Radboud Universiteit

What is special about being a theoretical physicist

Mikhail Katsnelson

IMM

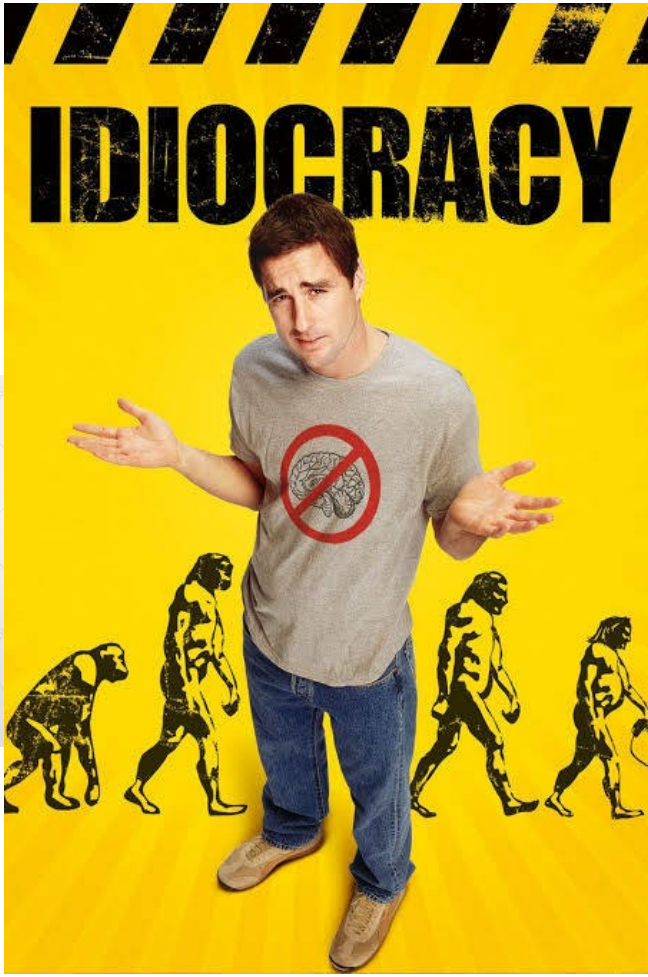
Institute for Molecules and Materials

Outline

- A bit on myself;
- On theoretical physics: a personal view
- Scientist and society: Problems at interface

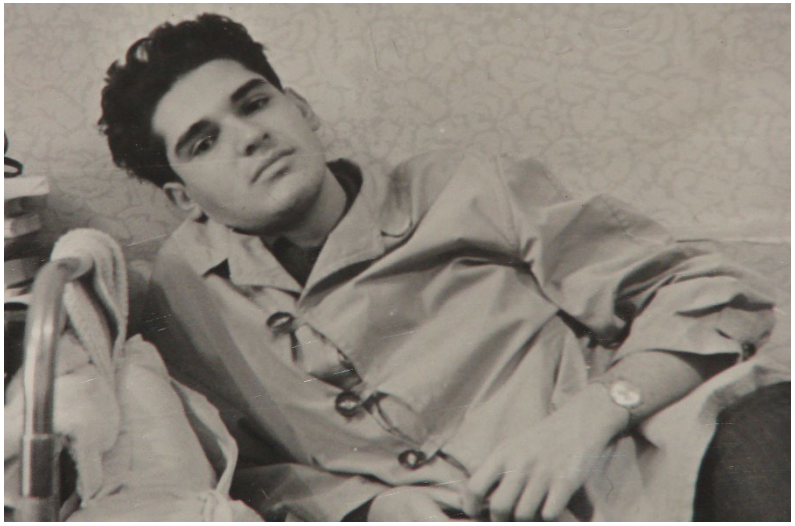
Ivory Tower © SELUXKANAUR on DeviantArt

(https://icons8.ru)



(Movie poster)

How to become a theoretical physicist



How to become a theoretical physicist II






Why I am a physicist?

Magnitogorsk: an industrial city in Ural Mountains (at a formal border of Europe and Asia)

My school teacher:
Ivan Kabanchuk (1920-1999)

11 hours of physics per week and all that

Why I am a theoretical physicist?

Ural State University, Dept. Physics
1972-1977

Boris Ishmukhametov (1929-2020)

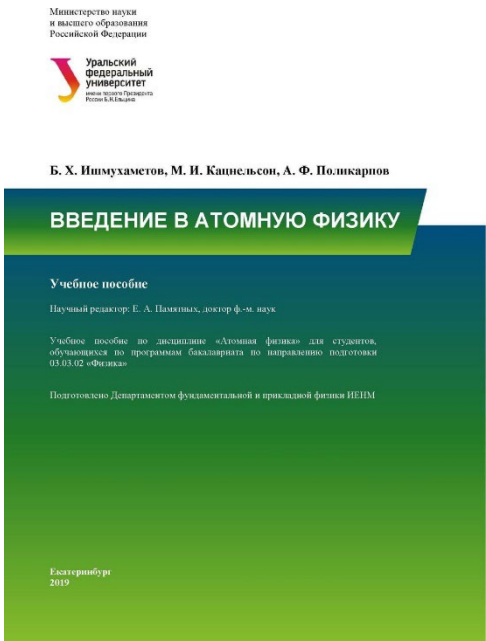
My first subject: Atomic plasmon
My first paper (with him): published 1975

Volume 82A, number 8 PHYSICS LETTERS 20 April 1981

ON THE EXISTENCE OF THE ATOMIC PLASMON

B. Kh. ISHMUKHAMETOV, M.I. KATSNELSON [a], V.N. LARIONOV and A.M. USTJUZHANIN [b]
Ural State University, Sverdlovsk, USSR
[a] *Institute for Metal Physics, Ural Scientific Centre, Sverdlovsk, USSR*
[b] *Institute for Mathematics and Mechanics, Ural Scientific Centre, Sverdlovsk, USSR*

Received 22 January 1981



Almost half a century later

Semiclassical theory for plasmons in spatially inhomogeneous media

Annals of Physics 446 (2022) 169116

K.J.A. Reijnders *, T. Tudorovskiy, M.I. Katsnelson

[41] B.Kh. Ishmukhametov, Phys. Status Solidi (B) 45 (1971) 669–678.
[42] B.Kh. Ishmukhametov, M.I. Katsnelson, Fiz. Met. Metalloved. 40 (1975) 736.

Appendix D. Review of a prior derivation

The derivations presented in Section 2 of this article arose after studying Refs. [41,42]. The formula $L_0(x, q) = 0$ was first presented in Ref. [41], in a slightly different notation. A justification of this formula was given in Ref. [42]. Unfortunately, the latter article is not available digitally and very hard to come by. In order to sketch the context of the present work and to show its inspiration, we repeat the arguments presented in Ref. [42] in this appendix. We emphasize that they are not completely rigorous, but may give the reader a more intuitive idea of the formal transformations presented in the main text.

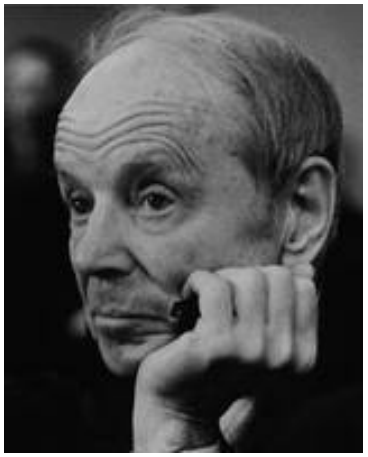
This appendix consists of two parts. In the first part, we briefly repeat the formulation of the RPA in real space, as presented in the textbook [5]. More precisely, we follow the three steps outlined in Section 2.1 to obtain an integro-differential equation for the induced potential $V(x, t)$.

Acknowledgments

We are grateful to Tjacco Koskamp, Malte Rösner, Sergey Dobrokhotov, Vladimir Nazaikinskii, Erik van Loon and Tim de Laat for helpful discussions. One of us (M.I.K.) started to work in this field long ago under the supervision of Boris Ishmukhametov (1929–2020). We dedicate this paper to his memory. The work of K.J.A.R. and M.I.K. was supported by the ERC Synergy Grant, Project No. 854843 FASTCORR.

Theoretical physics is Sverdlovsk

Semyon Shubin (1908-1938)
The founder of theoretical physics in Ural



Arrested 1929, professor and head of department 1933, arrested again 1937, killed 1938. Published 18 papers

Sergey Vonsovsky, 1910-1998
Pupil of Shubin and my main teacher

"Polar model" ("Mott insulators"), liquid metals, photoeffect, s-d exchange (Vonsovsky-Zener) model...

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

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

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

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

Fig. 1.

Fig. 2.

$$\begin{aligned}\{\varepsilon - s(\mathrm{A}+\mathrm{D}) - [\sum_{f<f'}(\mathrm{B}_{ff'}-\mathrm{J}_{ff'}) + \sum_{g<g'}(\mathrm{B}_{gg'}-\mathrm{J}_{gg'}) - \sum_{f,g}(\mathrm{B}_{fg}+\mathrm{J}_{fg})]\}\,\mathrm{C}(fgh)\\ + \sum_{h,k}\mathrm{J}_{hk}[\mathrm{C}(\mathrm{T}_{hk}|fgh) - \mathrm{C}(fgh)] + \sum_{f,g}\mathrm{J}_{fg}[\mathrm{C}(\mathrm{T}_{fg}|fgh) - \mathrm{C}(fgh)]\\ + \sum_{f,p}\mathrm{L}_{fp}\,\mathrm{C}(\mathrm{T}_{fp}|fgh) - \sum_{g,p}\mathrm{L}_{gp}\,\mathrm{C}(\mathrm{T}_{gp}|fgh) = 0, \qquad (9)\end{aligned}$$

Polar model II

Mott insulators and Mott transitions in 1934

(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.

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

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

Some types of instabilities in the electron energy spectrum of the polar model of the crystal: I. The maximum-polarity state

S V Vonsovsky and M I Katsnelson
Institute of Metal Physics, Ural Science Research Centre of the USSR Academy of Sciences, Sverdlovsk, USSR

Received 29 June 1978, in final form 9 October 1978

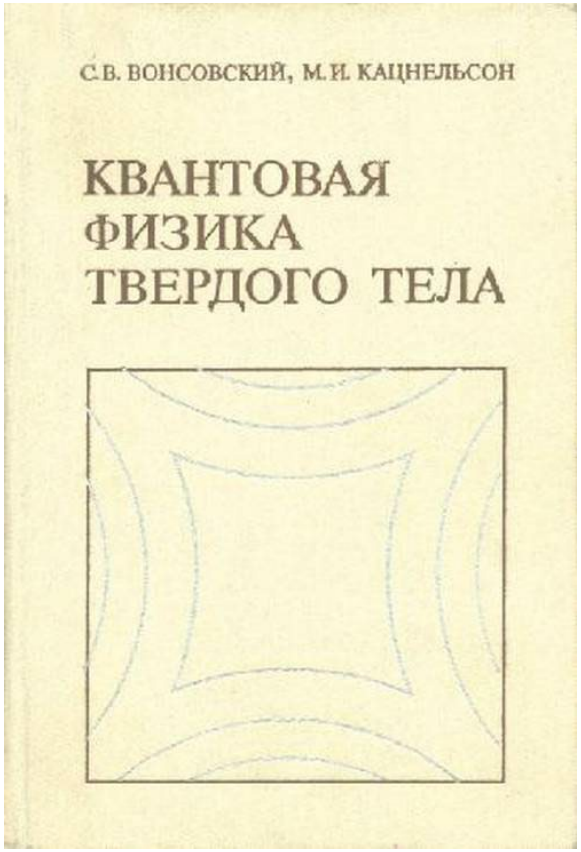
Some types of instabilities in the electron energy spectrum of the polar model of the crystal: II. The criterion of stability of a metallic state

S V Vonsovsky and M I Katsnelson
Institute of Metal Physics, Ural Science Research Centre of the USSR Academy of Sciences, Sverdlovsk, USSR

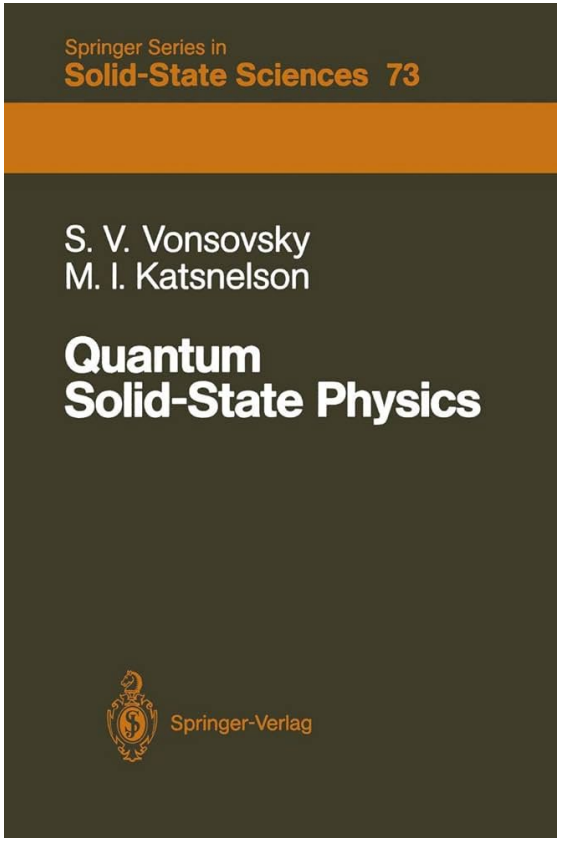
Received 29 June 1978, in final form 9 October 1978

J. Phys. C: Solid State Phys., Vol. 12, 1979. Printed in Great Britain.

Early writing of a book



Published in Russian
1983
Published in English
(extended and rewritten)
1989



In contemporary situation a young researcher cannot spend time on helping their supervisor to write books or reviews. Many letters in fancy journals is much better for the career

Also, replacing Vonsovsky at his lectures when he was away (from 1979)

A philosophical statement

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

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

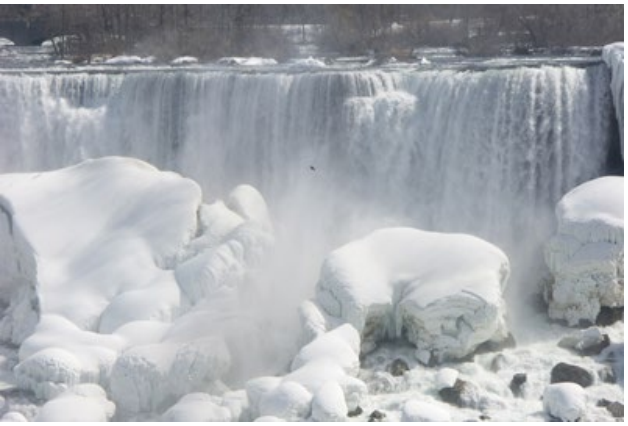
That is all. Please tell me why iridium is brittle and platinum is ductile, copper is red and silver is white, iron is ferromagnetic and vanadium is not... Not talking on biochemistry and biophysics!

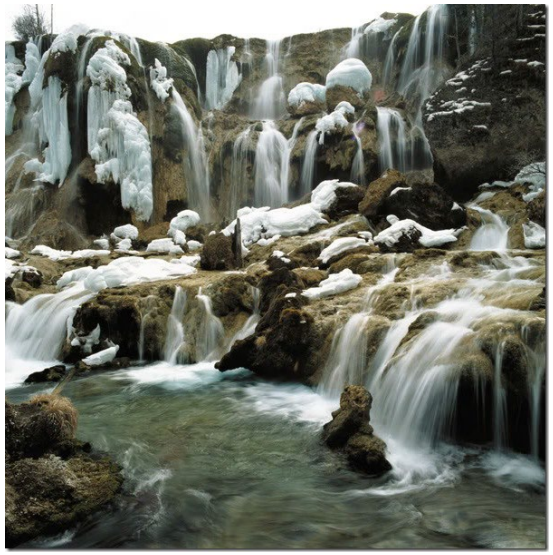
Does it help?

$$\nabla \cdot u = 0$$

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

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





Is fundamental physics fundamental?

Classical thermodynamics is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts (A. Einstein).

The laws describing our level of reality are essentially independent on the background laws. I wish our colleagues from true theory (strings, quantum gravity, etc....) all kind of success but either they will modify electrodynamics and quantum mechanics at atomic scale (and then they will be wrong) or they will not (and then I do not care). Our way is down.

How to pass from known basic laws of nature to understanding all richness and diversity of the world around us?

Pure chemical elements are already complicated enough to think very seriously

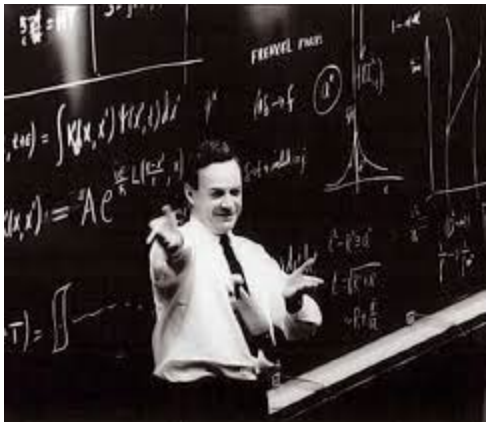
The aim of science: Understanding

Duality of understanding and knowledge

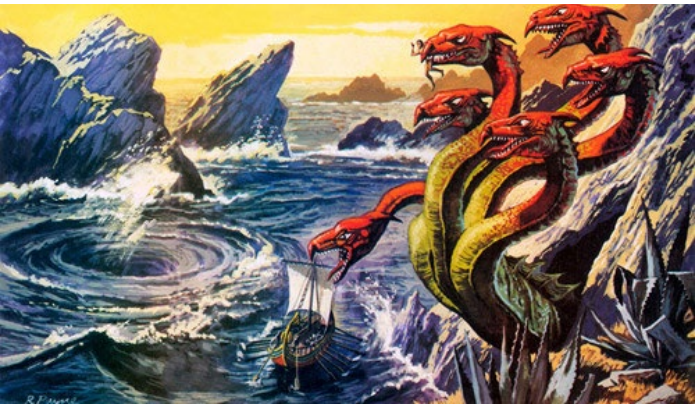
Newton laws... Rotation...
Air resistance... I know this stuff
but the result will be... well...

He does not know (?!) Newton Mechanics – but it works! He feels (=understands) what to do

I think I can safely say that nobody understands quantum mechanics
(R. P. Feynman)



Scylla and Charybdis

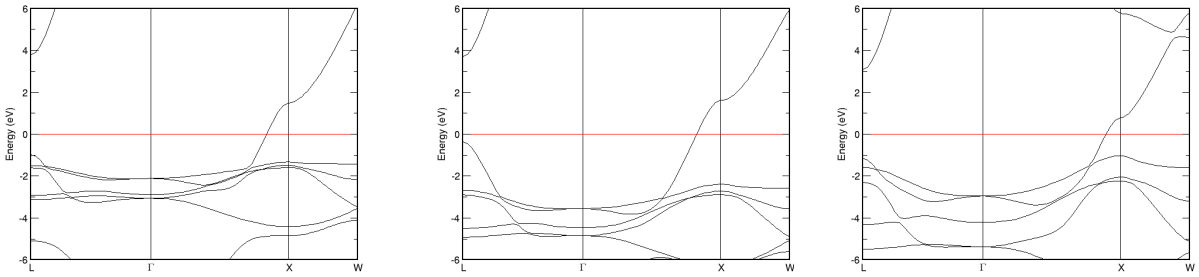


Understanding “in general”

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

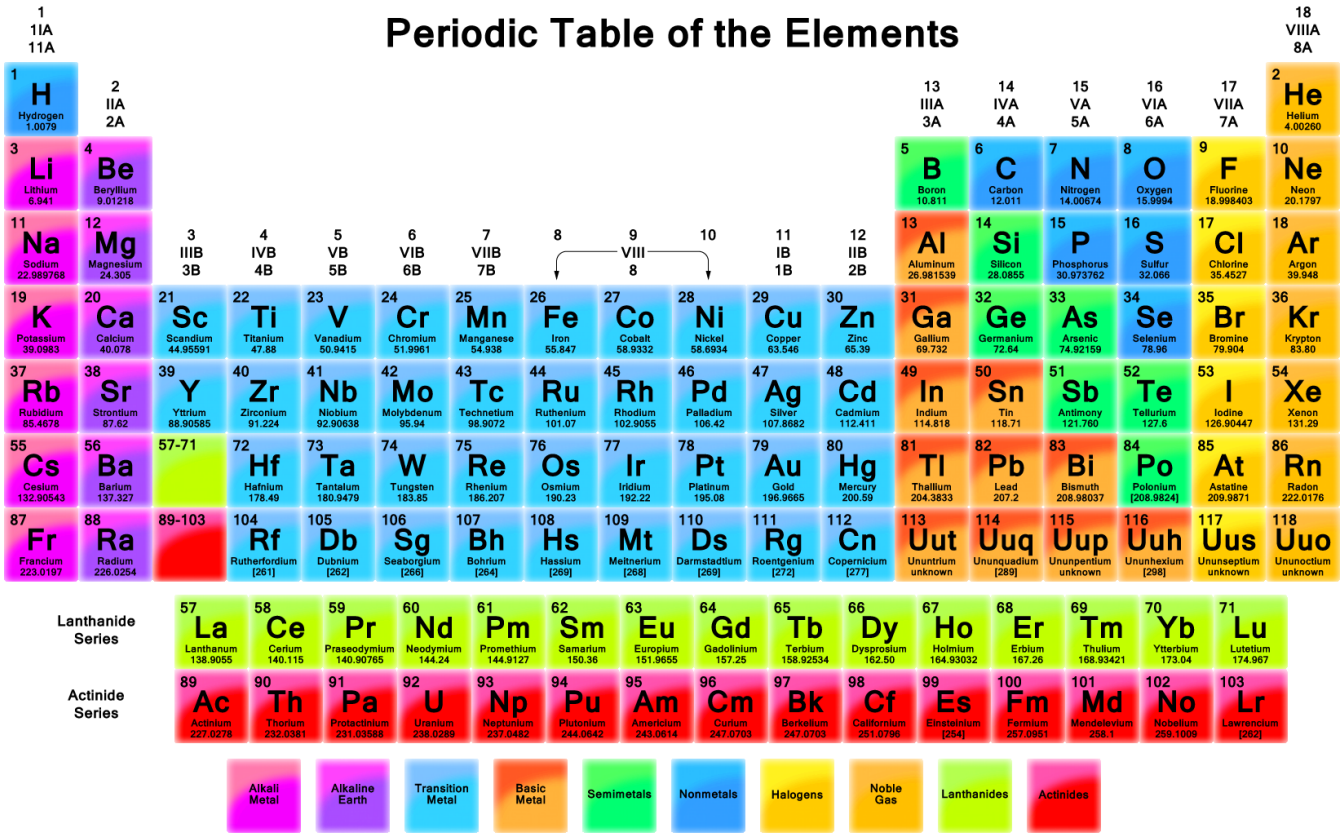
Reviews of Modern Physics, Vol. 50, No. 2, April 1978

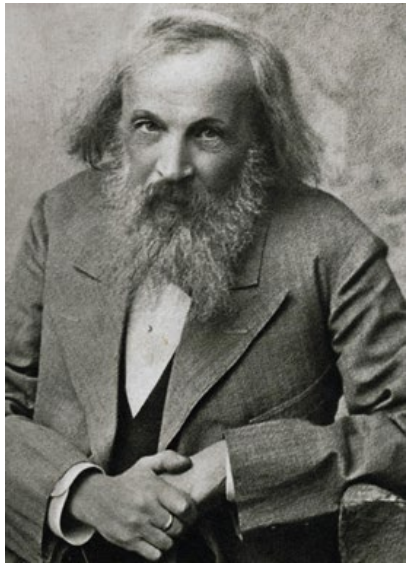
(Nobel lecture)

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?

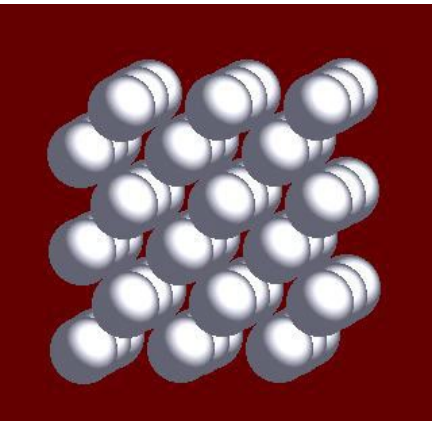




D. I. Mendeleev

An example: Alkali metals

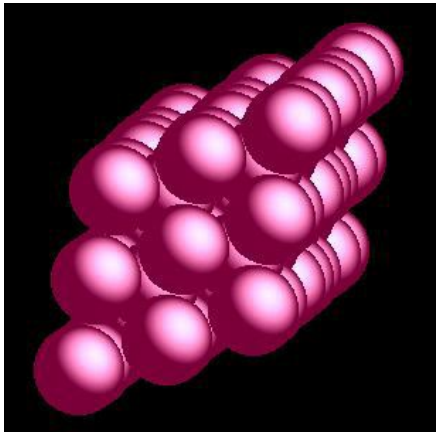
Ambient conditions: all body-centered cubic



Li, Na at low temperatures: 9R

Why? Well... Total energies are very, very close (difference $\approx 10^{-4}$)

Just numbers... Calculate!



J. Phys.: Condens. Matter **1** (1989) 5319–5335. Printed in the UK

An experimental and theoretical study of martensitic phase transitions in Li and Na under pressure

V G Vaks†, M I Katsnelson‡, V G Koreshkov‡, A I Likhtenstein§, O E Parfenov†, V F Skok‖, V A Sukhoparov‖, A V Trefilov† and A A Chernyshov†

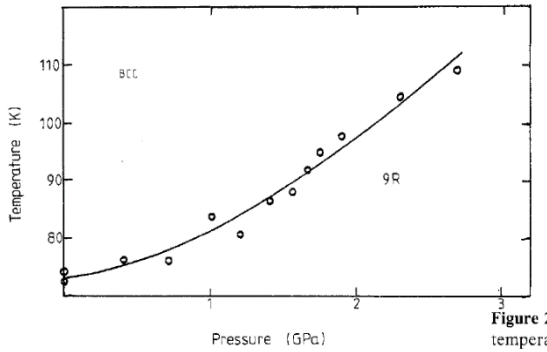


Figure 2. The martensitic transformation temperature M_s versus pressure in Li.

Why opposite behavior with pressure?

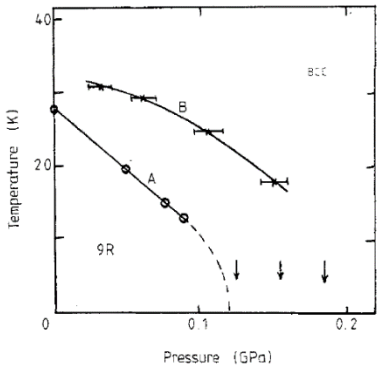
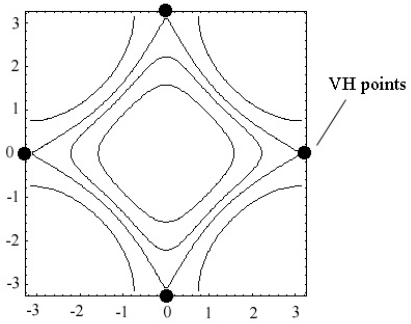
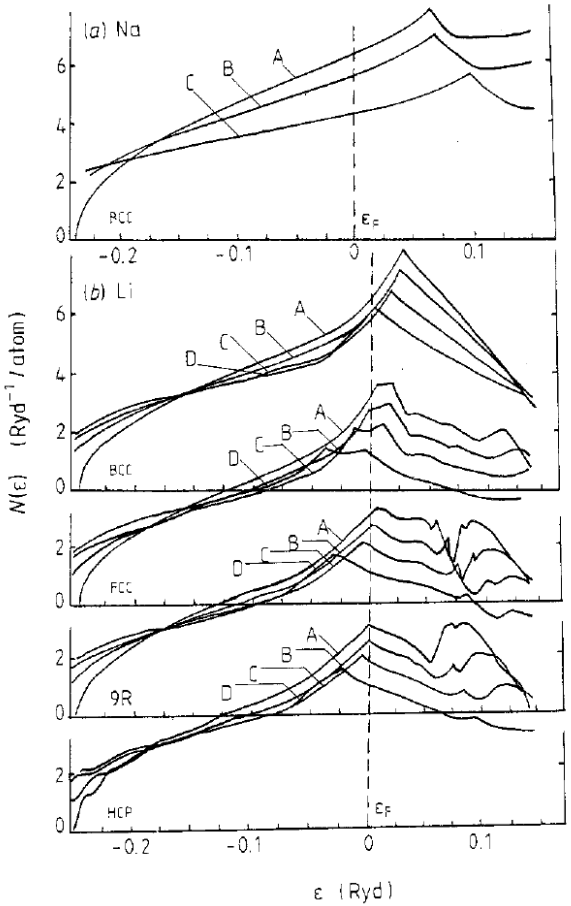


Figure 3. The martensitic transformation temperature M_s versus pressure in Na: A, the beginning of transformation, M_s, in cooling p = const; B, the beginning of transformation for decreasing pressure, T = const.

Understanding?!

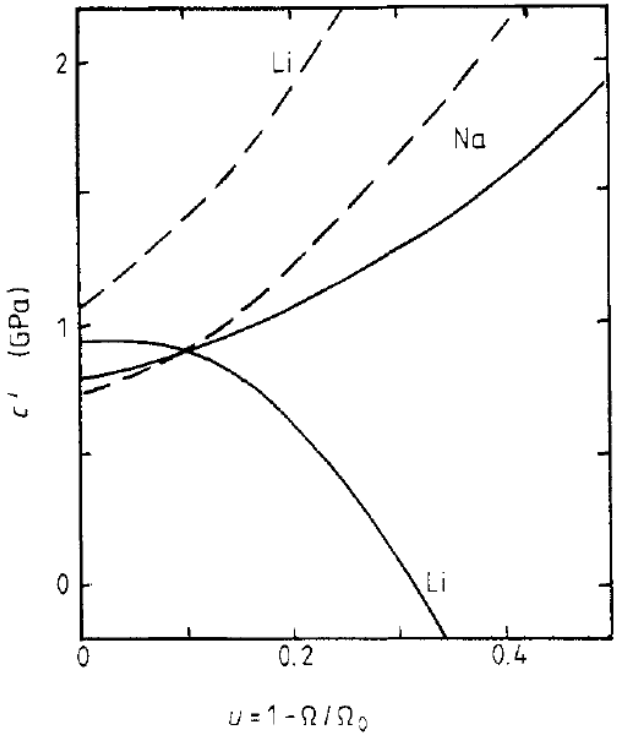


Van Hove singularities: topological property of any energy spectrum in crystals



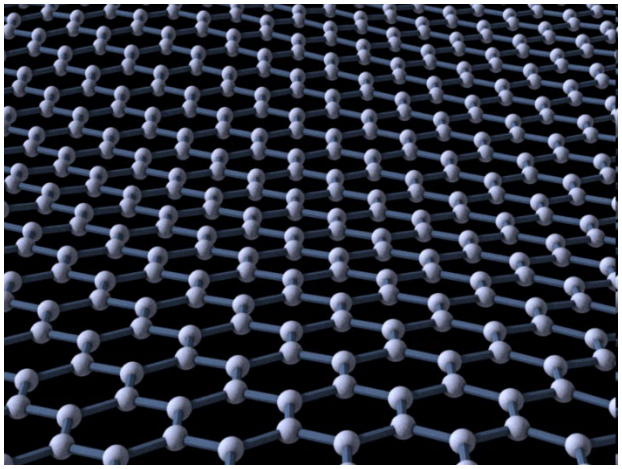
bcc Na: away from E_F
bcc Li: towards E_F

Different role of *p*-electrons

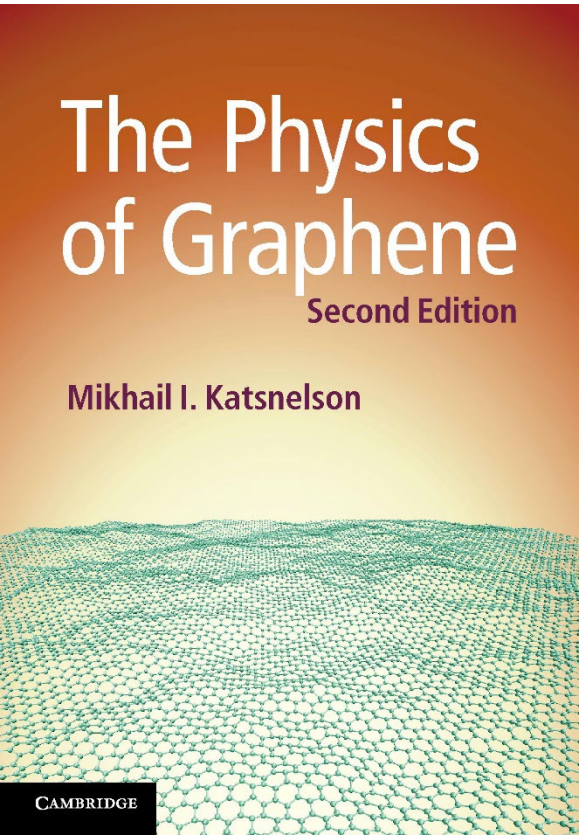


VHS near E_F destabilize crystal structure (a general theory)

Graphene!!! – Just elemental solid



Even insects understand what honeycomb lattice is



I am very grateful to Andre Geim and Kostya Novoselov, who involved me in this wonderful field before it became fashionable (otherwise I would probably never have dared to join such a brilliant company). I am especially grateful to Andre for regular and lengthy telephone conversations; when you have to discuss a theory using just words, without formulas and diagrams, and cannot even make faces, after several years it does improve your understanding of theoretical physics.

The end of my time line was only a start for further hard work involving many collaborators. Our rapid progress would be impossible without Misha Katsnelson who provided us with all the theoretical help an experimentalist can only dream of.

REVIEWS OF MODERN PHYSICS, VOLUME 83

Nobel Lecture: Random walk to graphene*

Andre K. Geim

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 of my type

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

Theoretical physics as a variety of mistique experience II

A miracle for yourself vs miracle for others

I have seen (and experienced) "miracle for myself" 3 or 4 times in my almost 50-year scientific career.

Resonance phenomena in a phonon subsystem in connection with anomalies of the structural state of metals

M. I. Katsnel'son and A. V. Trefilov
I. V. Kurchatov Institute of Atomic Energy, Moscow; Institute of Metal Physics, Ural Science Center, Academy of Sciences of the USSR

(Submitted 2 April 1987)
Pis'ma Zh. Eksp. Teor. Fiz. **45**, No. 10, 496–498 (25 May 1987)

PHYSICAL REVIEW B VOLUME 61, NUMBER 13 1 APRIL 2000-I

First-principles calculations of magnetic interactions in correlated systems

M. I. Katsnelson
Institute of Metal Physics, 620 219 Ekaterinburg, Russia

A. I. Lichtenstein

Real-space imaging of an orbital Kondo resonance on the Cr(001) surface

O. Yu. Kolesnychenko, R. de Kort, M. I. Katsnelson, A. I. Lichtenstein & H. van Kempen

NATURE | VOL 415 | 31 JANUARY 2002

Zitterbewegung, chirality, and minimal conductivity in graphene

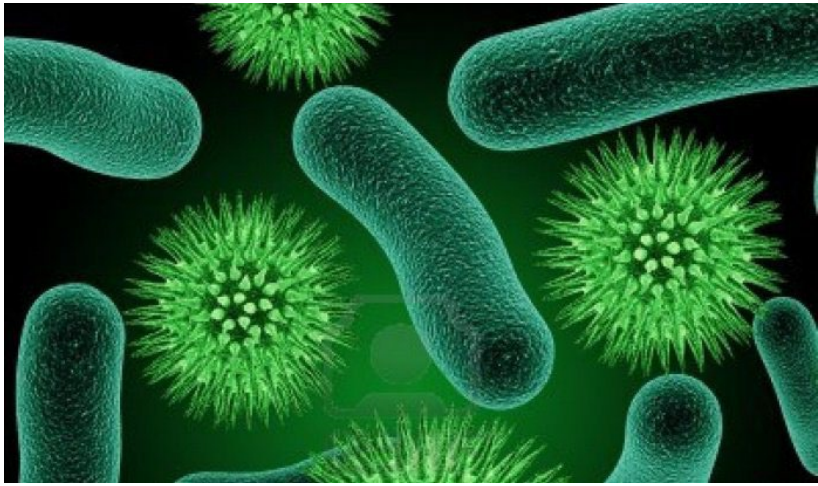
M.I. Katsnelson[a]

Eur. Phys. J. B **51**, 157–160 (2006)
DOI: 10.1140/epjb/e2006-00203-1

Science is necessary for survival of humankind

Agriculture ("green revolution")
Medicine (new antibiotics: arms race with bacteria)

We cannot just stop: too many will die



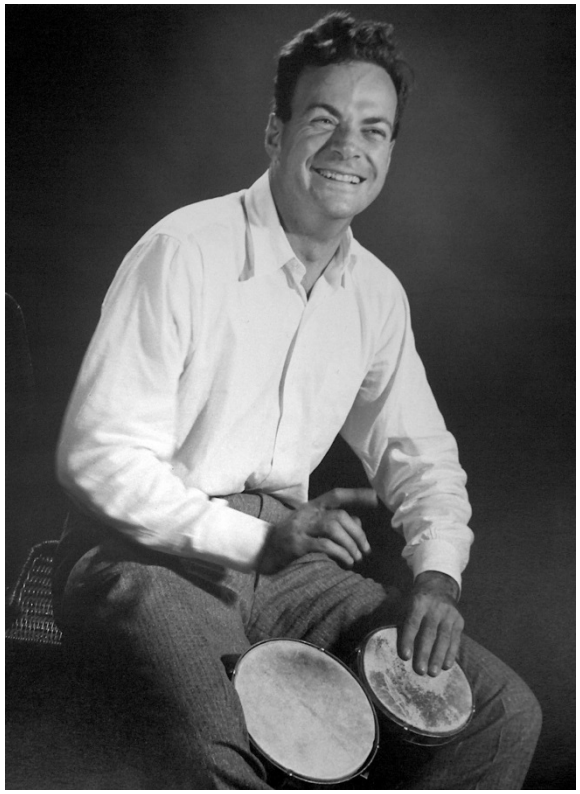
Our society is crucially dependent on communications, transport, computers... well... weapons...

Very important to know how science works

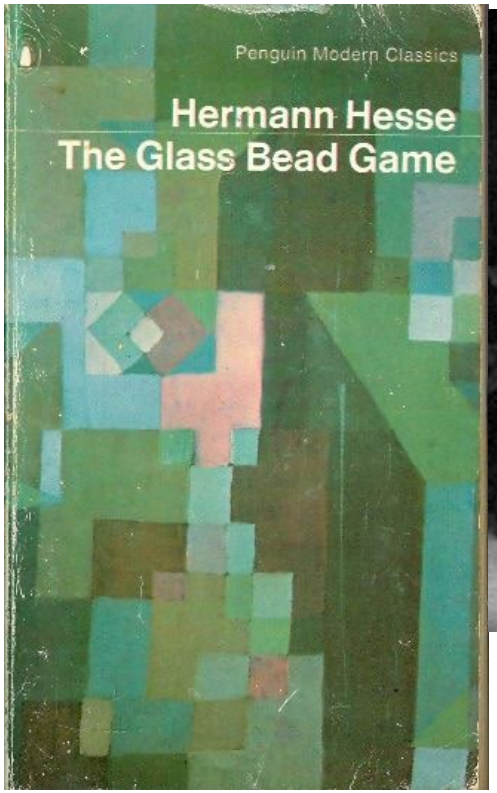
Curiosity-driven research

Physics is like sex: sure, it may give some practical results, but that's not why we do it

R. P. Feynman



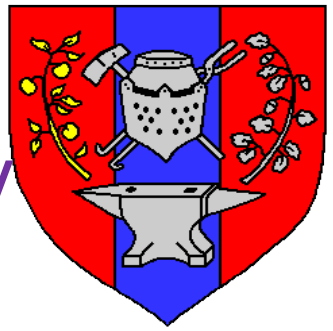
Motivations are very different...



Model of science

What to do?

1. Trust us, we are smart guys and we know what to do – medieval guilds principle



It will not work in modern society

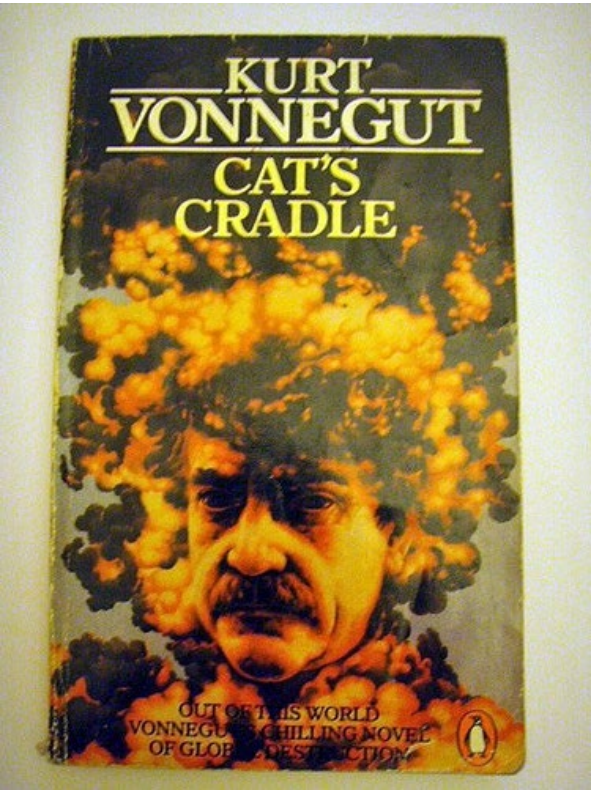
2. Convince people that we are useful

Well... We are useful but in a complicated way

Strong temptations: lie and intimidate
Polite version: tell on success only, overestimate practical importance, promise something too early...

Misuse of science

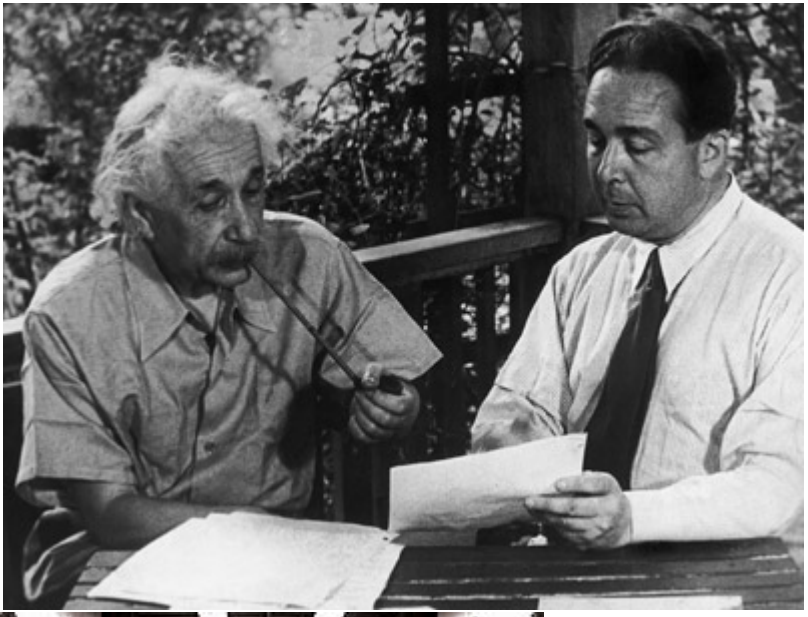
Everything a scientist did was destined to become a weapon (K. Vonnegut, Cat's Cradle)



Was/is arms race useful for science? Well...

Science as mass occupation

Starts with A-bomb making



Completely changes relations between scientists and society

How to be rational in irrational world?

A very simple answer: *I do not know*