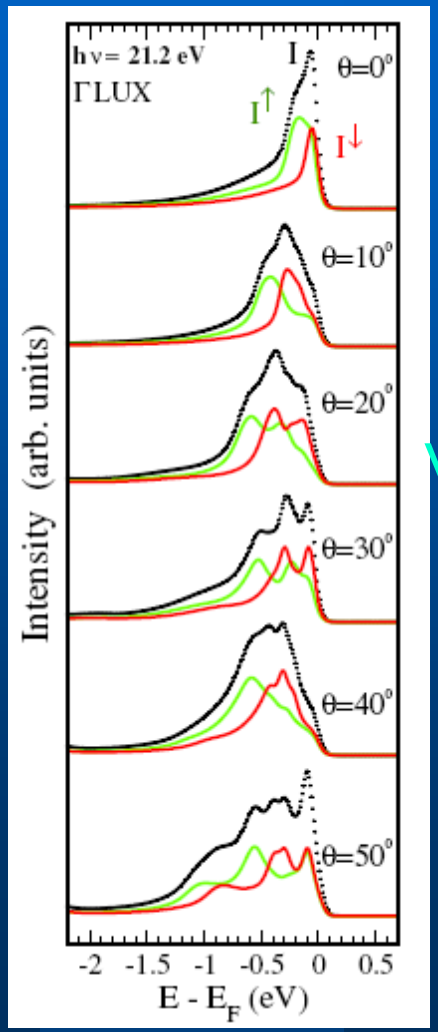
PRB 57, 6884 (1998)

JPCM 11, 1037 (1999)

Ferromagnetism of transition metals: LDA+DMFT

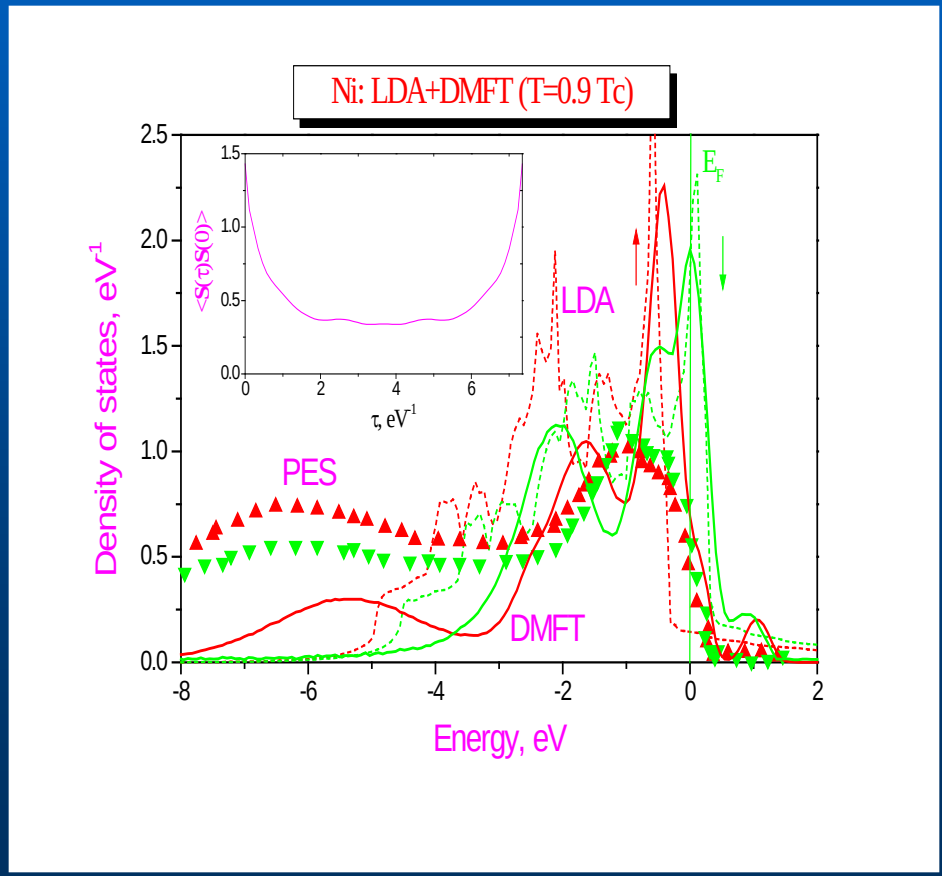
Ferromagnetic Ni DMFT vs. LSDA:

- 30% band narrowing
- 50% spin-splitting reduction
- -6 eV sattellite



LDA+DMFT with ME
J. Braun *et al*
PRL (2006)

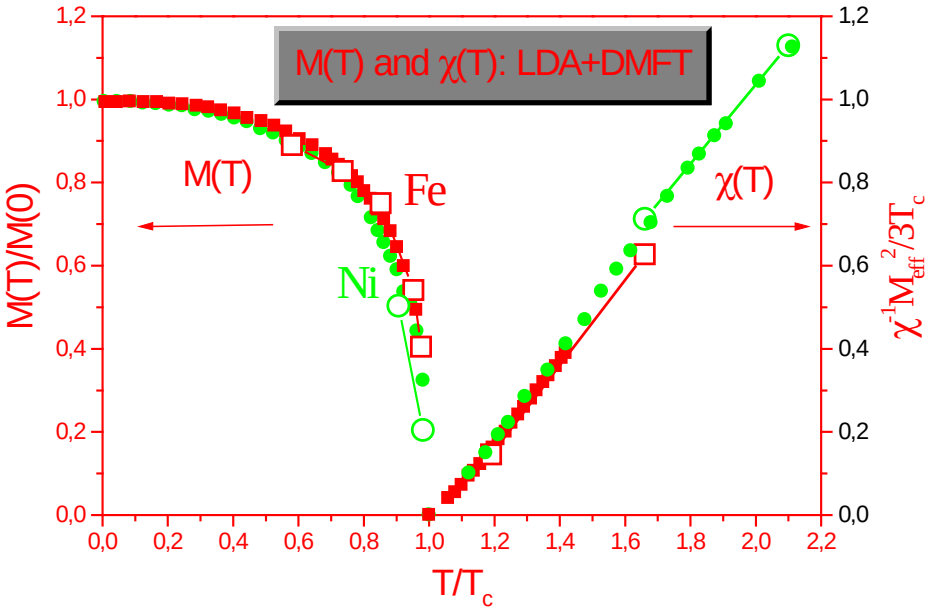
Very good for Ni



Lichtenstein, MIK, Kotliar, PRL (2001)

DMFT Effective Magnetic Moments: $T>T_c$

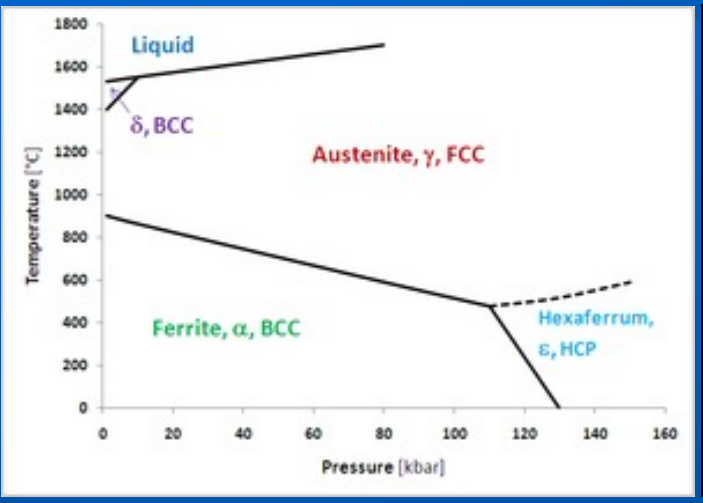
W	exp	eff	loc	DLM	Tc	exp
Fe	3.13	3.09	2.8	1.96	1900	1043
Ni	1.62	1.5	1.3	1.21	700	631

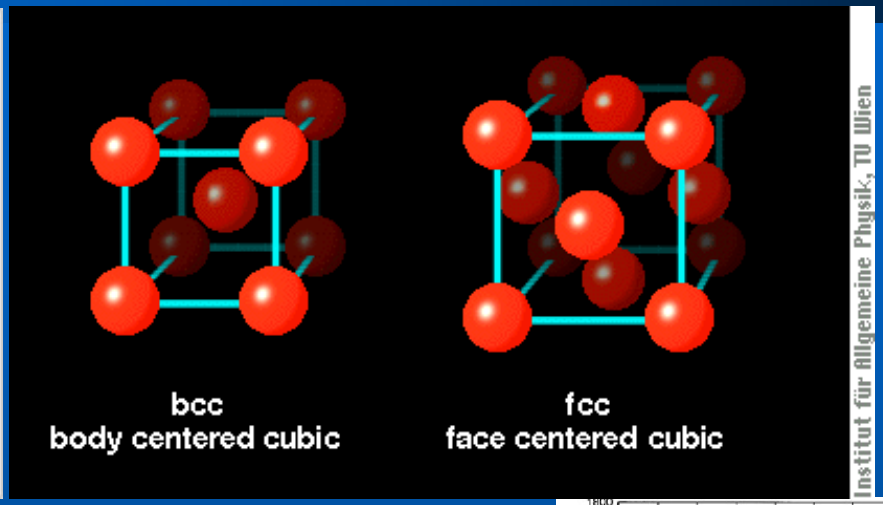


We are still in iron age

Steel (basically, Fe and a bit C) is one of the main materials of our civilization

Iron is polymorphous metal

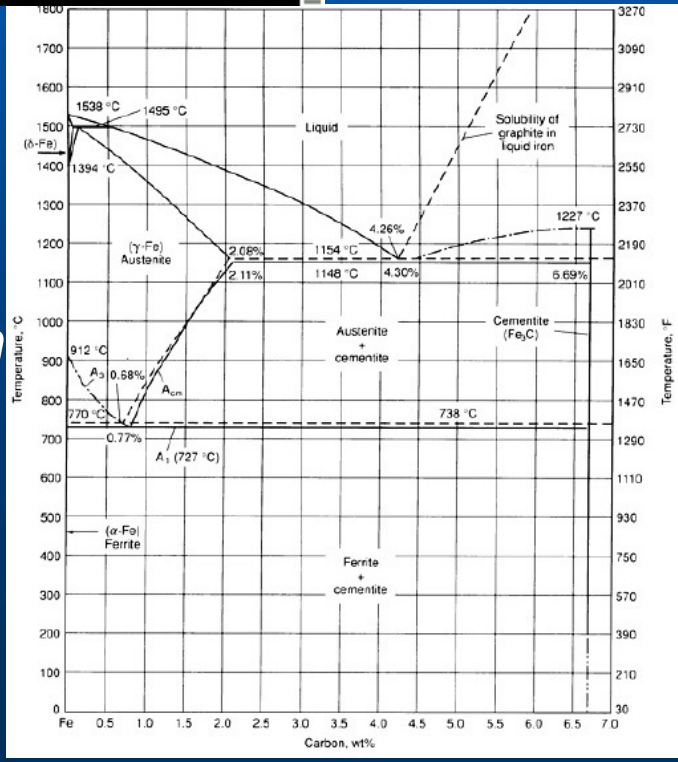




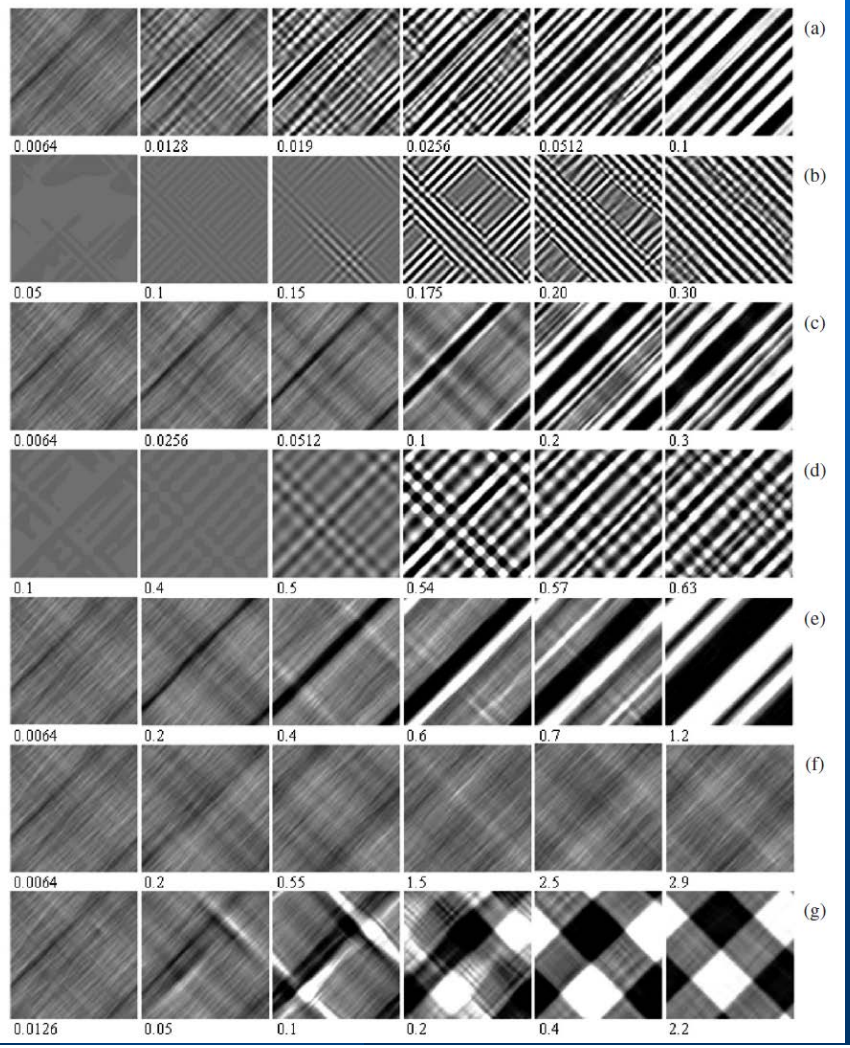
The only polymorphous metal where bcc phase is stable at lower temperatures than fcc or hcp: Role of magnetism (Zener)

Crucially important for Fe-C phase diagram and therefore for metallurgy

Should follow from electronic structure (quantum mechanical energy spectrum)



Morphology of two-phase state



J. Phys.: Condens. Matter **25** (2013) 135401 (9pp) doi:10.1088/0953-8984/25/13/135401

Effect of magnetism on kinetics of γ–α transformation and pattern formation in iron

I K Razumov[1,2], Yu N Gornostyrev[1,2] and M I Katsnelson[3]

Magnetic free energy plays crucial role in kinetics of transformation and morphology of the final structure in pure iron

Figure 2. Time evolution of the structure at exposure at $T = 400$ K ((a), (b)), 700 K ((c), (d)), 950 K (e), 1000 K ((f), (g)) after quenching of the high-temperature state ((a), (c), (e), (f)) or development of instability of the uniform fcc state ((b), (d)), under homogeneous ((a)–(f)) and heterogeneous nucleation (g). Gradations of gray color correspond to the values for the order parameter ϕ; black and white colors show the regions for the α-phase with two possible orientations ($\phi = \pm 1$).

What about steel?

Steel: composite material (hard carbide phase in ductile bcc Fe)
Morphology determines mechanical properties and therefore applications

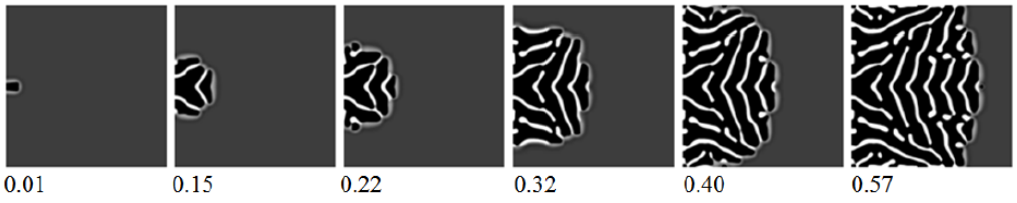


Fig.3. Kinetics of lamellar structure growth from a single ferrite nucleus placed on the grain boundary; T=675K, c_0=0.06; T=675K, c_0=0.06. The numbers under each fragments correspond to the dimensionless simulation time.

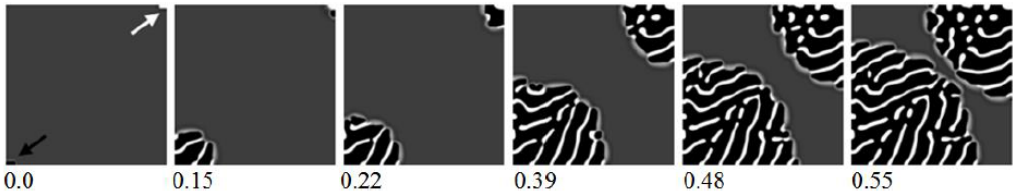


Fig.4. Kinetics of lamellar structure growth from a nucleus placed on the grain boundaries junctions (ferrite nucleus in the bottom left and cementite nucleus in the upper right corner are indicated by arrows); T=675K, c_0=0.06.

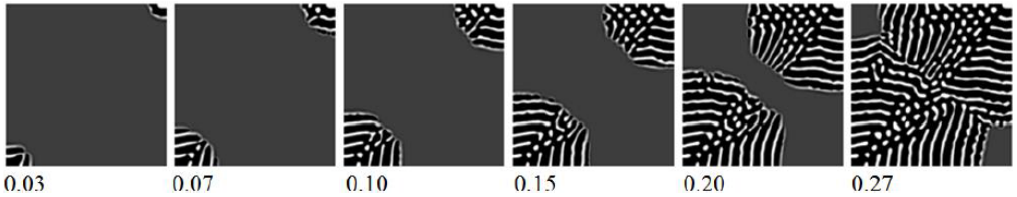


Fig.5. Kinetics of lamellar structure growth at shifting the line T_1 to the left by δc =0.03. The other parameters are the same as in Fig.4.

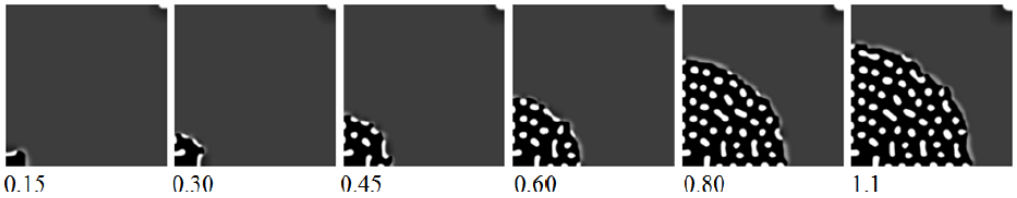
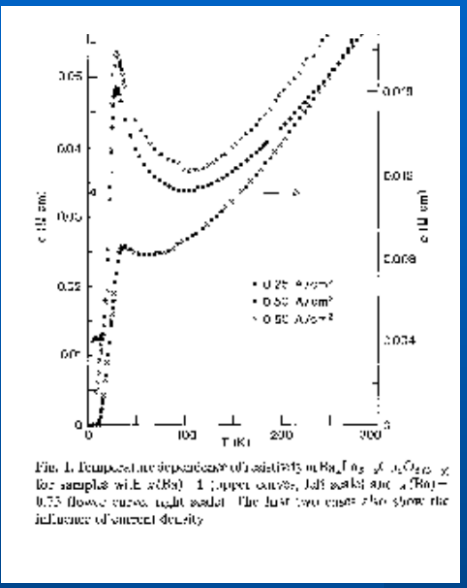


Fig.6. Kinetics of globular structure growth; T=800K, the other parameters are the same as in Fig.4.

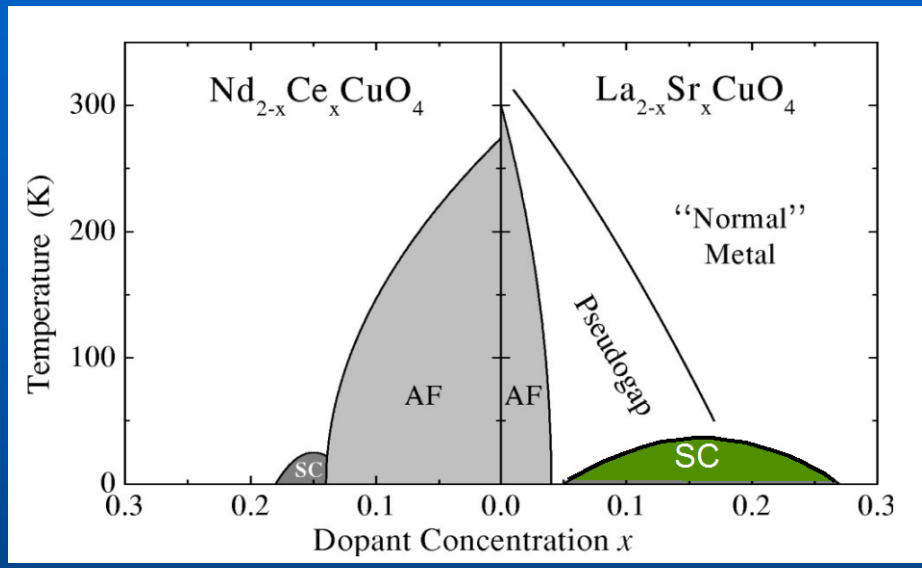
Razumov, Gornostyrev, MIK
Autocatalytic mechanism of perlite growth

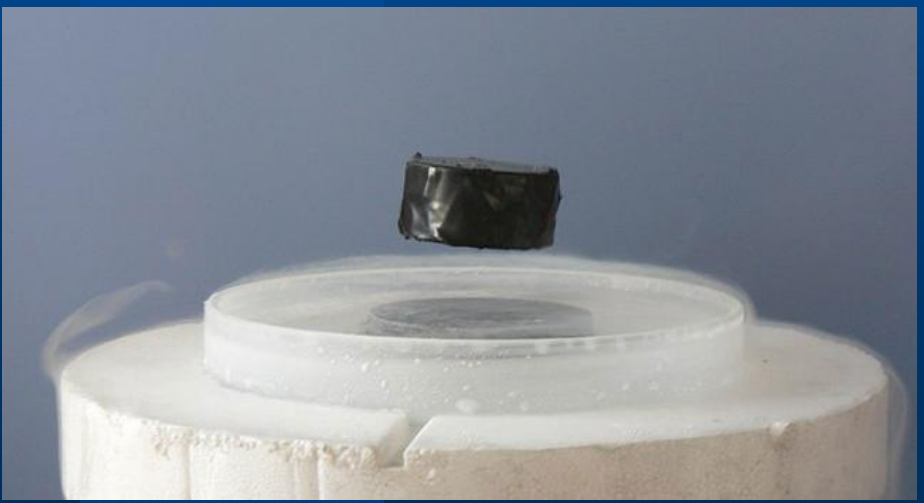
arXiv:1605.07508

30 years of high-temperature superconductivity



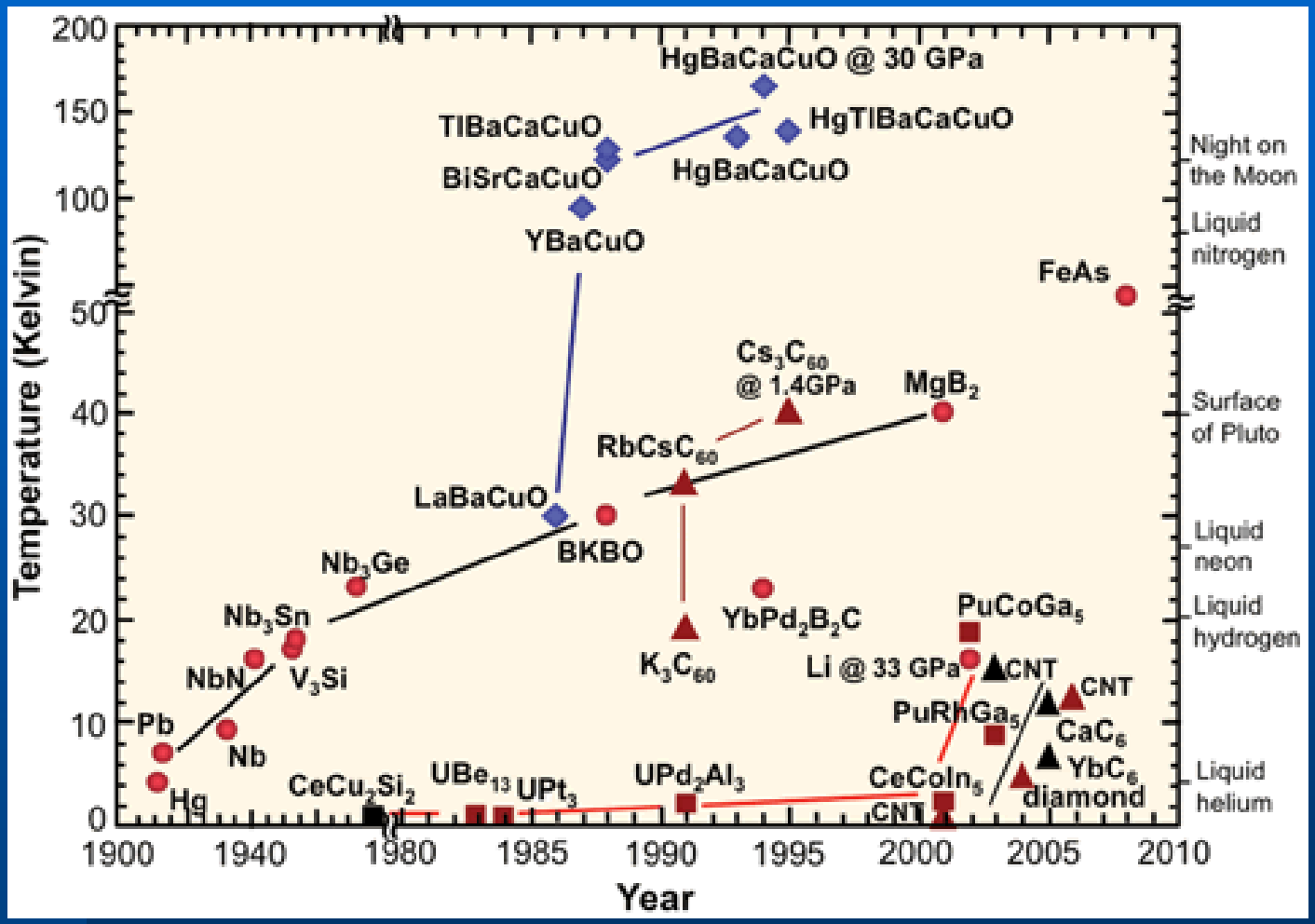
Bednorz and Müller
Zeitschrift für Physik
B 64, 189 (1986)





Magnetic levitation (Meissner effect) at liquid nitrogen temperature

High-Tc superconductivity II

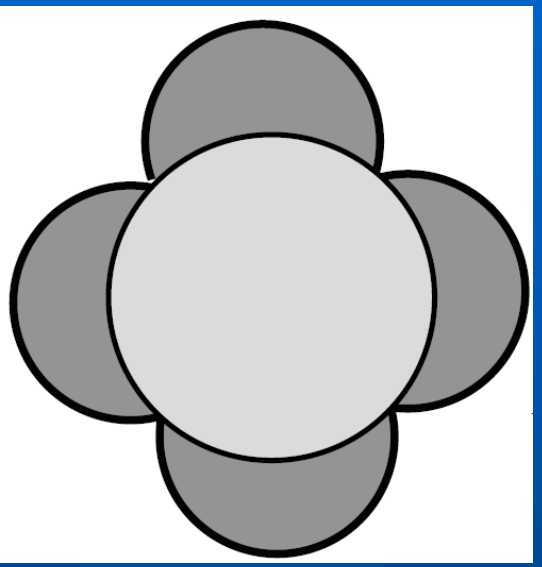


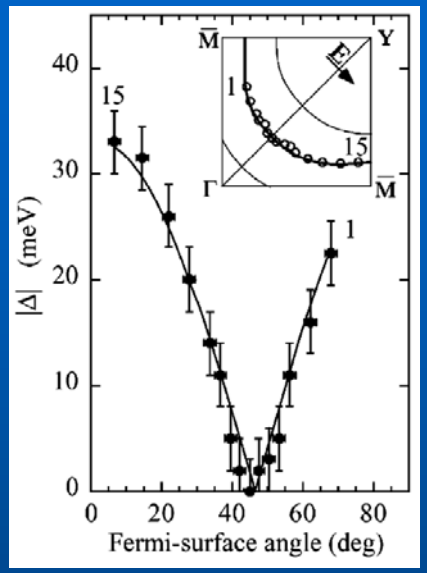
Cu-O compounds seem to be special!

(Very recently – H_3S under pressure, different physics)

High-Tc superconductivity III

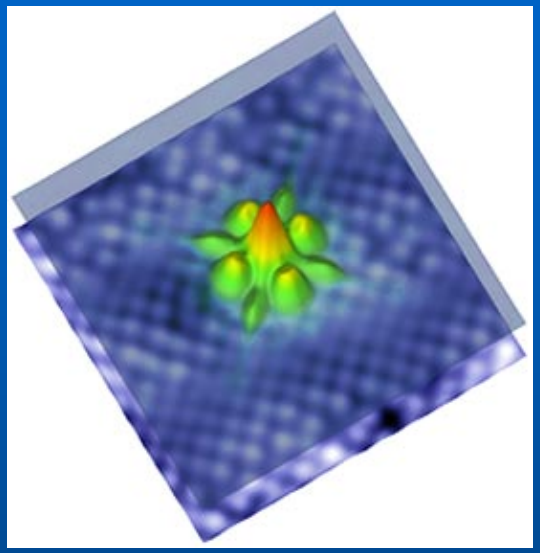
d-wave pairing





Electronic structure in superconducting state (ARPES)

Damascelli *et al.*, Rev. Mod. Phys 75, 2 (2003)



Visualization of the order parameter around Zn impurity by STM

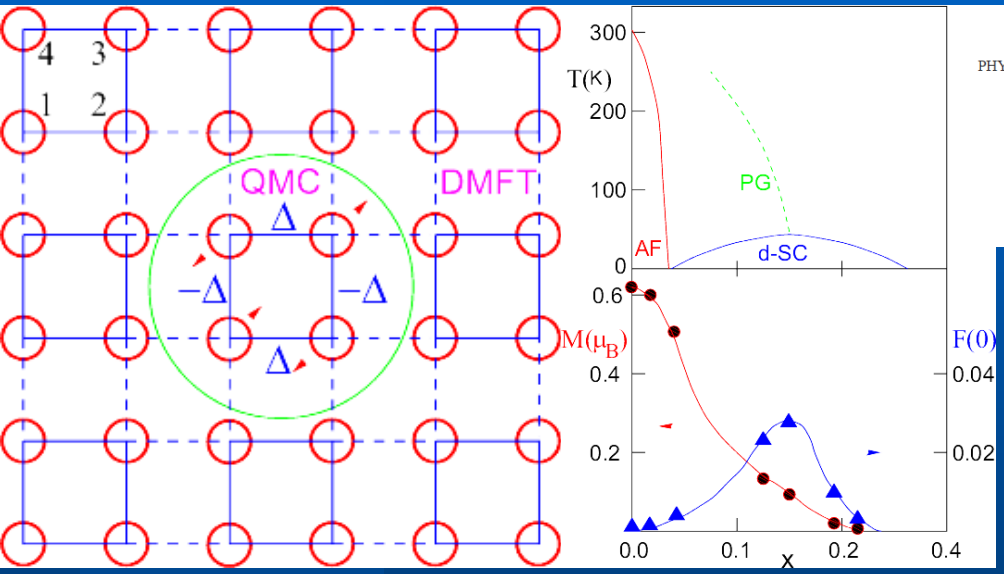
S. Davis group, Nature 2000

Btw, another example of massless Dirac fermions in cond. matter

Also, Josephson junctions etc

High-T_c superconductivity IV

d-wave paring itself is nonlocal effect (cannot be introduced on site)



RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 62, NUMBER 14 1 OCTOBER 2000-II

Antiferromagnetism and *d*-wave superconductivity in cuprates: A cluster dynamical mean-field theory

A. I. Lichtenstein[1] and M. I. Katsnelson[2]
[1]*University of Nijmegen, 6525 ED Nijmegen, The Netherlands*
[2]*Institute of Metal Physics, 620219 Ekaterinburg, Russia*
(Received 22 November 1999)

Cluster DMFT as the first step
Order parametrer on the bond rather than on site

Important role of (antiferro)magnetic fluctuations, interplay of magnetism and superconductivity

Pseudogap formation, node and antinode points at the Fermi surface, shadow Fermi surface etc. etc.

High-Tc superconductivity V

PHYSICAL REVIEW B **94**, 125133 (2016)

Plaquette valence bond theory of high-temperature superconductivity

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(Received 10 April 2016; revised manuscript received 26 July 2016; published 19 September 2016)

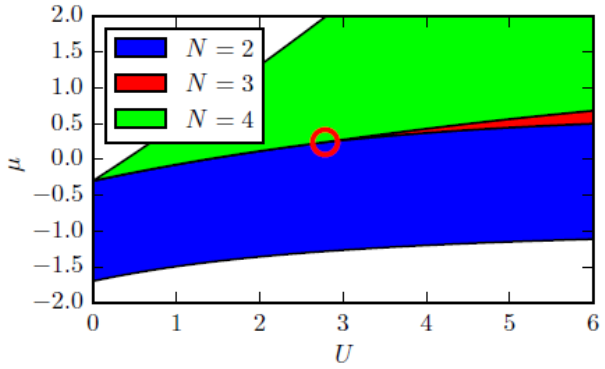


FIG. 1. Zero-temperature phase diagram of the isolated plaquette as a function of the Hubbard U and chemical potential μ in the proximity of the quantum critical point (circle) for $t'/t = -0.3$.

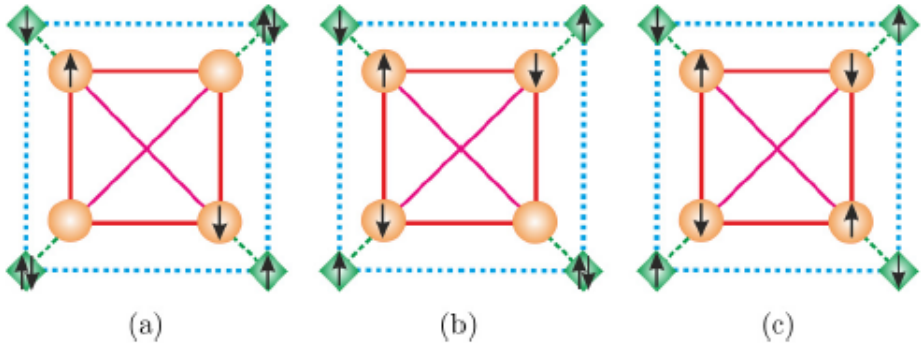


FIG. 3. The main contributions to the plaquette's singlet ground state in a four-site bath with the $d_{x^2-y^2}$-wave order parameter is the hybridization $V = 0.2\Delta_d = 0.05$ for $U = 3$ and $\mu = 0.27$. (a) Sector $N = 2$ with coefficient $=0.05$ and four antisymmetric contributions. (b) Sector $N = 3$ with coefficient $=0.06$ and eight antisymmetric contributions. (c) Sector $N = 4$ with coefficient $=0.08$ and two antisymmetric contributions.

Quantum critical point in plaquette?

"Understanding?!" – The simplest model which catches the essence

High-Tc superconductivity VI

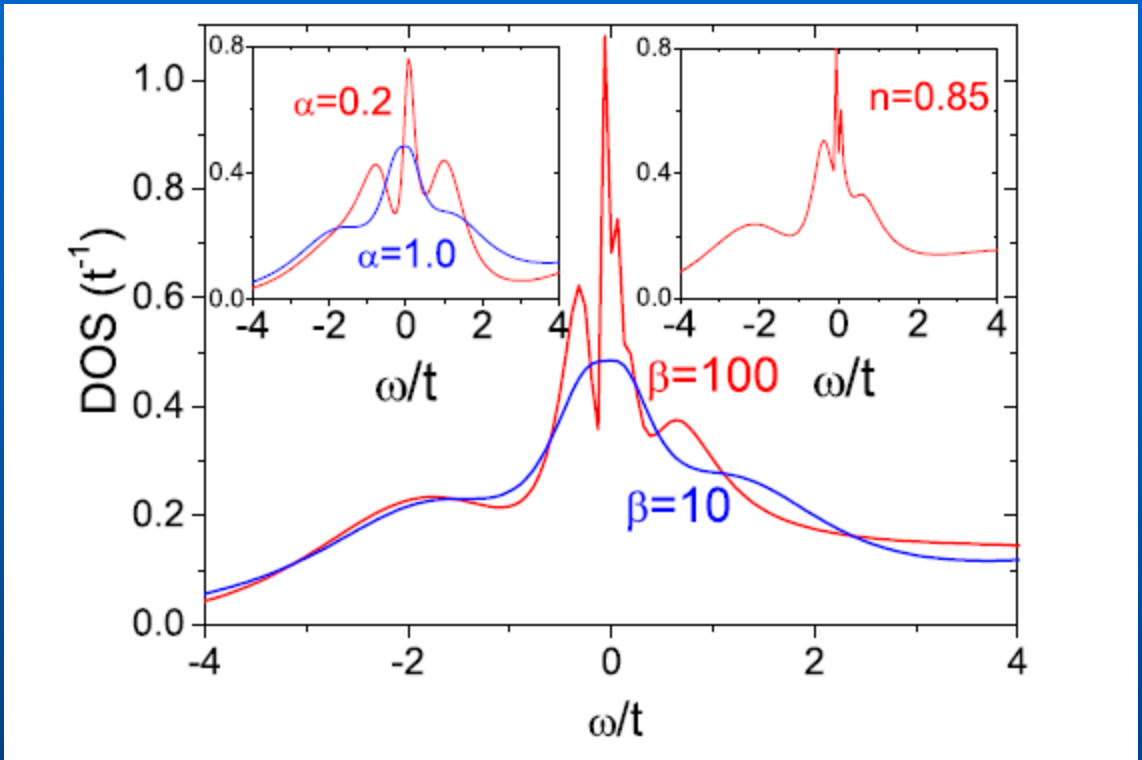


FIG. 5. Density of states for both spins of the plaquette CDMFT for $U = 6$ and $\mu = 0.54$ for different temperatures, (the left inset) with plaquette-lattice hoppings scaled by a factor of α at $\beta = 10$ and (the right inset) for optimal doping $n = 0.85$ at $\beta = 100$.

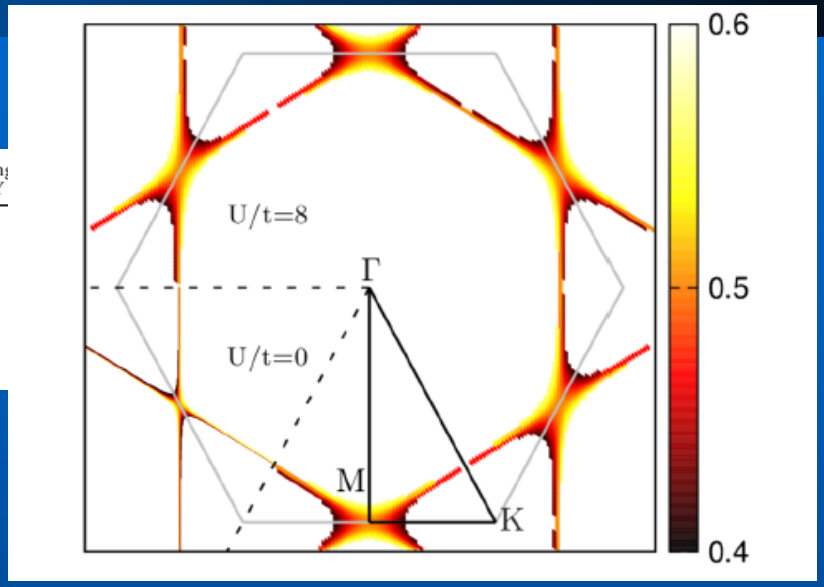
Pseudogap as “Fano anti-resonance”

Relation to ultracold gases

PRL 112, 070403 (2014) PHYSICAL REVIEW LETTERS week ending 21 FEBRUARY

Fermi Condensation Near van Hove Singularities Within the Hubbard Model on the Triangular Lattice

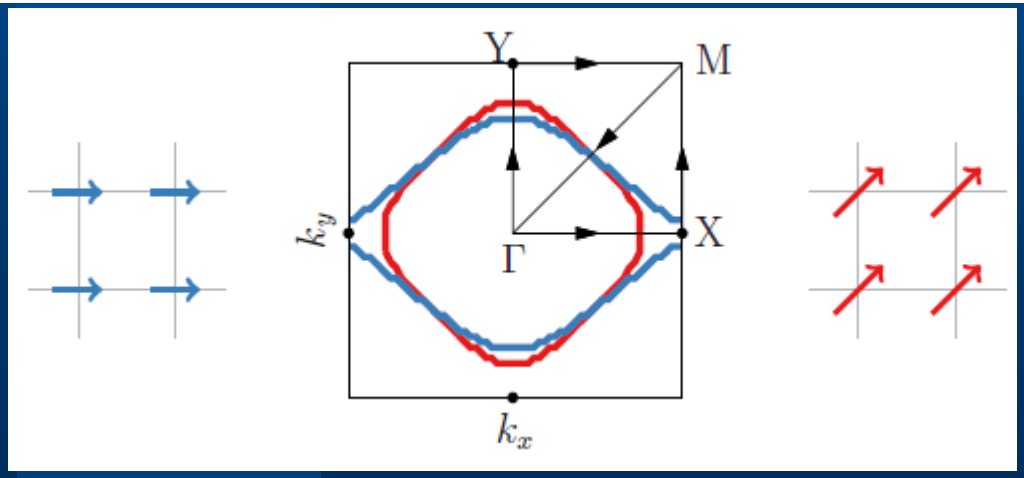
Dmitry Yudin,[1] Daniel Hirschmeier,[2] Hartmut Hafermann,[3] Olle Eriksson,[1]
Alexander I. Lichtenstein,[2] and Mikhail I. Katsnelson[4,5]

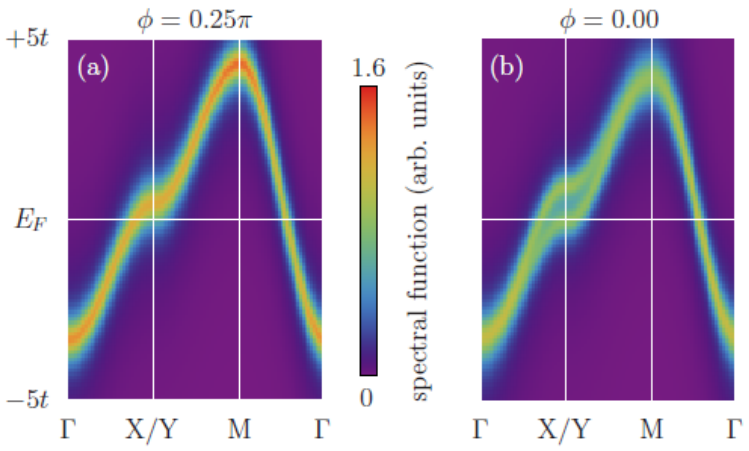


PHYSICAL REVIEW B 93, 195145 (2016)

Interaction-driven Lifshitz transition with dipolar fermions in optical lattices

E. G. C. P. van Loon,[1] M. I. Katsnelson,[1] L. Chomaz,[2,3] and M. Lemeshko[4,*]





What to do next?

Out-of-equilibrium phenomena...

Topological matter...

Quantum theoretical design of new materials...

Materials science not only uses quantum physics, it stimulates its further development