MAGNETISM IN MATERIALS

Lecture 7: Itinerant Magnetism

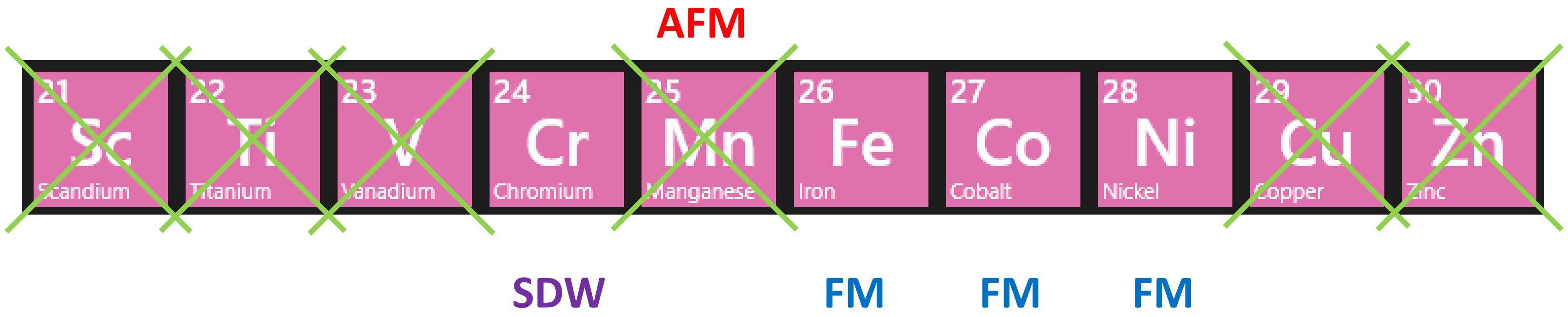
Ivica Zivkovic

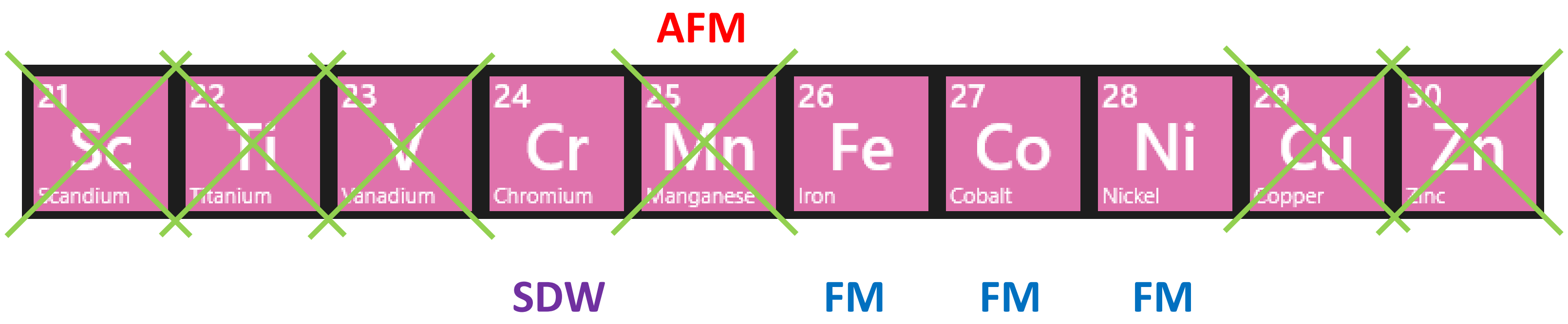
01.04.2025

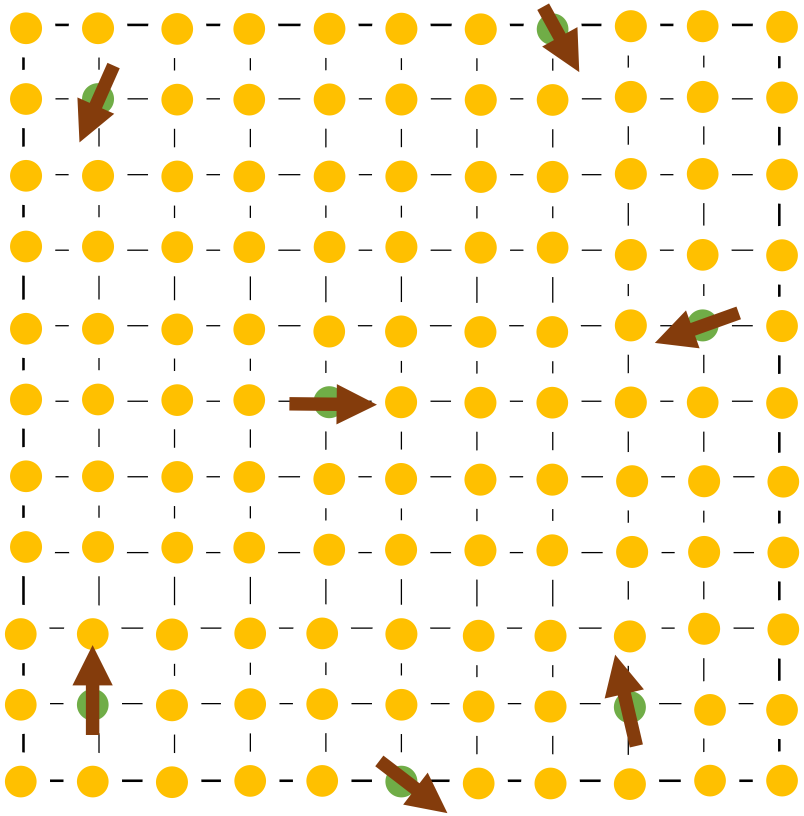
EPFL

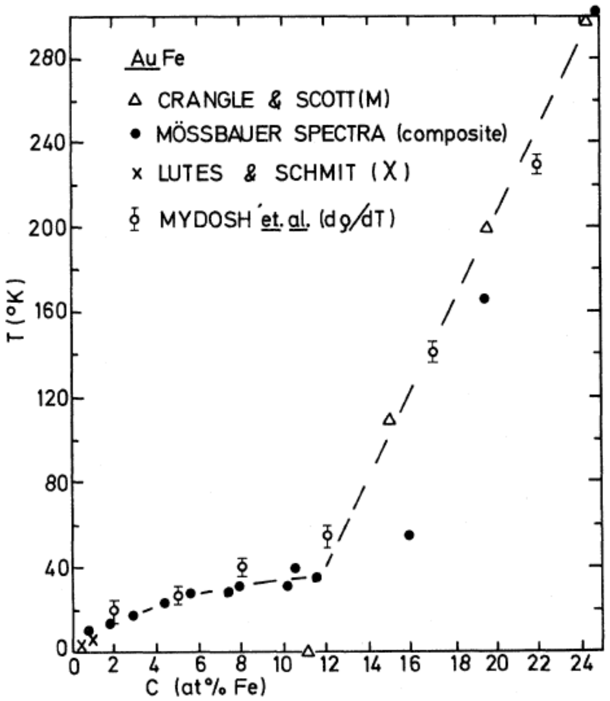
ITINERANT MAGNETISM

- elemental magnets
- free electron model
- Pauli paramagnetism
- spontaneous band polarization
- Landau levels

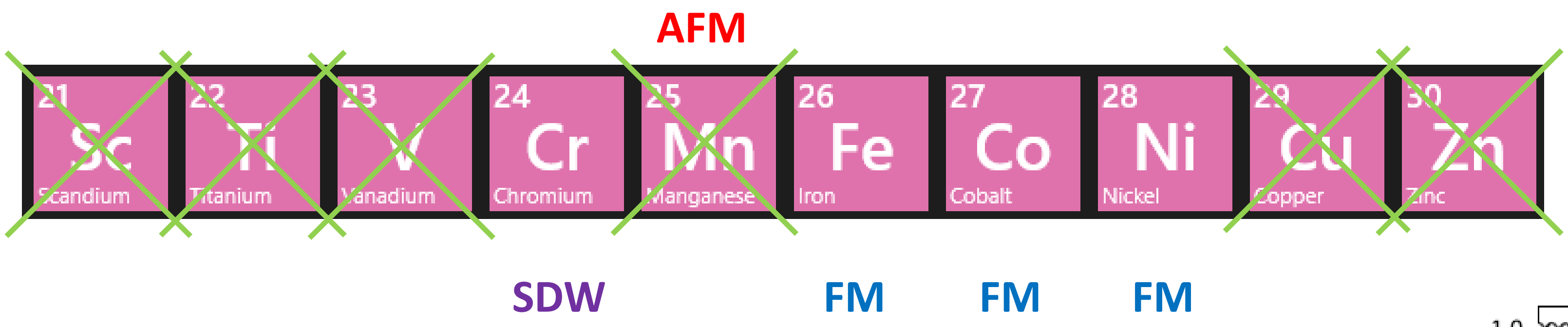

AFM
21 Sc Scandium
22 Ti Titanium
23 V Vanadium
24 Cr Chromium
25 Mn Manganese
26 Fe Iron
27 Co Cobalt
28 Ni Nickel
29 Cu Copper
30 Zn Zinc
SDW
FM
FM
FM



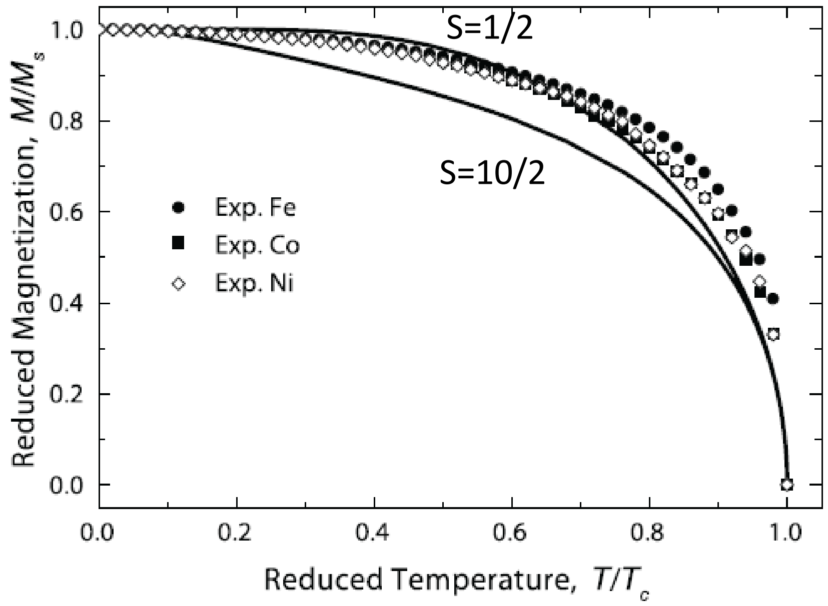




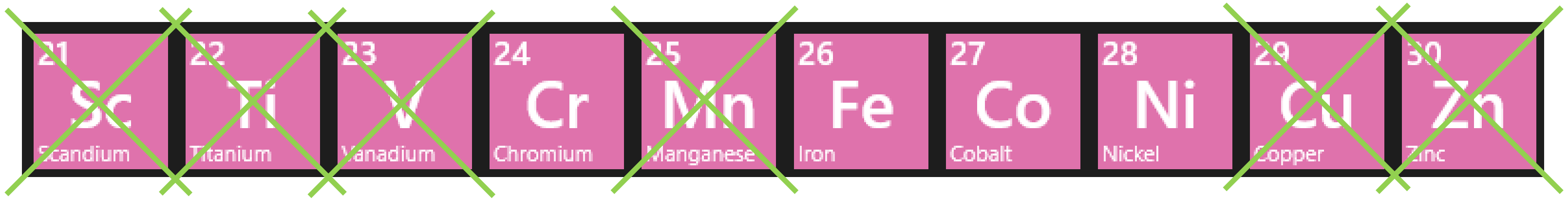
d^5	d^6	d^7	d^8
Mn^{2+}/Fe^{3+}	Fe^{2+}/Co^{3+}	Co^{2+}	Ni^{2+}
S = 5/2	S = 2	S = 3/2	S = 1
S = 1/2	S = 0	S = 1/2	



saturation magnetization (μ_B/atom)	2.216	1.715	0.616
Curie temperature (K)	1044	1388	627
magnetic moments from Curie-Weiss (μ_B/atom)	2.29	2.29	0.9
ratio CW/saturation	1.03	1.34	1.46



AFM



SDW FM FM FM

	Fe	Co	Ni
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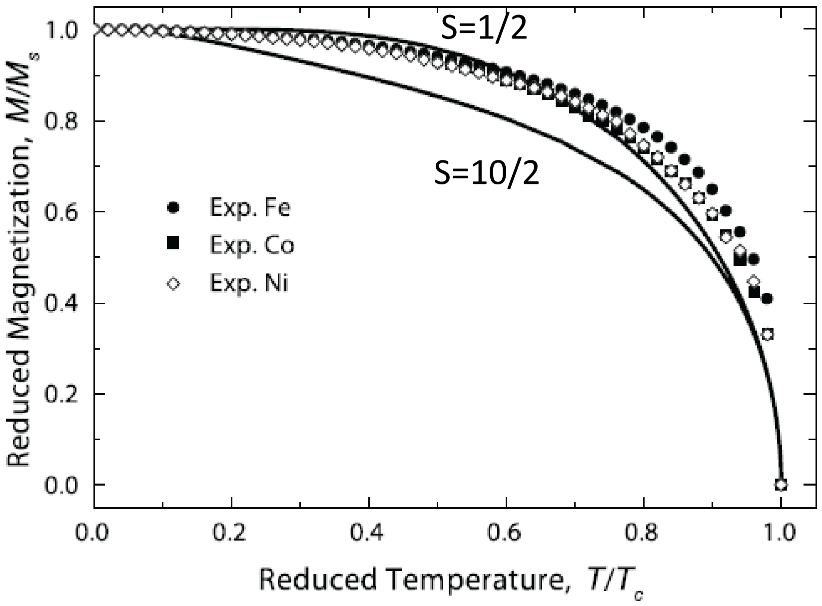
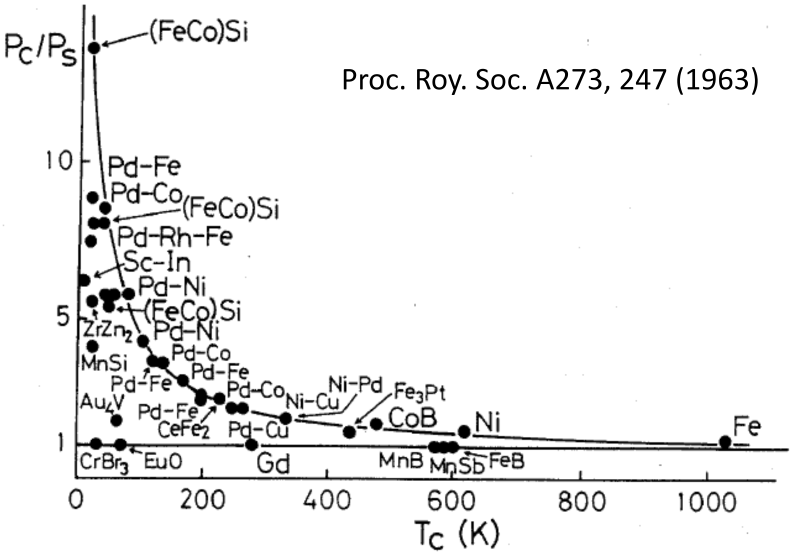
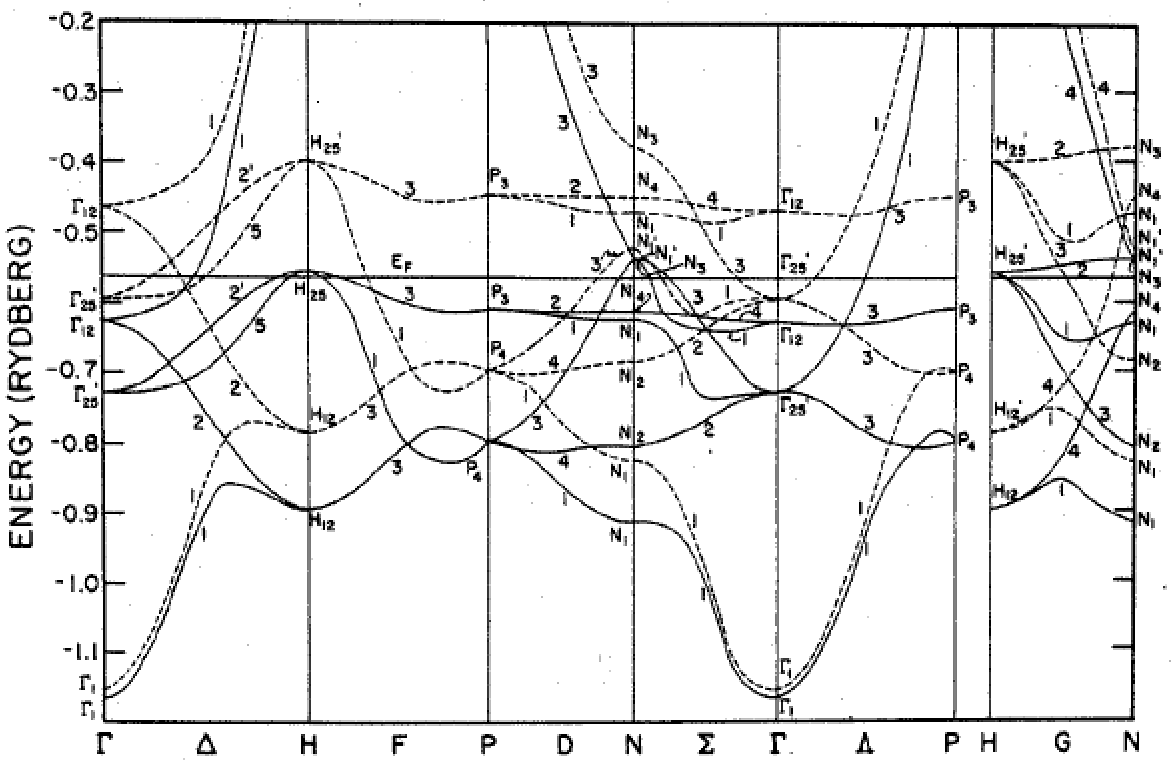
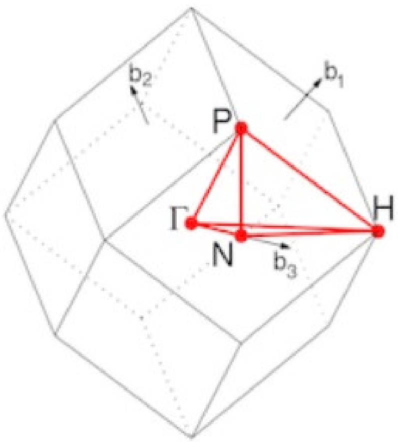




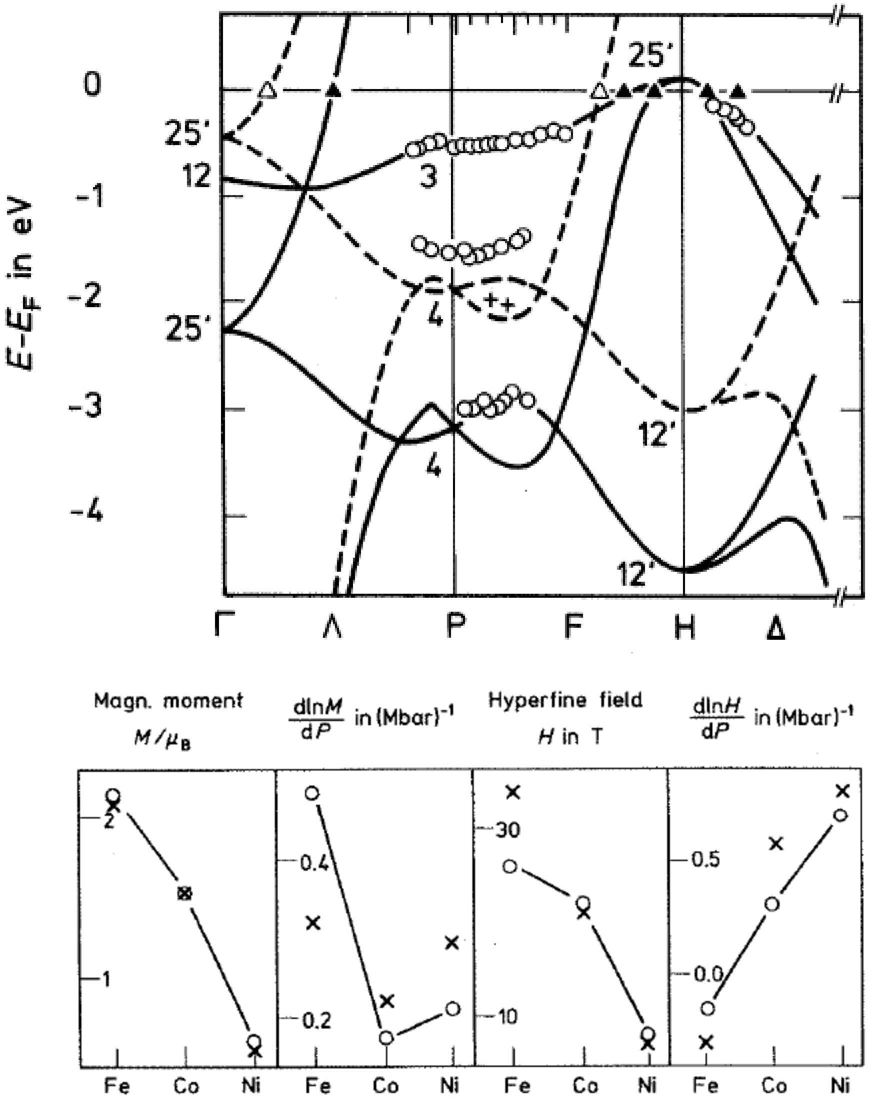
Proc. Roy. Soc. A273, 247 (1963)

Phys. Rev. B 16, 2095 (1977)





J. Appl. Phys. 50, 7423 (1979)



- ignoring the periodic potential of the lattice
- at T=0 states are filled up to k_F (spherical symmetry)

up/down

spherical shell

$$g(k)dk = 2\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3}$$

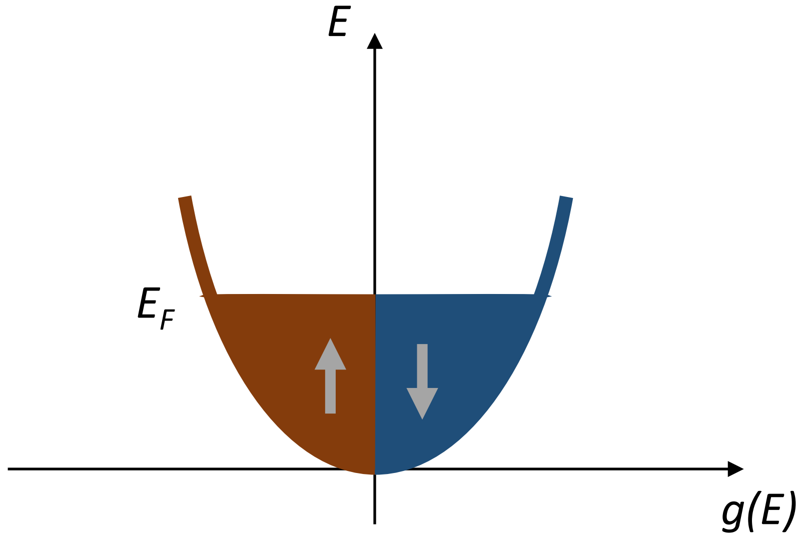
volume of one *k*-point

density of states (s-band)

$$g(E) \sim \sqrt{E}$$

$$g(E_F) = \frac{4 m_e k_F}{h^2}$$

$$E_F \sim n^{2/3}$$

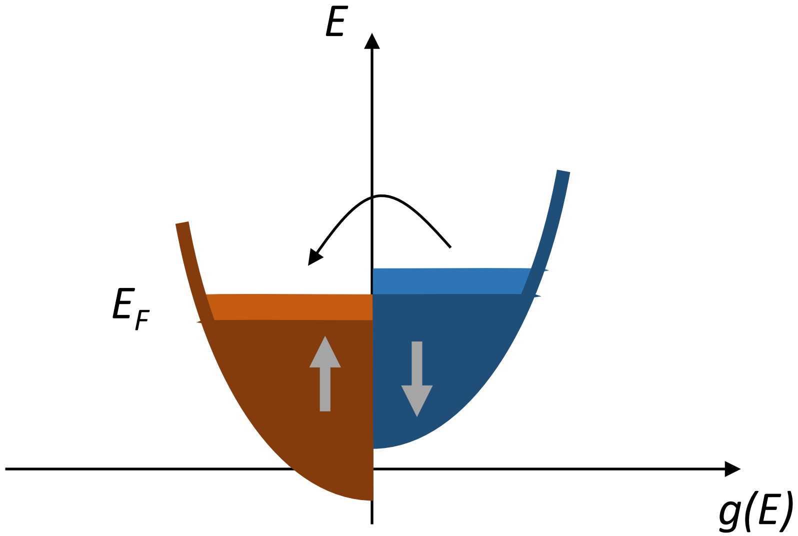


- applied field raises one sub-band and lowers the other

$$M = \mu_B(n_\uparrow - n_\downarrow) = \mu_B[g_\uparrow(E_F)\mu_B B - g_\downarrow(E_F)(-\mu_B B)] = g(E_F)\mu_B^2 B$$

$$g_\uparrow(E_F) = g_\downarrow(E_F) = \frac{1}{2}g(E_F)$$

$$\chi_P = g(E_F)\mu_0\mu_B^2 \ll \chi_{INSULATOR}$$



$$\Delta E_\uparrow = -gS\mu_B B = -\mu_B B$$

$$\Delta E_\downarrow = gS\mu_B B = \mu_B B$$

$$\mu_B B \ll E_F$$

- itinerant vs localized behavior

$$n_{\uparrow} = \frac{1}{2}\int_0^{\infty} g(E+\mu_B B) f(E) dE \qquad f(E) = \frac{1}{e^{(E-\mu)/k_B T}+1}$$

$$n_{\downarrow} = \frac{1}{2}\int_0^{\infty} g(E-\mu_B B) f(E) dE$$

$$M = \mu_B(n_{\uparrow} - n_{\downarrow}) \approx \mu_B^2 B \int_0^{\infty} \frac{dg(E)}{dE} f(E) dE = -\mu_B^2 B \int_0^{\infty} \frac{df(E)}{dE} g(E) dE$$

degenerate limit ($T << E_F$): $\frac{df}{dE} \approx -\delta(E-E_F)$ $\chi_P = g(E_F)\mu_0\mu_B^2$

non-degenerate limit *(n <<)*: $\frac{df}{dE} \approx -\frac{f}{k_B T}$ $\chi_C = \frac{n\mu_0\mu_B^2}{k_B T}$

- on-site repulsion U has to be considerable

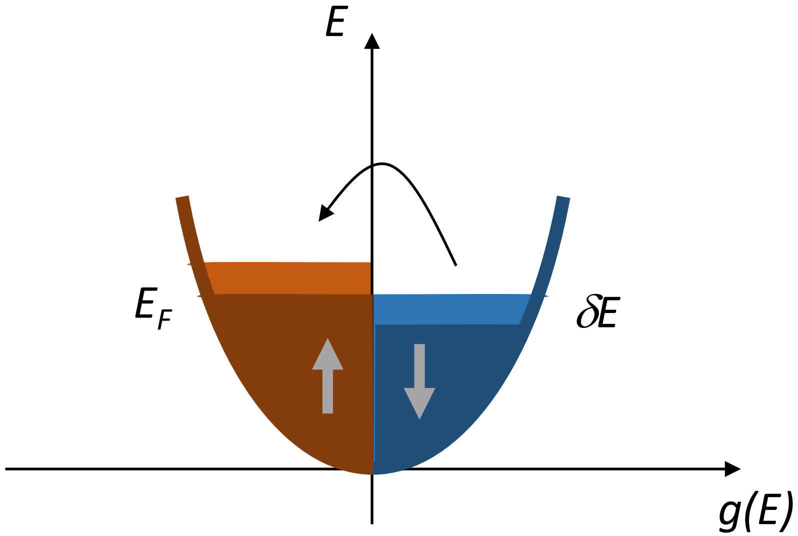
$$\Delta E_K = \frac{1}{2} g(E_F)(\delta E)^2$$

$$\Delta E_P = -\frac{1}{2} U\, [g(E_F)\delta E]^2$$

$$\Delta E = \Delta E_K - \Delta E_P = \frac{1}{2} g(E_F)(\delta E)^2 - \frac{1}{2} U\, [g(E_F)\delta E]^2$$

$$\Delta E = \frac{1}{2} g(E_F)(\delta E)^2 [1 - U g(E_F)] < 0 \overset{FM}{\Longrightarrow} U g(E_F) > 1$$

Stoner criterion



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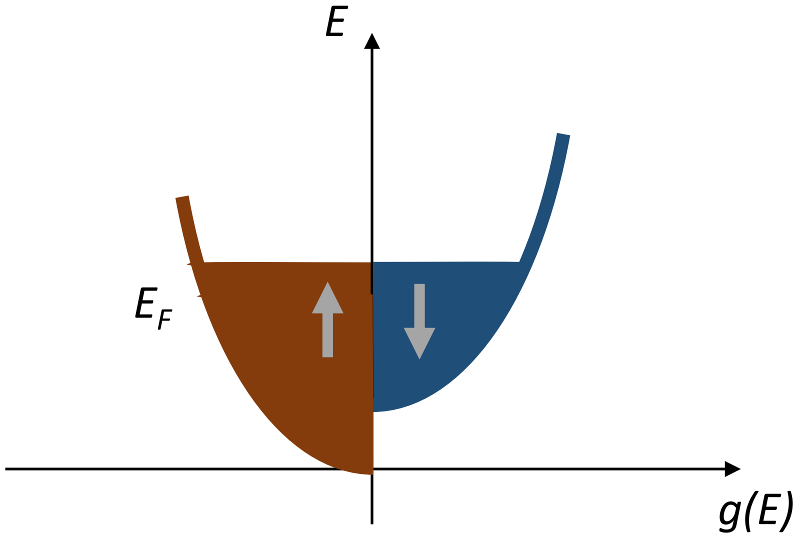

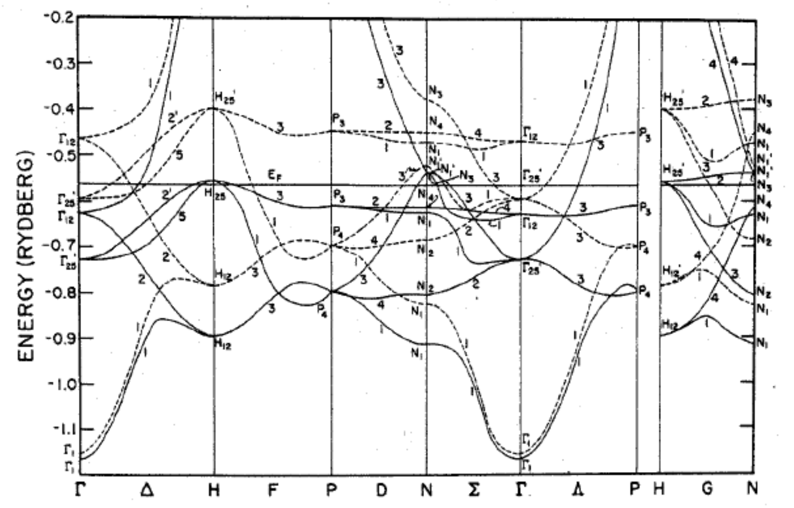

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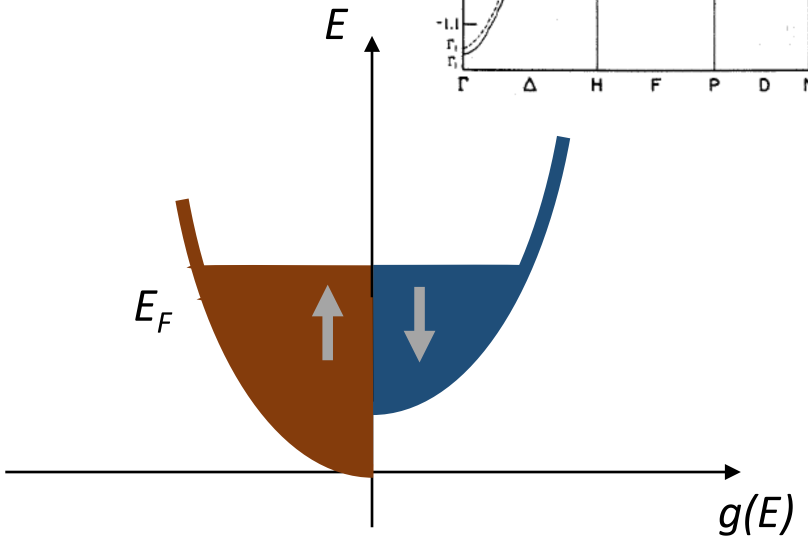

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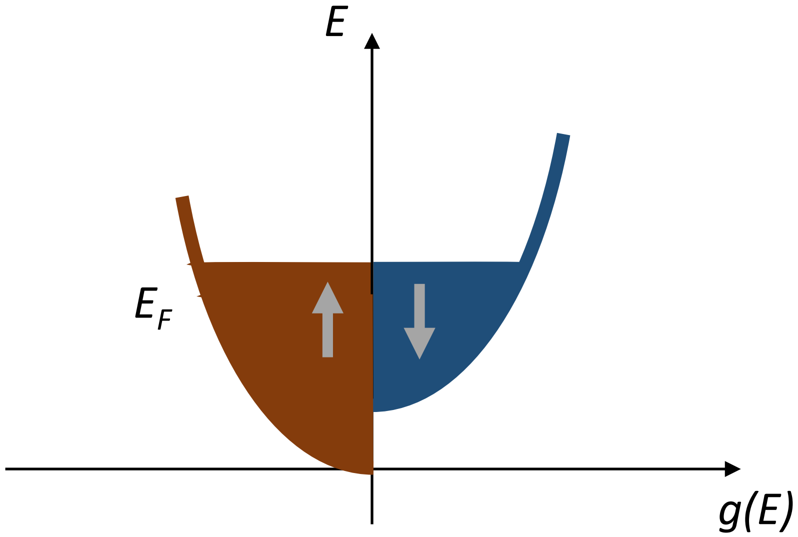
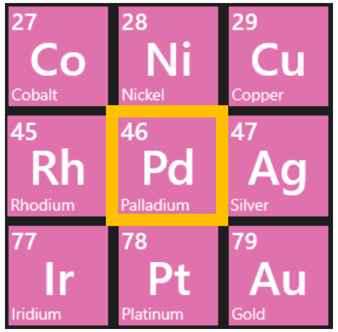
Stoner criterion



$U g(E_F) \lesssim 1 \longrightarrow$ $\chi = \dfrac{\chi_P}{1 - U g(E_F)}$ Stoner enhancement (Pd, Pt) $\rightarrow$ doping with Fe



- pressure effect

PHYSICAL REVIEW B **105**, 024404 (2022)

Pressure-induced collapse of ferromagnetism in nickel

A. Ahad[1,*] and M. S. Bahramy[2,†]
[1]*Department of Physics, Aligarh Muslim University, Aligarh 202002, India*
[2]*Department of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom*

(Received 26 August 2021; revised 22 December 2021; accepted 23 December 2021; published 4 January 2022)

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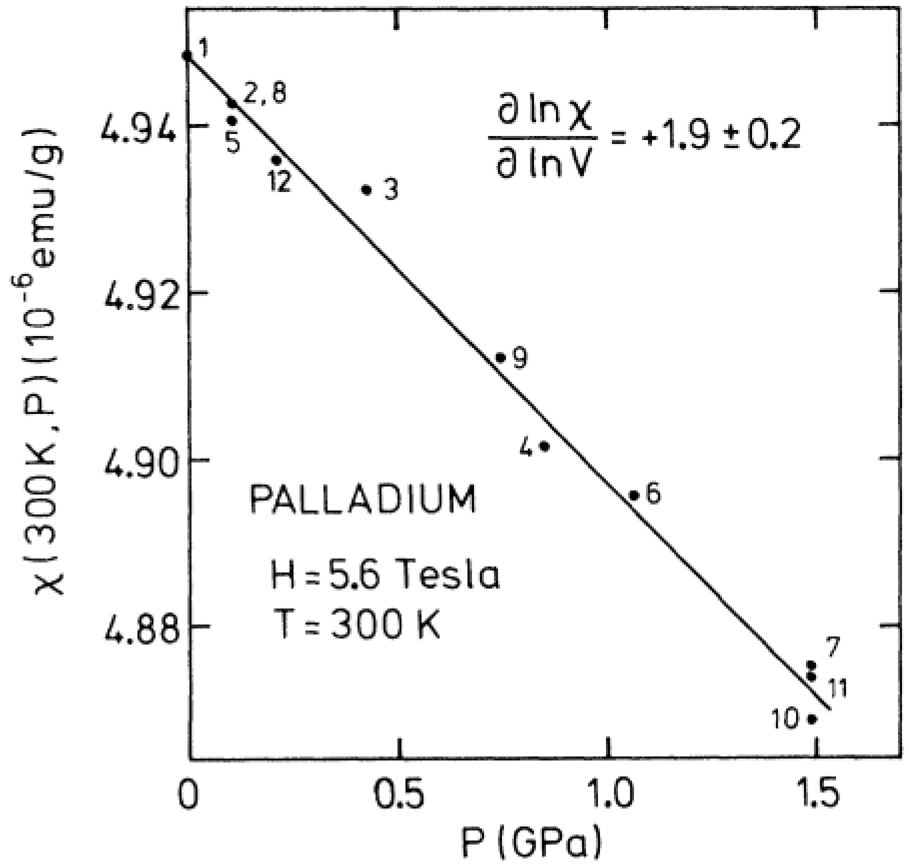
PRB 24, 6744 (1981)

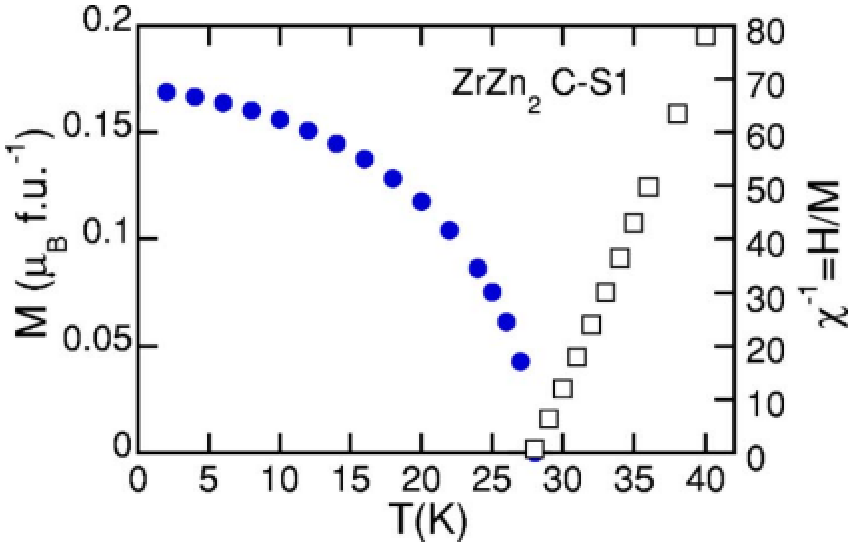


❖ 'non-magnetic' ferromagnets

PHYSICAL REVIEW B **72**, 184436 (2005)

Ferromagnetic properties of $ZrZn_2$

E. A. Yelland, S. J. C. Yates, O. Taylor, A. Griffiths, S. M. Hayden, and A. Carrington
H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom
(Received 15 August 2005; revised manuscript received 14 October 2005; published 30 November 2005)



$$M(T) = M_0\sqrt{1-\left(\frac{T}{T_C}\right)^2}$$

$$\chi(T) = \frac{C_{Stoner}}{T^2 - T_C^2}$$

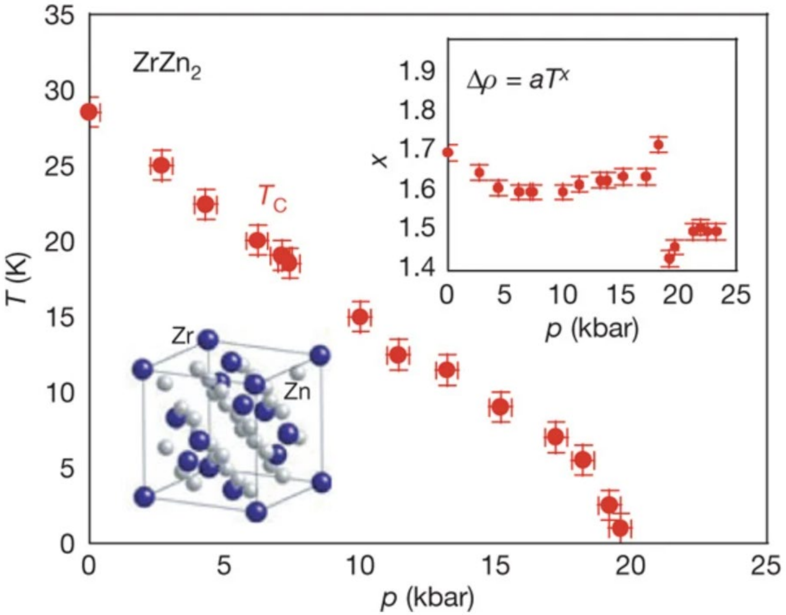
	Mean-field	Heisenberg	This work
β	0.5	0.326	0.52±0.05
δ	3	4.78	3.20±0.08

❖ non-Fermi liquid behavior

Marginal breakdown of the Fermi-liquid state on the border of metallic ferromagnetism

R. P. Smith, M. Sutherland, G. G. Lonzarich, S. S. Saxena, N. Kimura, S. Takashima, M. Nohara & H. Takagi

Nature **455**, 1220–1223 (2008) | Cite this article



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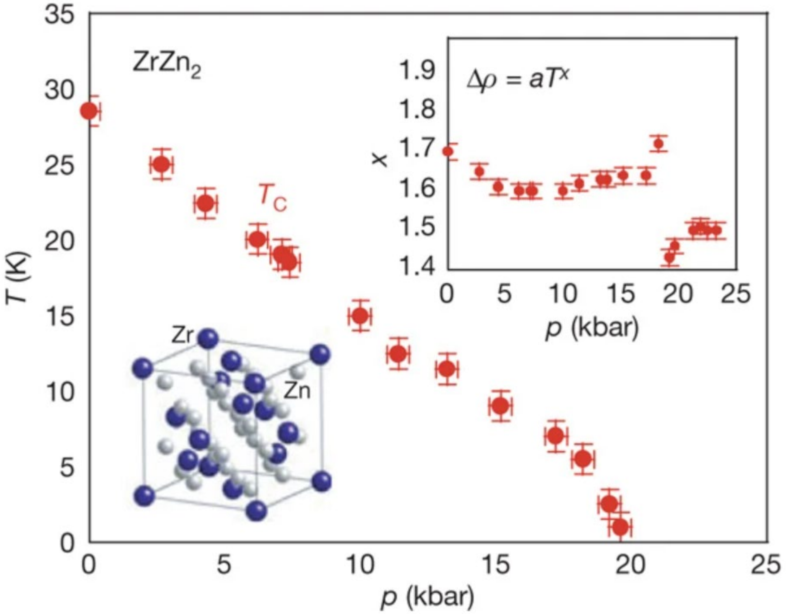
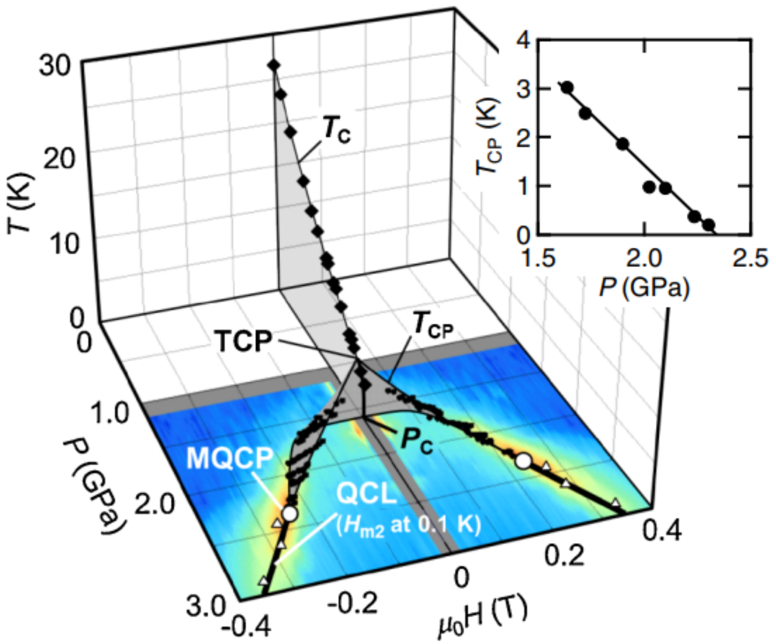
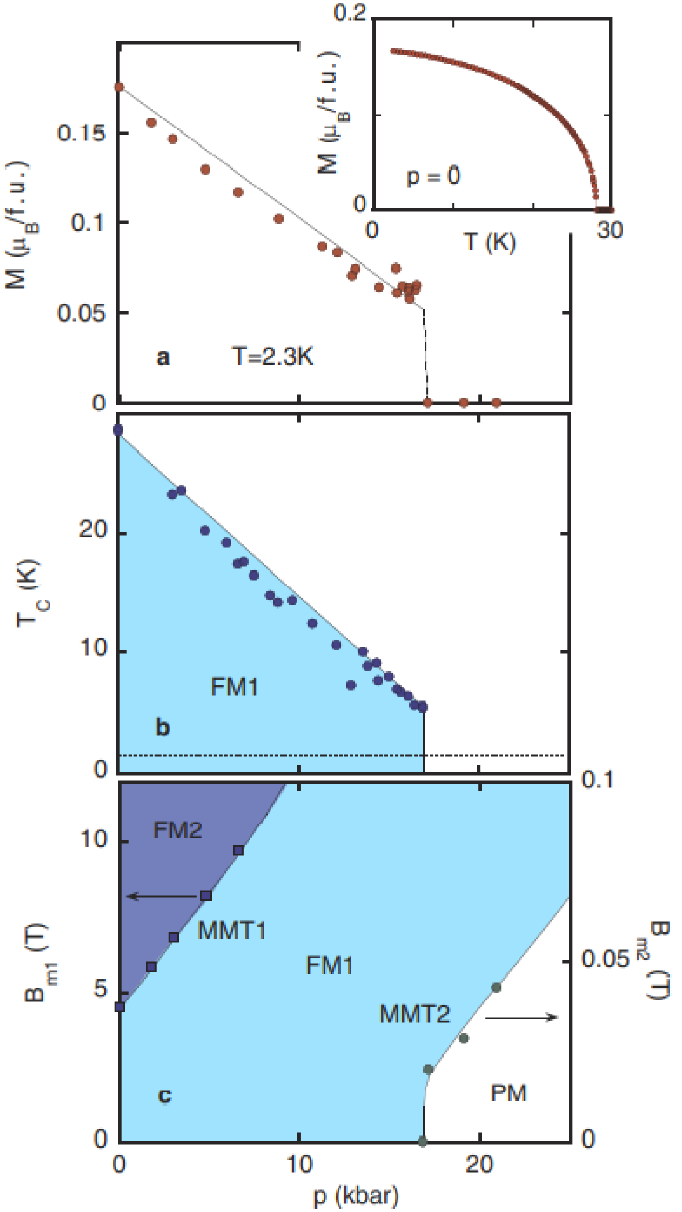


JPSJ 81, 073706 (2012)



PRL 93, 256404 (2004)

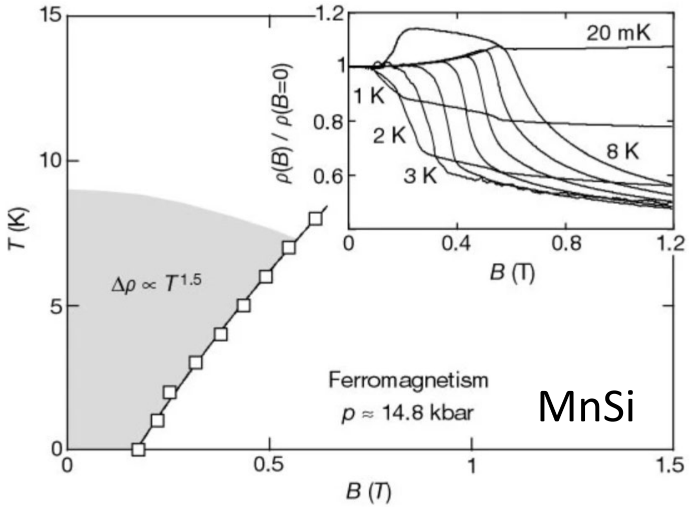


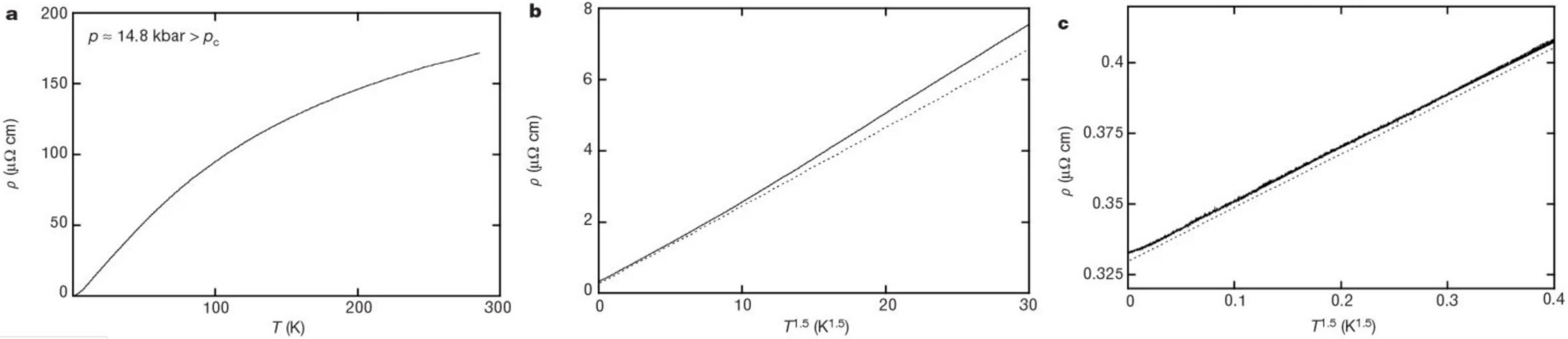
❖ non-Fermi liquid behavior

Non-Fermi-liquid nature of the normal state of itinerant-electron ferromagnets

C. Pfleiderer, S. R. Julian & G. G. Lonzarich

Nature 414, 427–430 (2001) | Cite this article



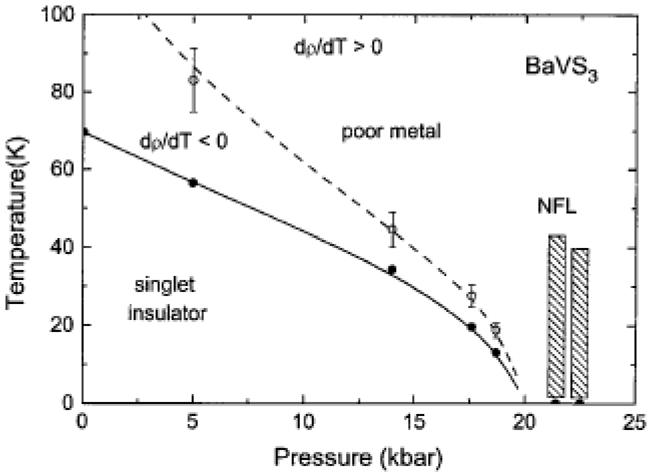


- non-Fermi liquid behavior

VOLUME 85, NUMBER 9 PHYSICAL REVIEW LETTERS 28 AUGUST 2000

Pressure Induced Quantum Critical Point and Non-Fermi-Liquid Behavior in $BaVS_3$

L. Forró,[1] R. Gaál,[1] H. Berger,[1] P. Fazekas,[2] K. Penc,[2] I. Kézsmárki,[1,3] and G. Mihály[1,3]
[1]*Department of Physics, Ecole Politechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*
[2]*Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.B. 49, Hungary*
[3]*Department of Physics, Technical University of Budapest, H-1111 Budapest, Hungary*
(Received 24 January 2000)



- orbital contribution of itinerant electrons when B>0

$$H = \frac{\boldsymbol{p}^2}{2m_e} \longrightarrow H = \frac{1}{2m_e}(\boldsymbol{p} + e\boldsymbol{A})^2$$

$$H\psi = E\psi \qquad \psi_{\boldsymbol{k}} = \frac{1}{\sqrt{V}} e^{i\boldsymbol{kr}}$$

$$E_{\boldsymbol{k}} = \frac{\hbar^2}{2m_e}(k_x^2 + k_y^2 + k_z^2)$$

$$\boldsymbol{B} = (0,0,B)$$

$$\boldsymbol{A} = (0, Bx, 0) \qquad \text{or } \boldsymbol{A} = (-By, 0,0)$$

$$H = \frac{1}{2m_e}\left[\hat{p}_x^2 + \left(\hat{p}_y + eB\hat{x}\right)^2 + \hat{p}_z^2\right]$$

$$H = \frac{1}{2m_e}[\hat{p}_x^2 + m_e^2\omega_c^2(\hat{x} - x_0)^2 + \hbar^2 k_z^2]$$

harmonic oscillator

plain wave

$$\sqrt{k_x^2 + k_y^2}$$

$$x_0 = -\frac{\hbar k_y}{eB}$$

$$\omega_c = \frac{eB}{m_e}$$

$$E = \left(l + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m_e}$$

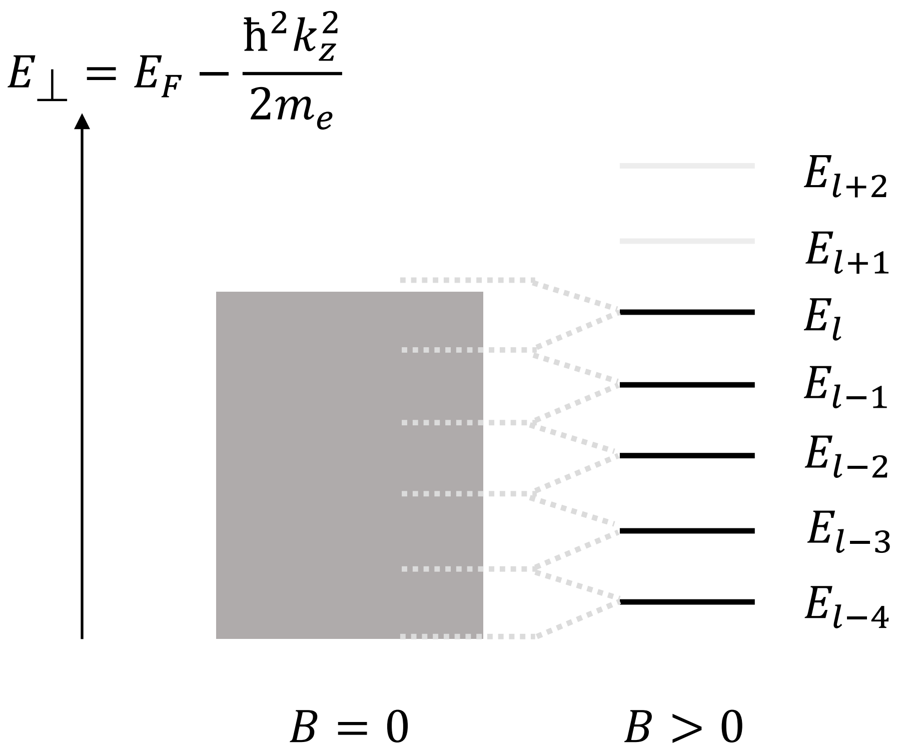
❖ orbital contribution of itinerant electrons when B>0

$$E = \left(l + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m_e}$$

degeneracy: $p = \dfrac{m_e L^2 \omega_c}{\pi\hbar}$

Landau diamagnetism

$$\chi_L = -\frac{1}{3}\left(\frac{m_e}{m^*}\right)^2 \chi_P$$



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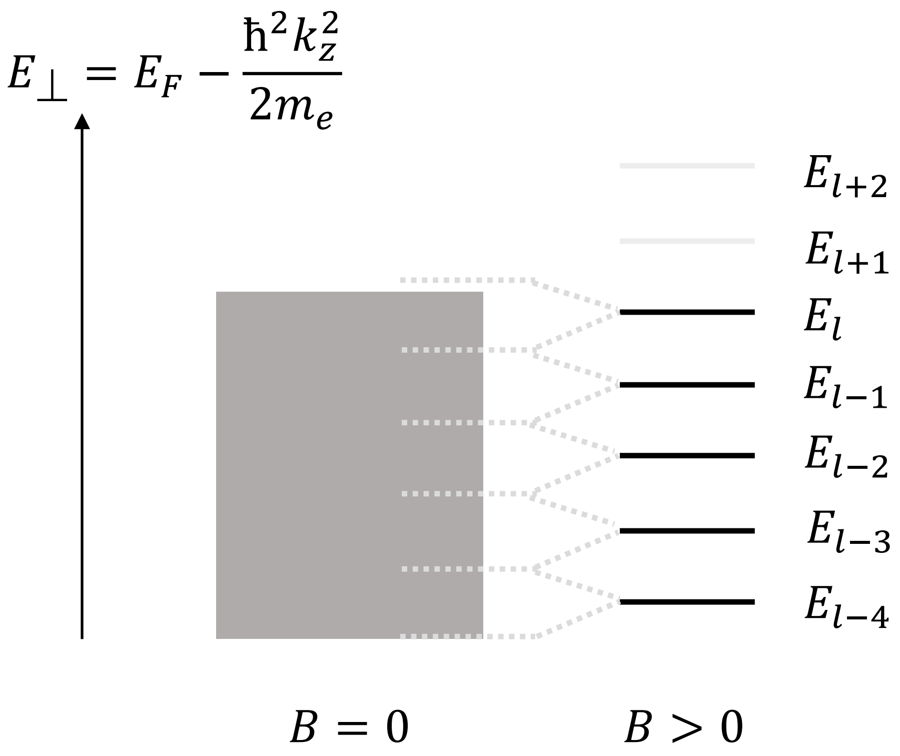
Landau diagnetism

$$\chi_L = -\frac{1}{3}\left(\frac{m_e}{m^*}\right)^2 \chi_P$$

Bi metal is strongly diamagnetic

$$m^* \sim 0.01 m_e$$



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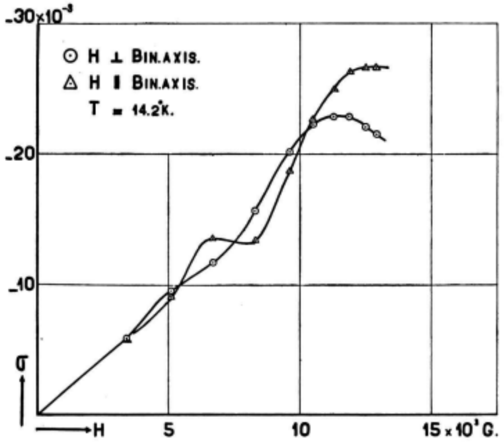
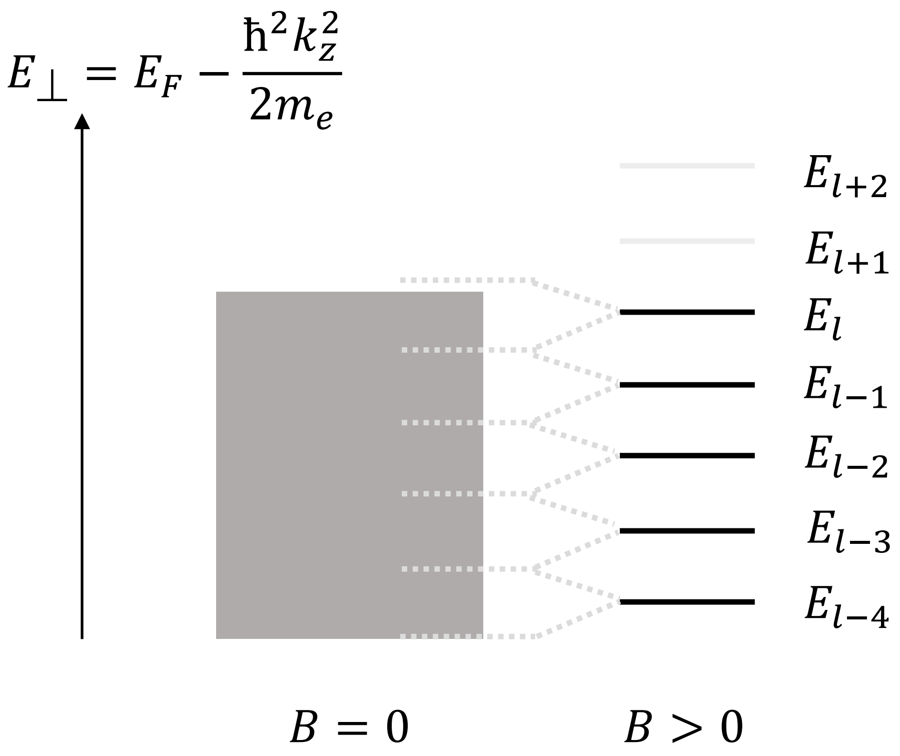
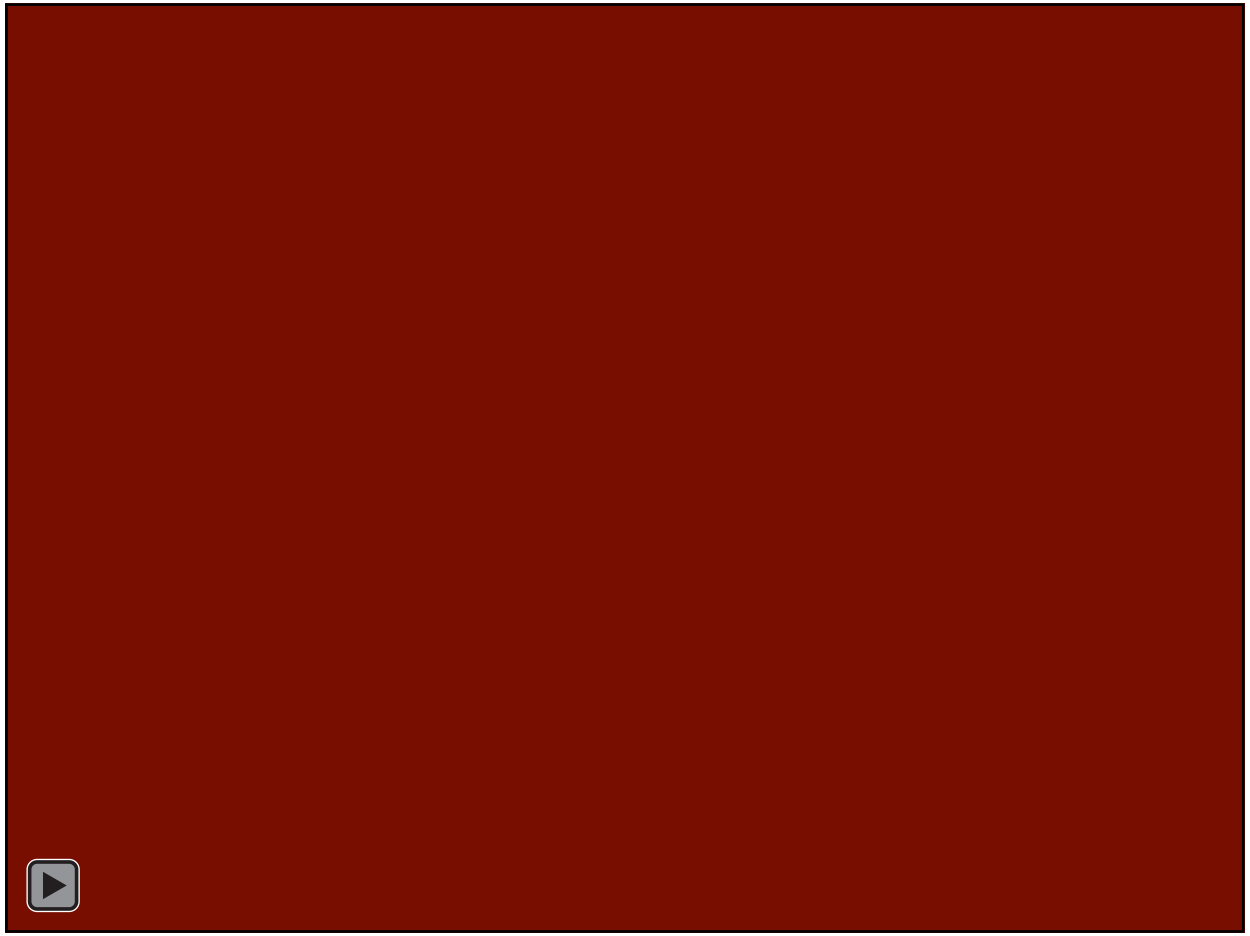




de Haas – van Alphen effect
M(B) oscillations

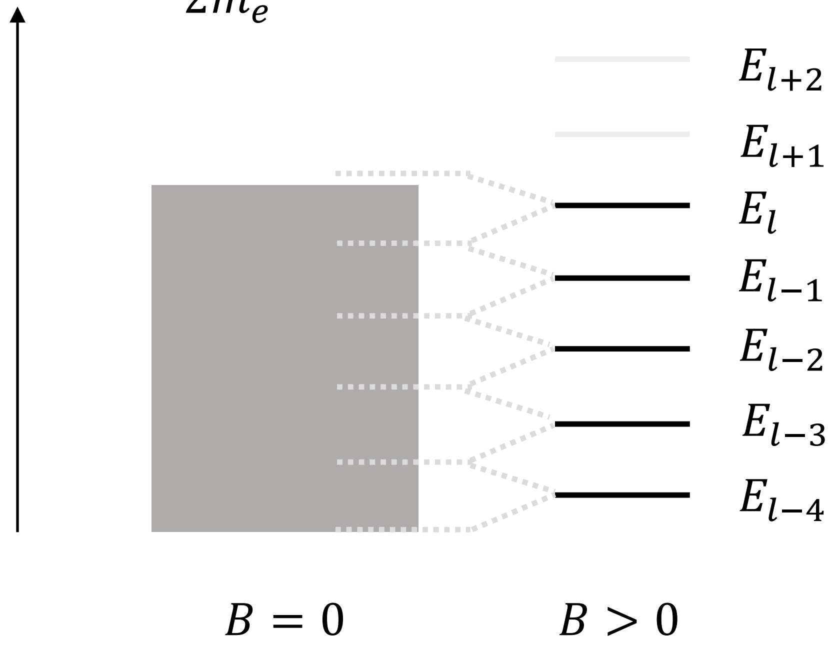
Shubnikov – de Haas effect
R(B) oscillations

$$\Delta\left(\frac{1}{B}\right) = \frac{e}{h}\frac{1}{S}$$



animation

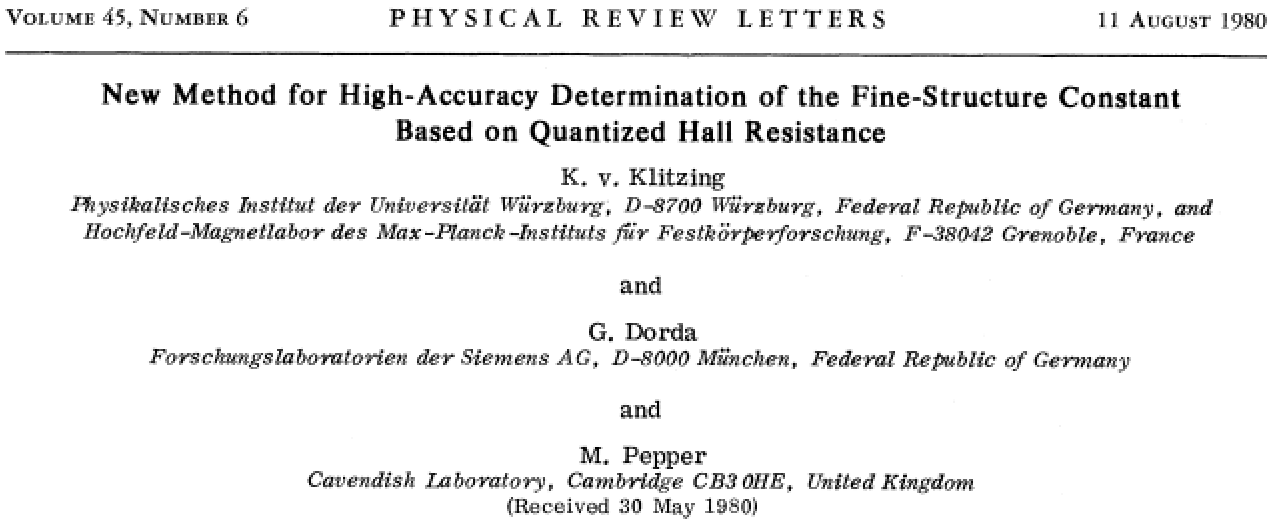
$$E_\perp = E_F - \frac{\hbar^2 k_z^2}{2m_e}$$



Shubnikov – de Haas effect
R(B) oscillations

$$\Delta\left(\frac{1}{B}\right) = \frac{e}{h}\frac{1}{S}$$

image source: wikimedia.org



Volume 45, Number 6 PHYSICAL REVIEW LETTERS 11 August 1980

New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance

K. v. Klitzing
Physikalisches Institut der Universität Würzburg, D-8700 Würzburg, Federal Republic of Germany, and Hochfeld-Magnetlabor des Max-Planck-Instituts für Festkörperforschung, F-38042 Grenoble, France

and

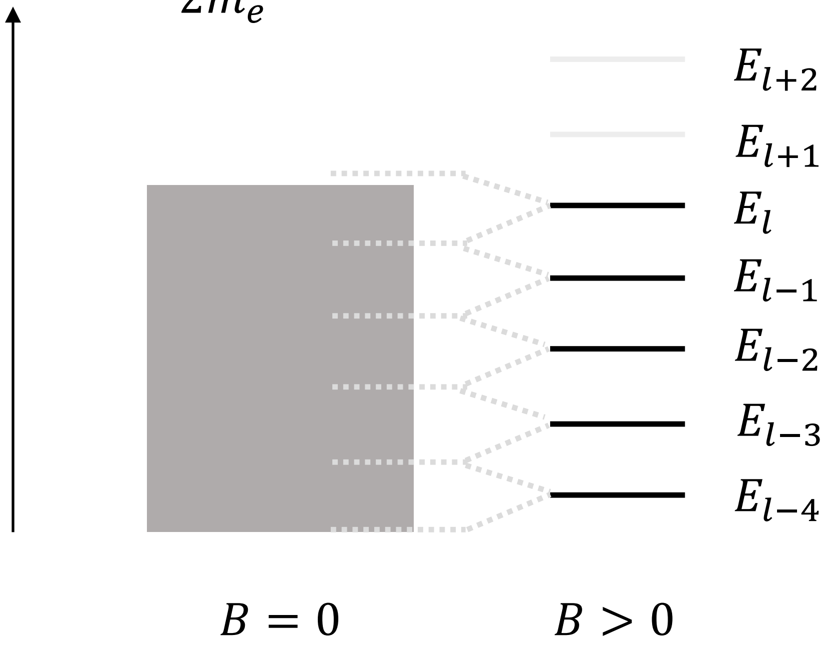
G. Dorda
Forschungslaboratorien der Siemens AG, D-8000 München, Federal Republic of Germany

and

M. Pepper
Cavendish Laboratory, Cambridge CB3 0HE, United Kingdom

(Received 30 May 1980)

$$E_{\perp} = E_F - \frac{\hbar^2 k_z^2}{2m_e}$$



Shubnikov – de Haas effect
R(B) oscillations

$$\Delta\left(\frac{1}{B}\right) = \frac{e}{h}\frac{1}{S}$$

$$R_K = \frac{h}{e^2} = 25812.80745\ \Omega$$

image source: wikimedia.org

VOLUME 45, NUMBER 6 PHYSICAL REVIEW LETTERS 11 AUGUST 1980

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Two-Dimensional Magnetotransport in the Extreme Quantum Limit

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(Received 5 March 1982)

$$R_K = \frac{h}{e^2} = 25812.80745\ \Omega$$

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New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance

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