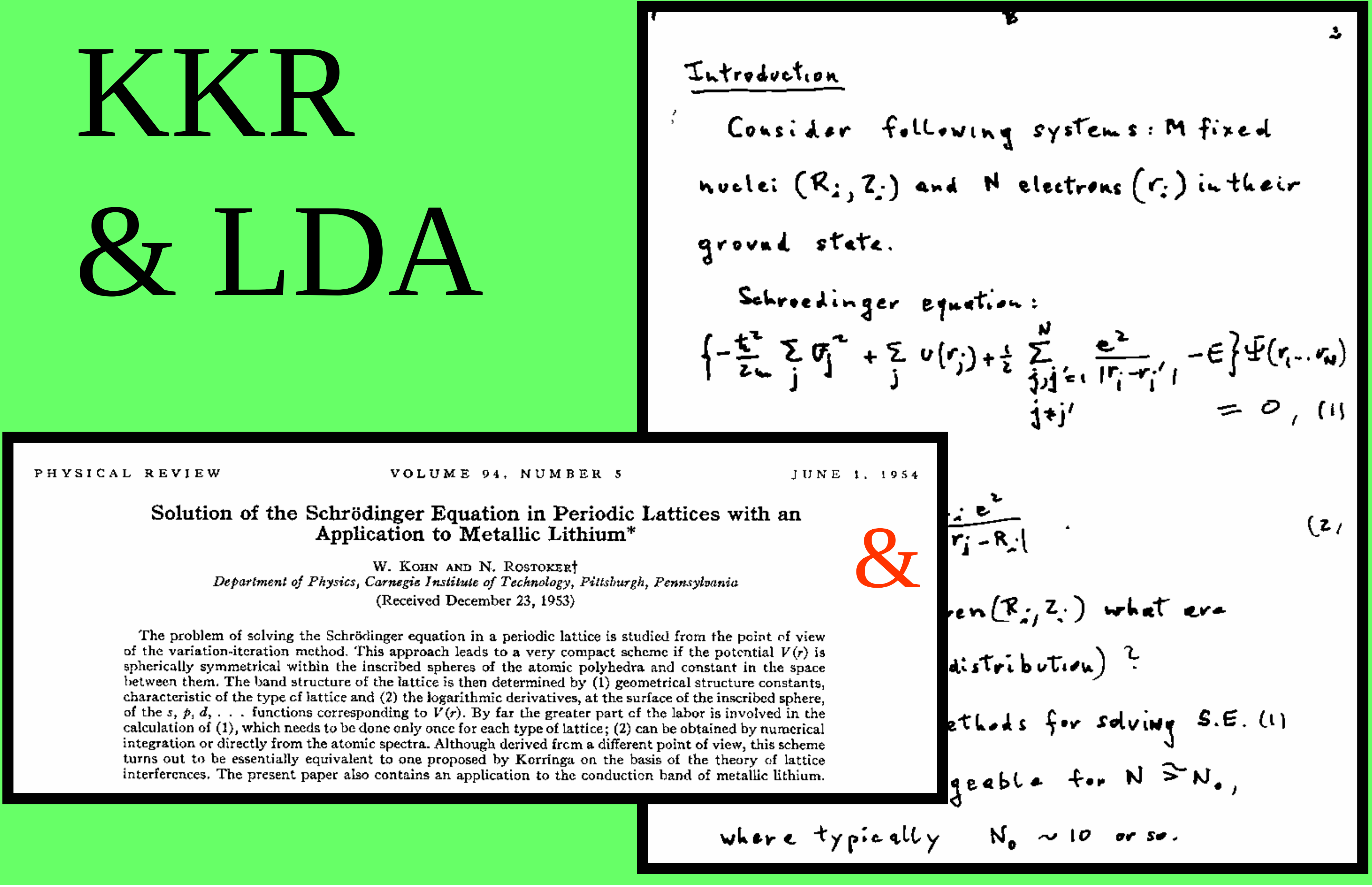
KKR
& LDA



2

Introduction

Consider following systems: M fixed nuclei (R_i, Z_i) and N electrons (r_i) in their ground state.

Schroedinger equation:

$$\left\{-\frac{\hbar^2}{2m}\sum_j \nabla_j^2 + \sum_j v(r_j) + \frac{1}{2}\sum_{\substack{j,j'=1\\ j\neq j'}}^{N} \frac{e^2}{|r_j - r_{j'}|} - E\right\}\Psi(r_1 \ldots r_N) = 0, \quad (1)$$

$$\frac{e^2}{|r_j - R_i|} \quad (2)$$

en (R_i, Z_i) what are

distribution) ?

ethods for solving S.E. (1)

geable for $N \gtrsim N_0$,

where typically $N_0 \sim 10$ or so.

&

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Solution of the Schrödinger Equation in Periodic Lattices with an Application to Metallic Lithium*

W. Kohn and N. Rostoker†
Department of Physics, Carnegie Institute of Technology, Pittsburgh, Pennsylvania

(Received December 23, 1953)

The problem of solving the Schrödinger equation in a periodic lattice is studied from the point of view of the variation-iteration method. This approach leads to a very compact scheme if the potential $V(r)$ is spherically symmetrical within the inscribed spheres of the atomic polyhedra and constant in the space between them. The band structure of the lattice is then determined by (1) geometrical structure constants, characteristic of the type of lattice and (2) the logarithmic derivatives, at the surface of the inscribed sphere, of the s, p, d, . . . functions corresponding to $V(r)$. By far the greater part of the labor is involved in the calculation of (1), which needs to be done only once for each type of lattice; (2) can be obtained by numerical integration or directly from the atomic spectra. Although derived from a different point of view, this scheme turns out to be essentially equivalent to one proposed by Korringa on the basis of the theory of lattice interferences. The present paper also contains an application to the conduction band of metallic lithium.

Resolvents:

- $G(z) = (z - H)^{-1}$ resolvent: analytic in the complex plane with exception of the poles on the real axis; Green‘s functions: e.g., $\langle \mathbf{r}|G(z)|\mathbf{r}'\rangle$ are representations of G(z)
- H : non-relativistic or relativistic (Dirac)
- G(z) and H have the same symmetry
- physical properties can be formulated as mappings of G(z)

Lippmann-Schwinger equation

$$G(z) = G_0(z)[1+VG(z)]$$

$G_0(z)$: structure constants, V = const.,
„screened KKR“, semi-infinite systems

$G_0(z)$: semi-infinite system, V = set of „impurity“
potentials: „embedded cluster method“,
nanostructures

Configurational averages

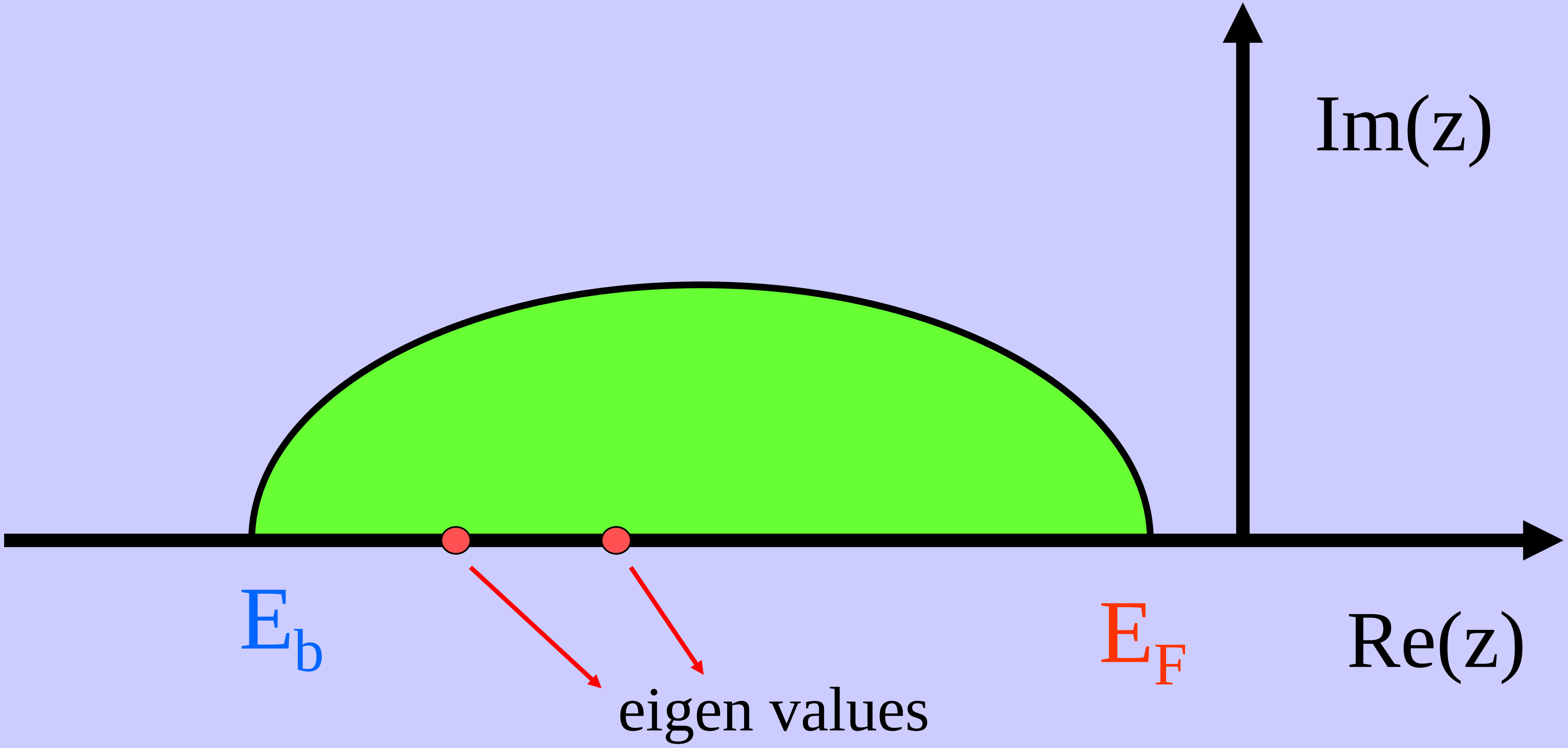
$$\langle G(z)\rangle_{conf} = c_A \langle G(z)\rangle_A + c_B \langle G(z)\rangle_B$$

$\langle G(z)\rangle_{A,B}$: partial average

c: can be inhomogeneous (layered systems)

Coherent Potential Approximation (CPA)

Contour integrations



Im(z)

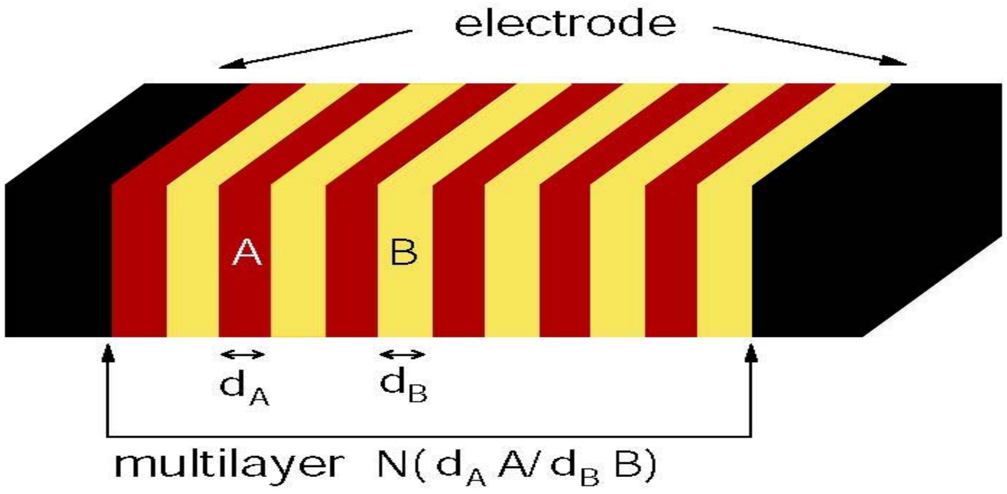
Re(z)

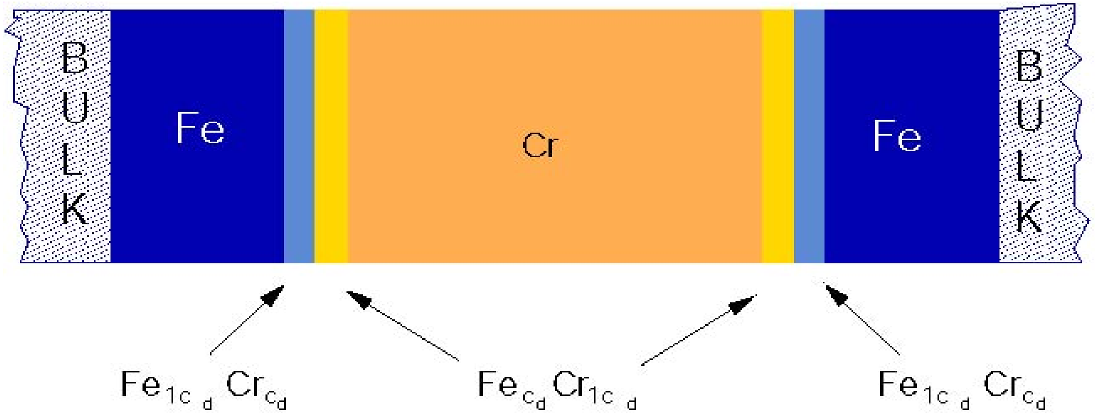
E_b

E_F

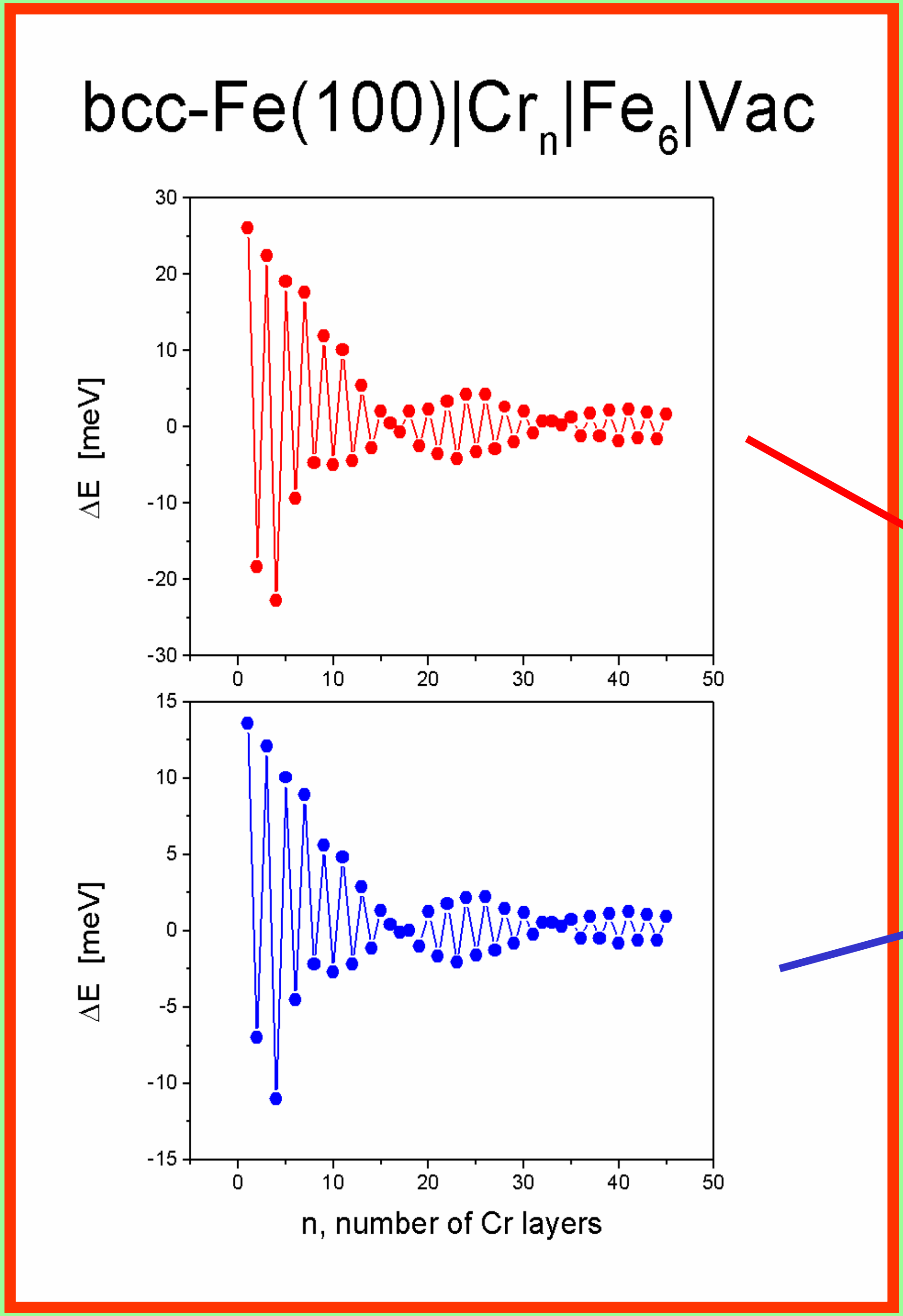
eigen values

Magnetic multilayers





Interlayer exchange coupling (IEC)

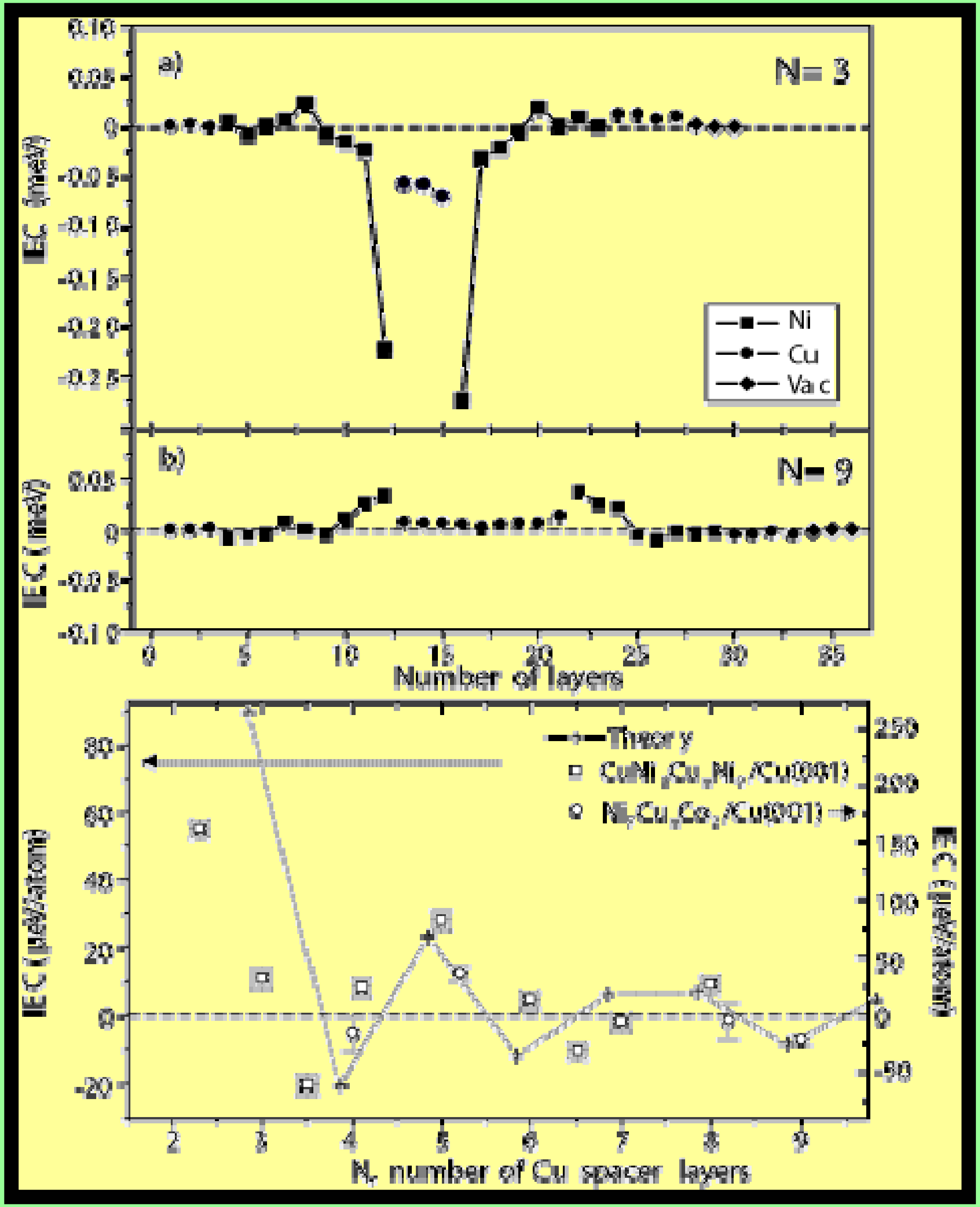

bcc-Fe(100)|Cr_n|Fe_6|Vac

180^0 coupling

90^0 coupling

(1) Phase slip
(2) Oscillatory, two periods

IEC & experiment



$Cu_4Ni_8Cu_5Ni_9/Cu(100)$

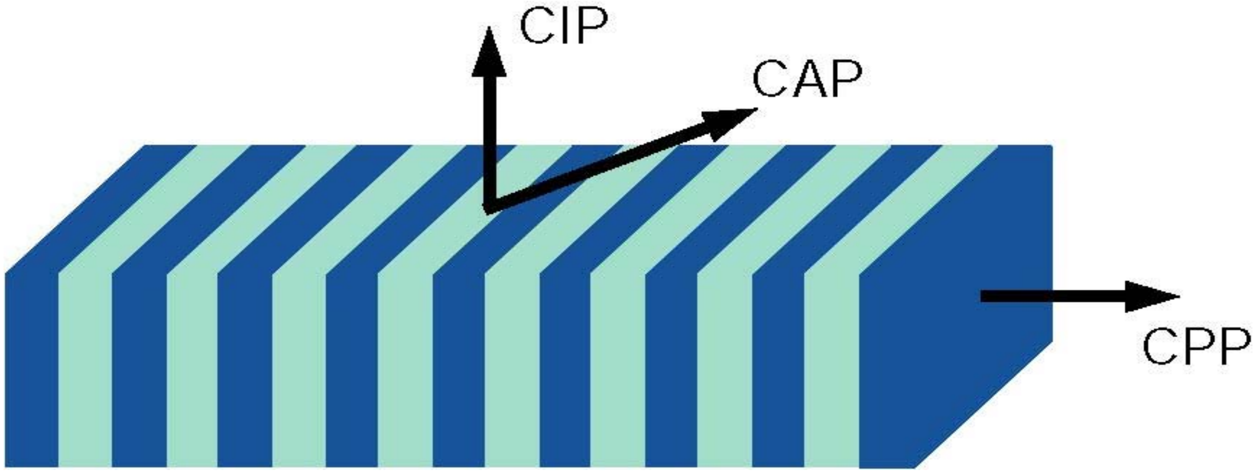
Electric transport

CIP: „current-in-plane“

CPP: „current-perpendicular to the planes of atoms

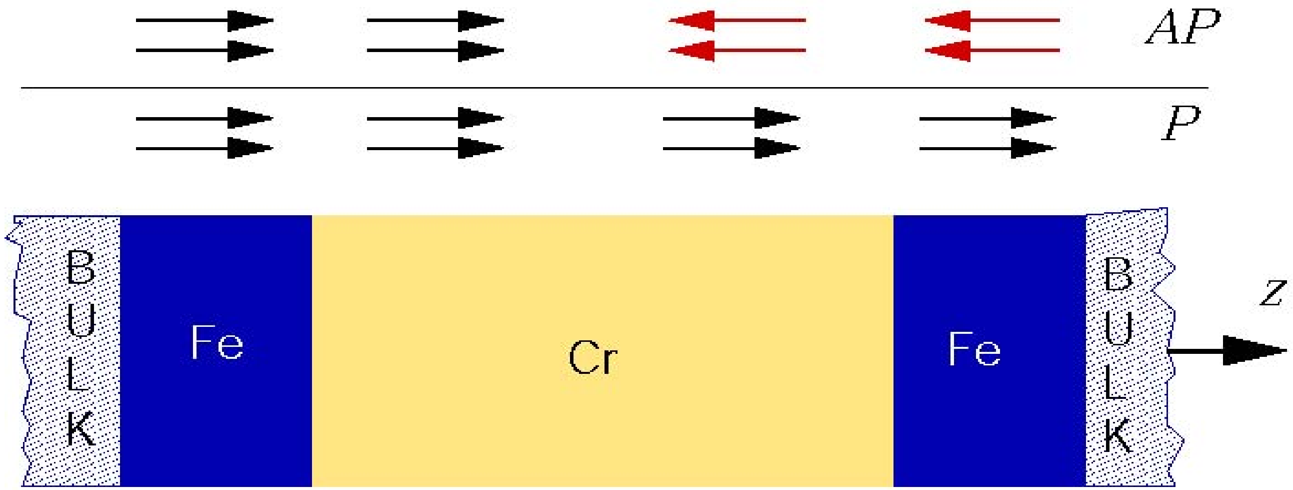
GMR: giant magnetoresistance

TMR: tunneling magnetoresistance

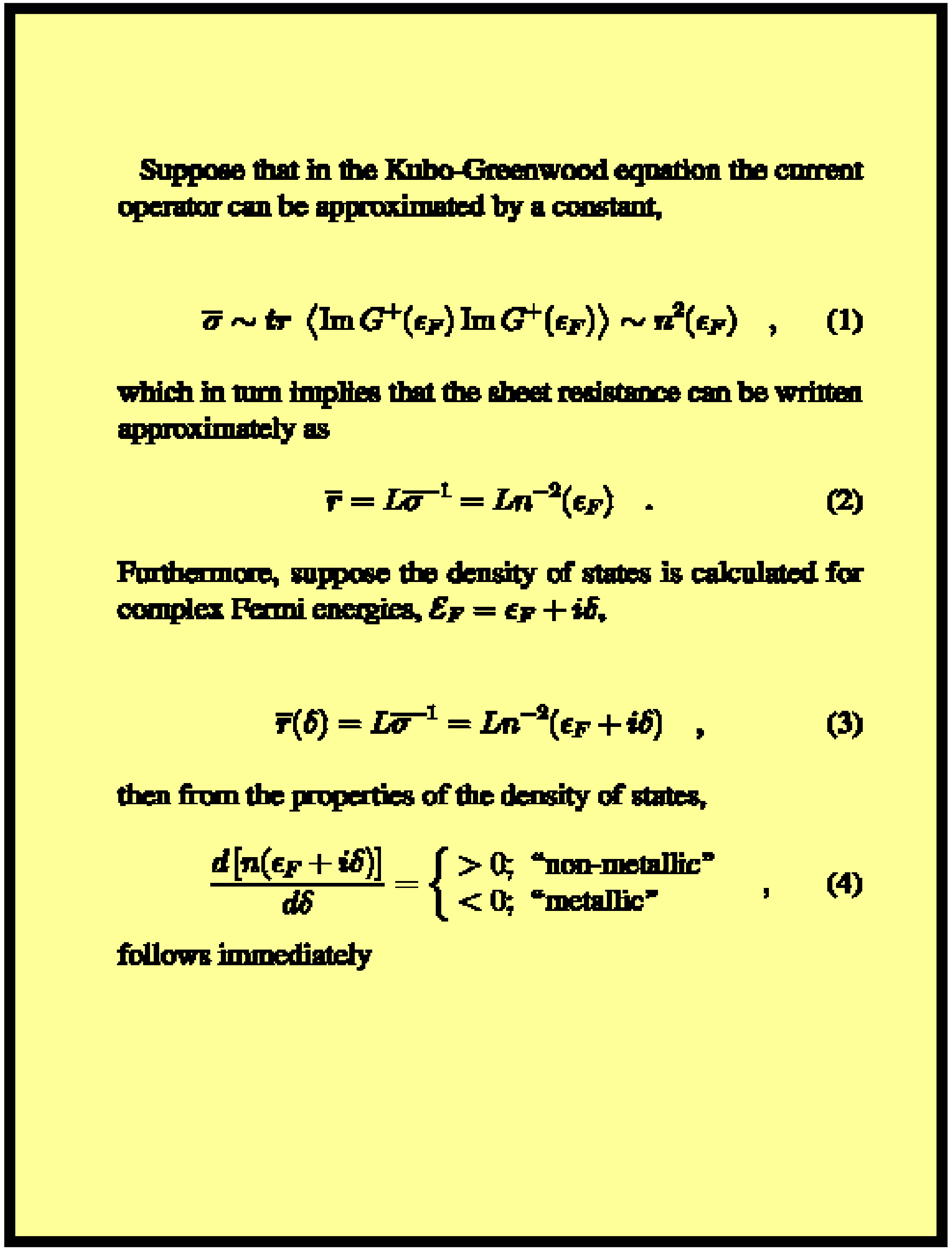


Magnetic configurations

P: parallel („ferromagnetic“)
AP: antiparallel („antiferromagnetic“)



Physical meaning of complex Fermi energies I



Suppose that in the Kubo-Greenwood equation the current operator can be approximated by a constant,

$$\overline{\sigma} \sim tr \ \langle \mathrm{Im}\, G^{+}(\epsilon_F)\, \mathrm{Im}\, G^{+}(\epsilon_F) \rangle \sim n^2(\epsilon_F) \quad , \qquad (1)$$

which in turn implies that the sheet resistance can be written approximately as

$$\overline{r} = L\overline{\sigma}^{-1} = Ln^{-2}(\epsilon_F) \quad . \qquad (2)$$

Furthermore, suppose the density of states is calculated for complex Fermi energies, $\mathcal{E}_F = \epsilon_F + i\delta$,

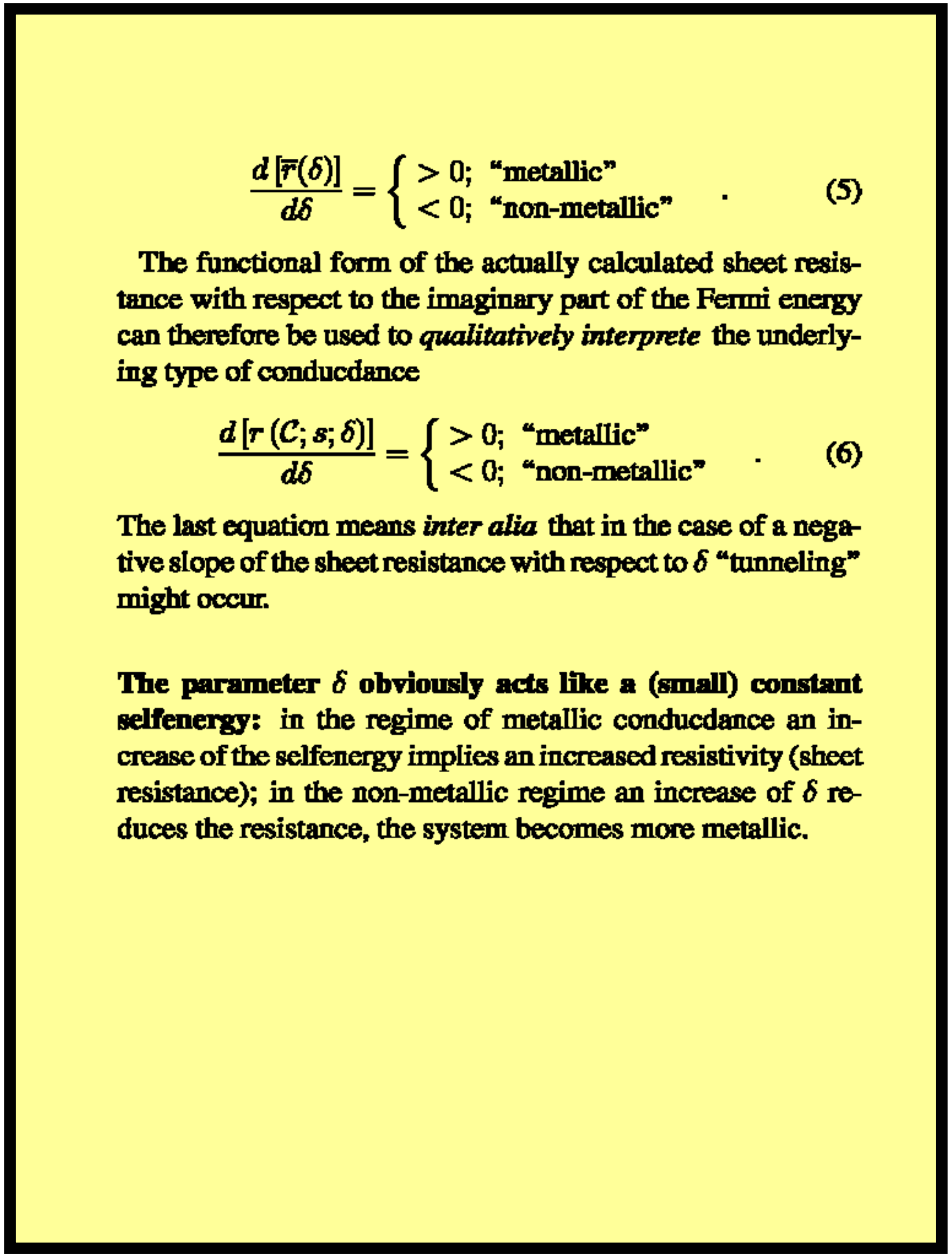
$$\overline{r}(\delta) = L\overline{\sigma}^{-1} = Ln^{-2}(\epsilon_F + i\delta) \quad , \qquad (3)$$

then from the properties of the density of states,

$$\frac{d\left[n(\epsilon_F + i\delta)\right]}{d\delta} = \begin{cases} > 0; & \text{“non-metallic”} \\ < 0; & \text{“metallic”} \end{cases} \quad , \qquad (4)$$

follows immediately

Physical meaning of complex Fermi energies II



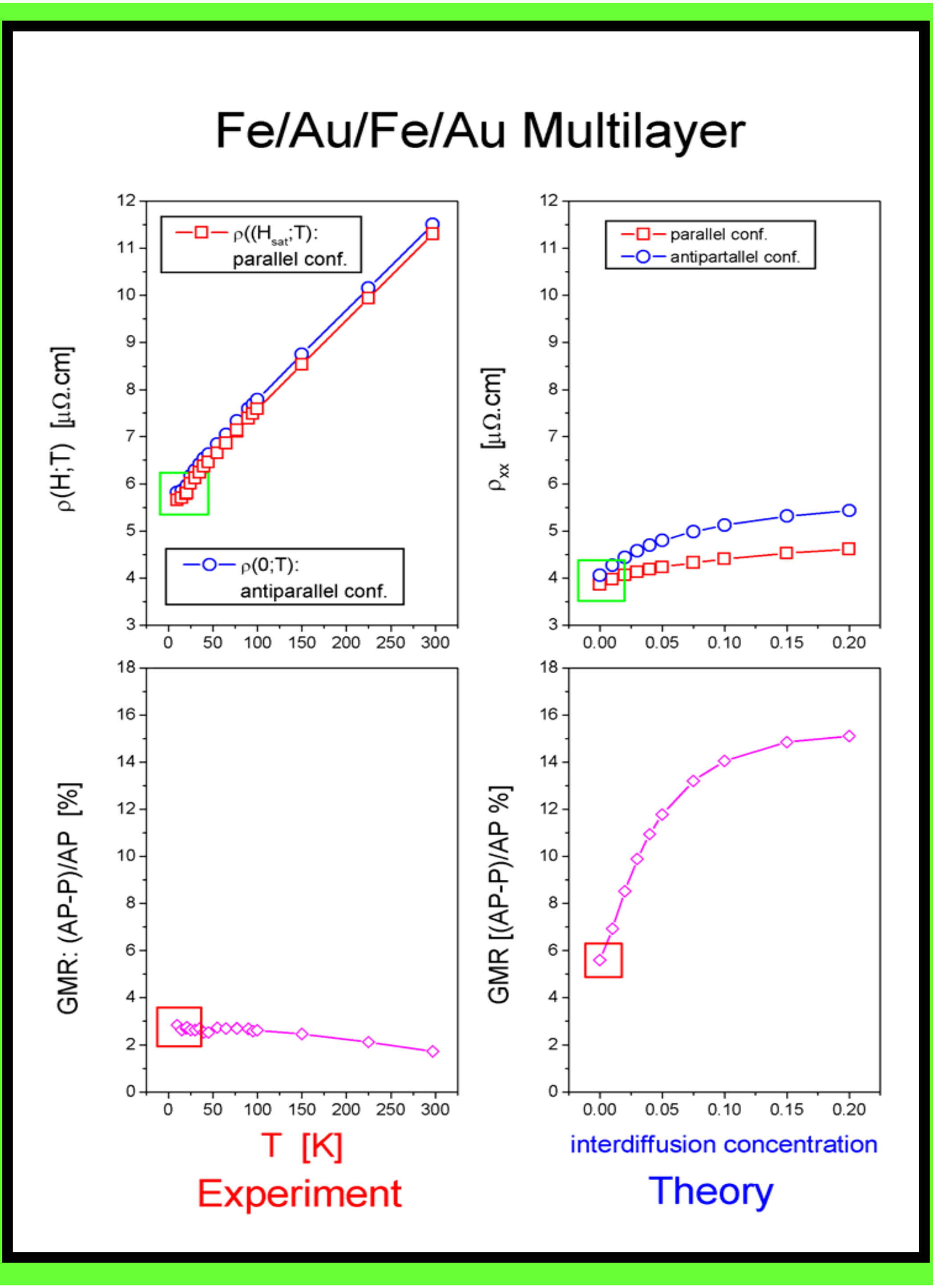
$$\frac{d\left[\overline{r}(\delta)\right]}{d\delta} = \begin{cases} > 0; & \text{“metallic”} \\ < 0; & \text{“non-metallic”} \end{cases} \quad . \qquad (5)$$

The functional form of the actually calculated sheet resistance with respect to the imaginary part of the Fermi energy can therefore be used to *qualitatively interprete* the underlying type of conducdance

$$\frac{d\left[r\left(C; s; \delta\right)\right]}{d\delta} = \begin{cases} > 0; & \text{“metallic”} \\ < 0; & \text{“non-metallic”} \end{cases} \quad . \qquad (6)$$

The last equation means *inter alia* that in the case of a negative slope of the sheet resistance with respect to δ “tunneling” might occur.

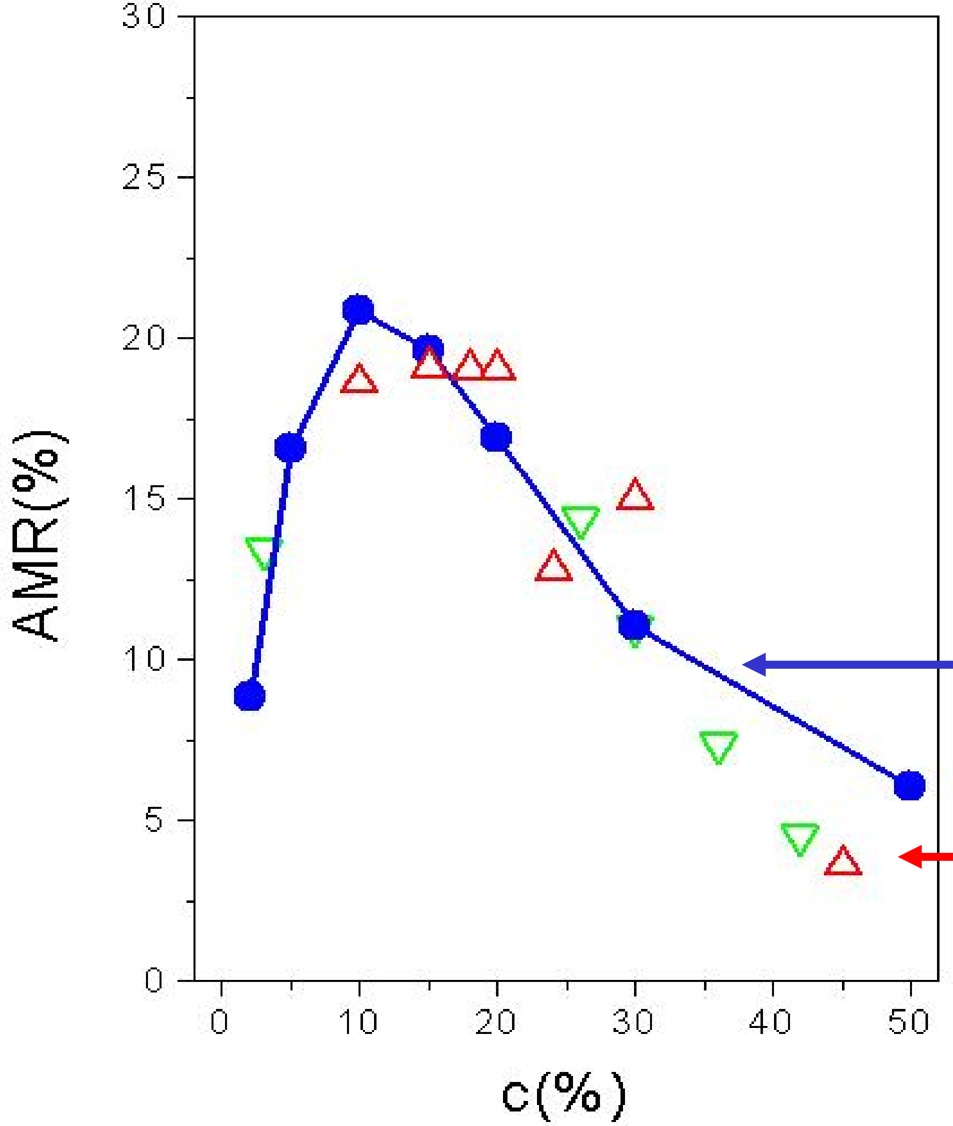
The parameter δ obviously acts like a (small) constant selfenergy: in the regime of metallic conducdance an increase of the selfenergy implies an increased resistivity (sheet resistance); in the non-metallic regime an increase of δ reduces the resistance, the system becomes more metallic.



Resistivities & GMR in magnetic multilayers

AMR
in Permalloy

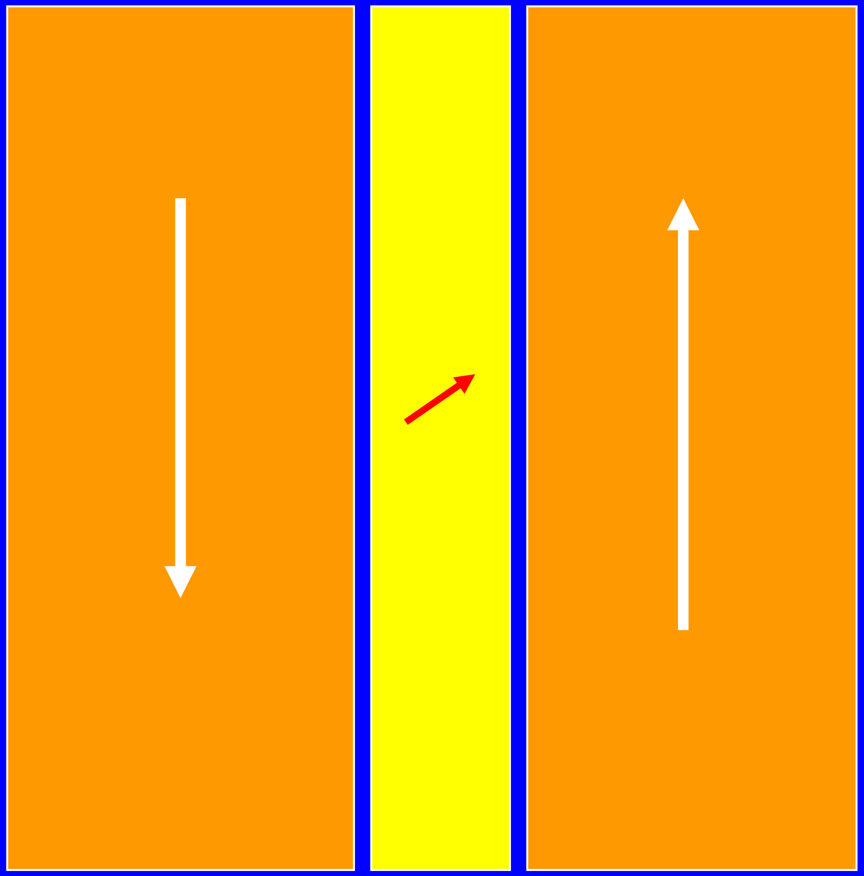
Fe_cNi_{1-c}



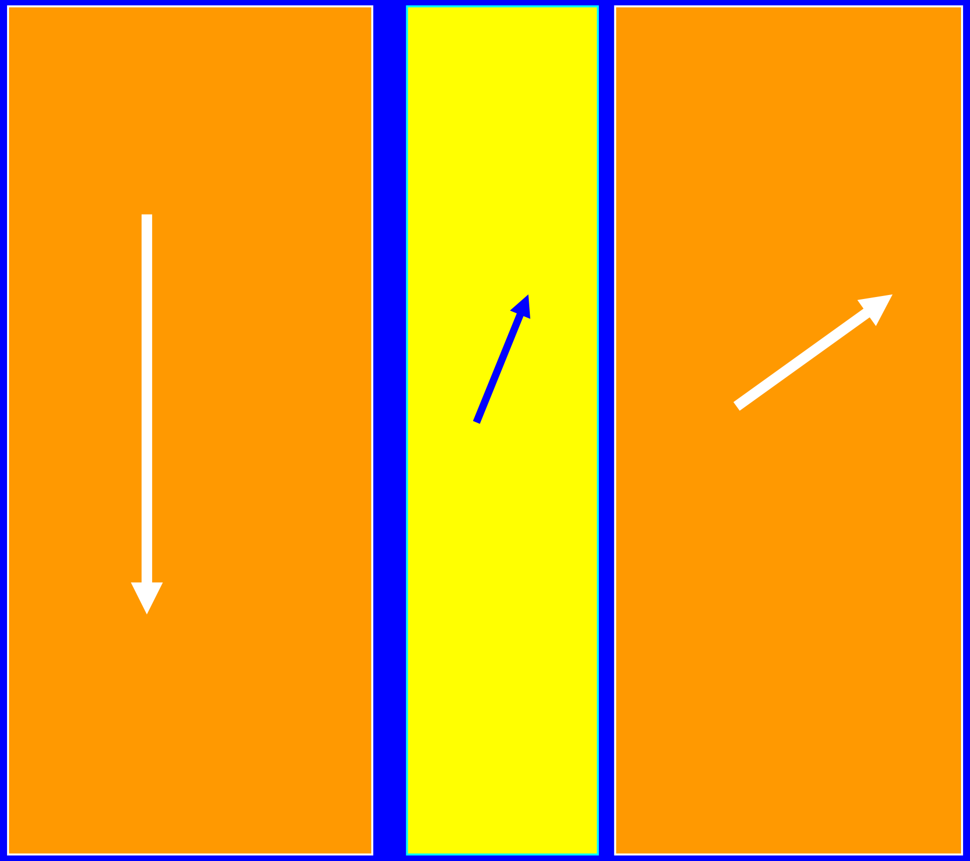
Theory

Experiment

Magnetic domains



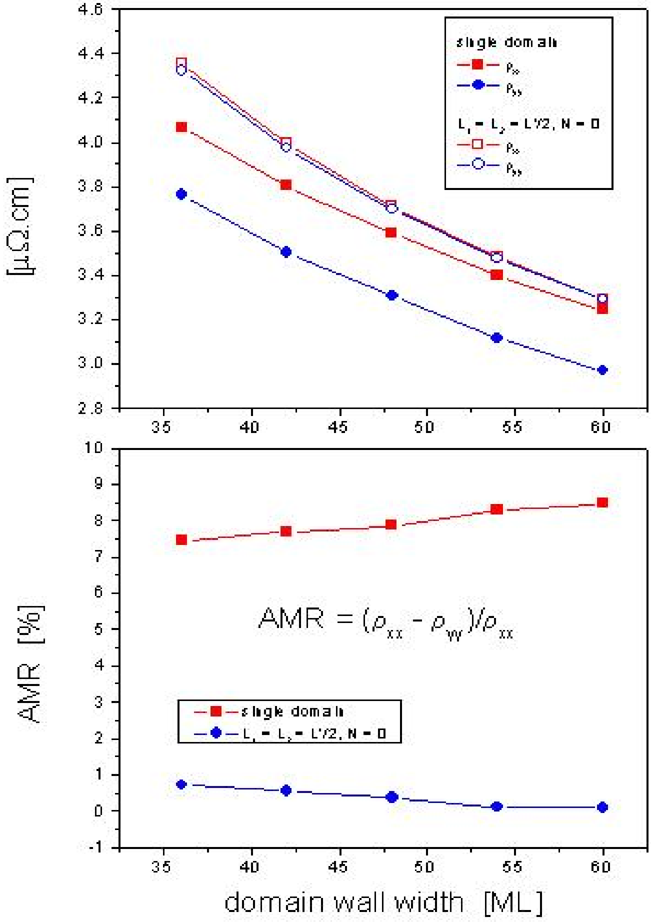
180^0 domains



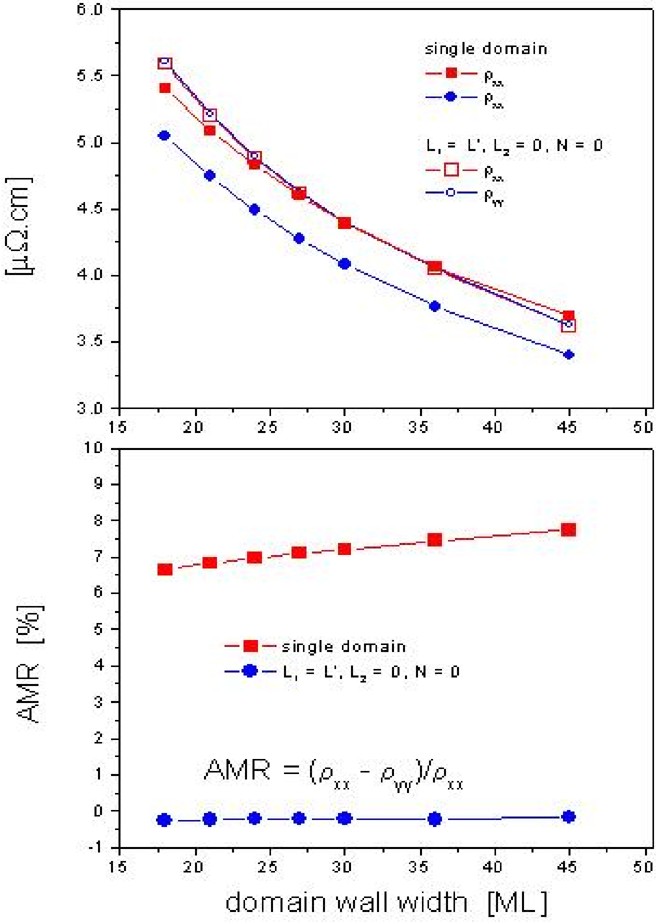
90^0 domains

CIP-AMR in permalloy domain walls

180^0 domain wall



90^0 domain wall



Exchange bias

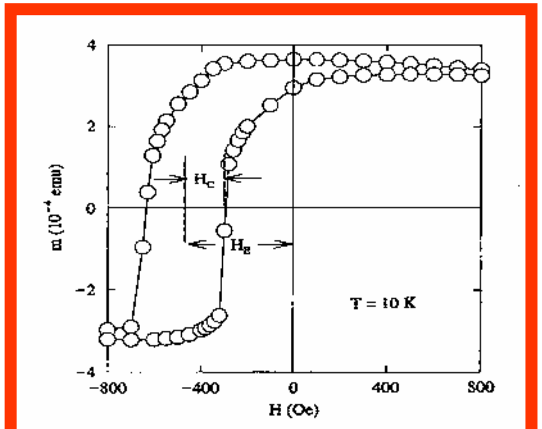


Fig. 1. Hysteresis loop, $m(H)$, of a FeF_2/Fe bilayer at $T = 10$ K after field cooling [72]. The exchange bias, H_E, and the coercivity, H_C, are indicated in the figure.

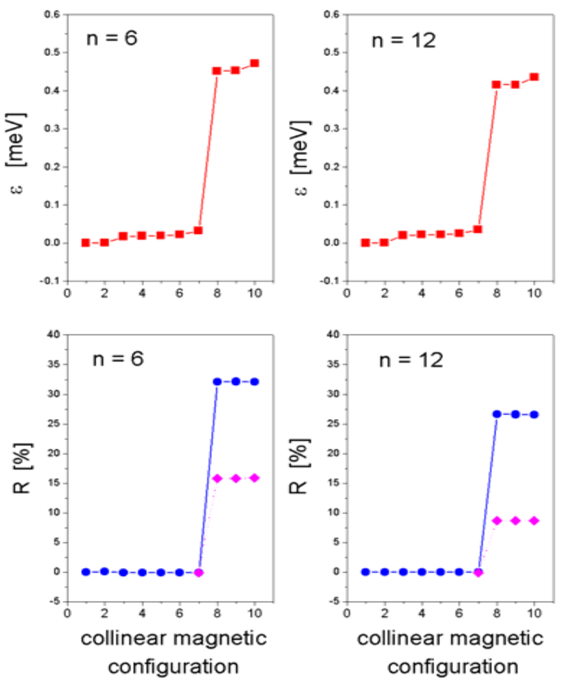
AFM/FM systems: Magnetic pinning

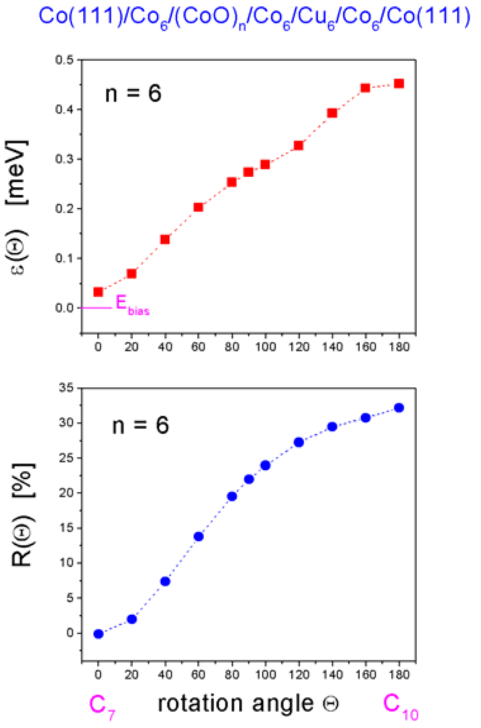
Exchange bias for GMR-devices:

$0 < E < E_{bias} : R(E) = 0$

$E > E_{bias} : R(E) > 0$

E: interlayer exchange energy



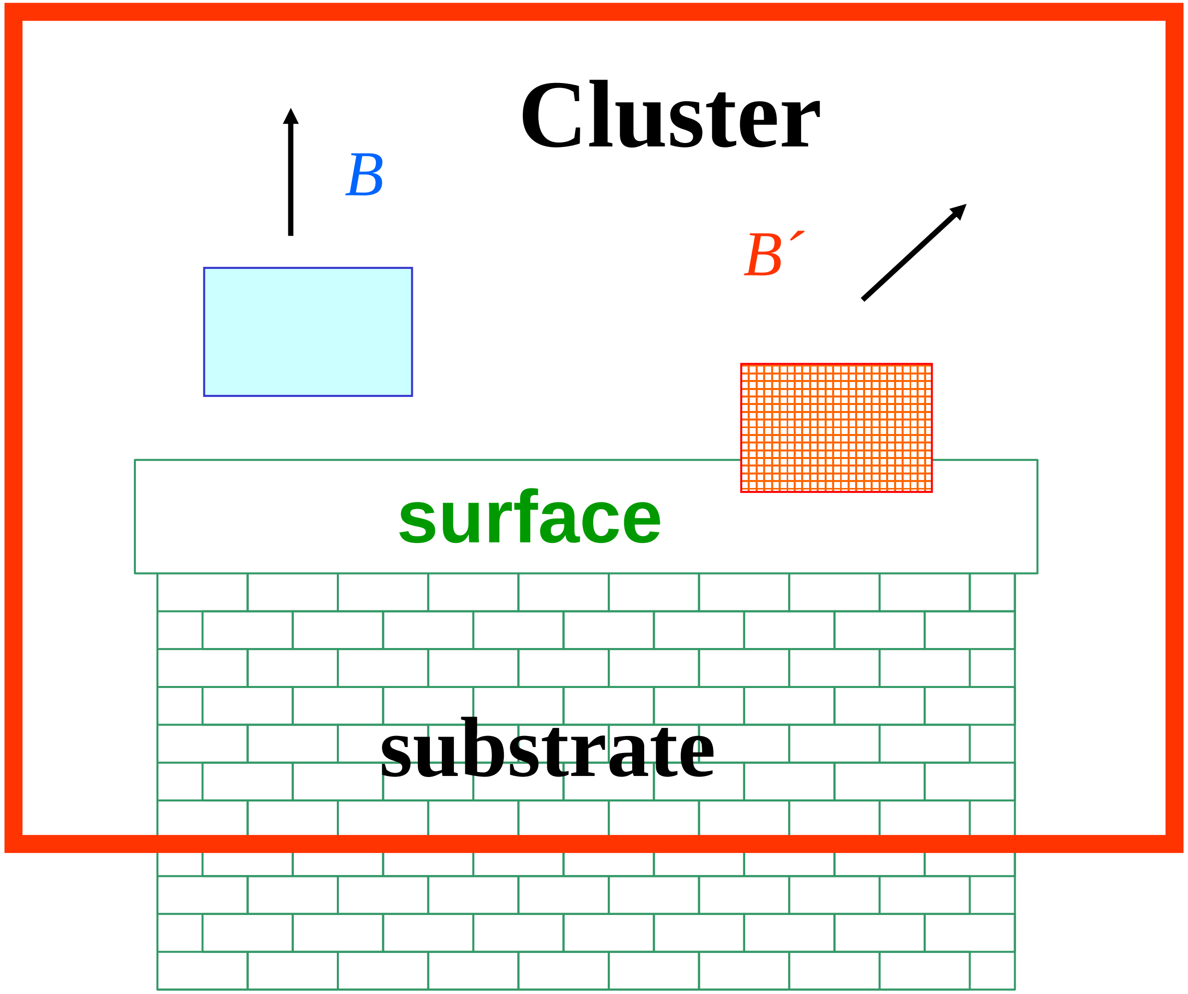


CoO/Co:

E_{bias}(exp.) < 9.5 kO

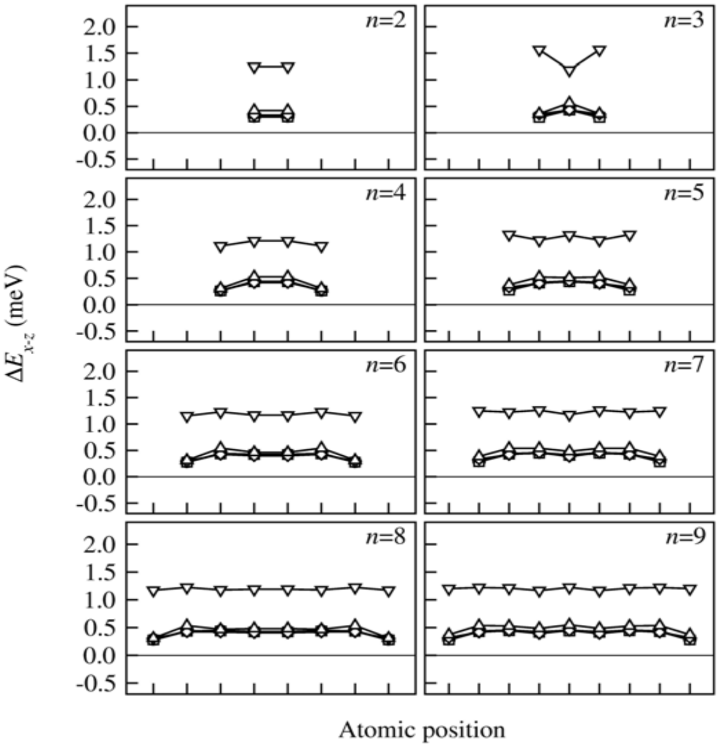
E_{bias} (theor.) = 6 kO

Nanostructures

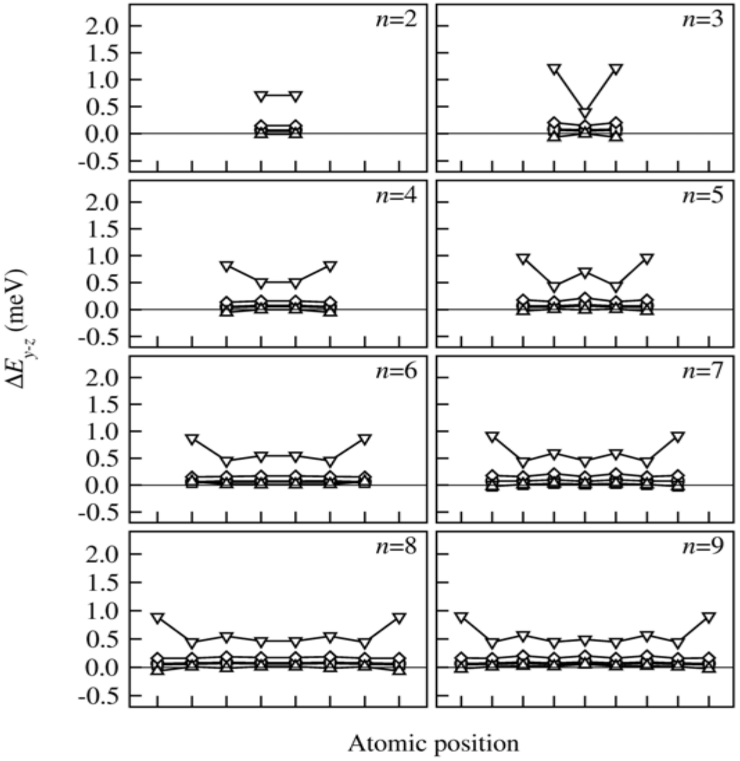


Magnetic anisotropy of nanostructures

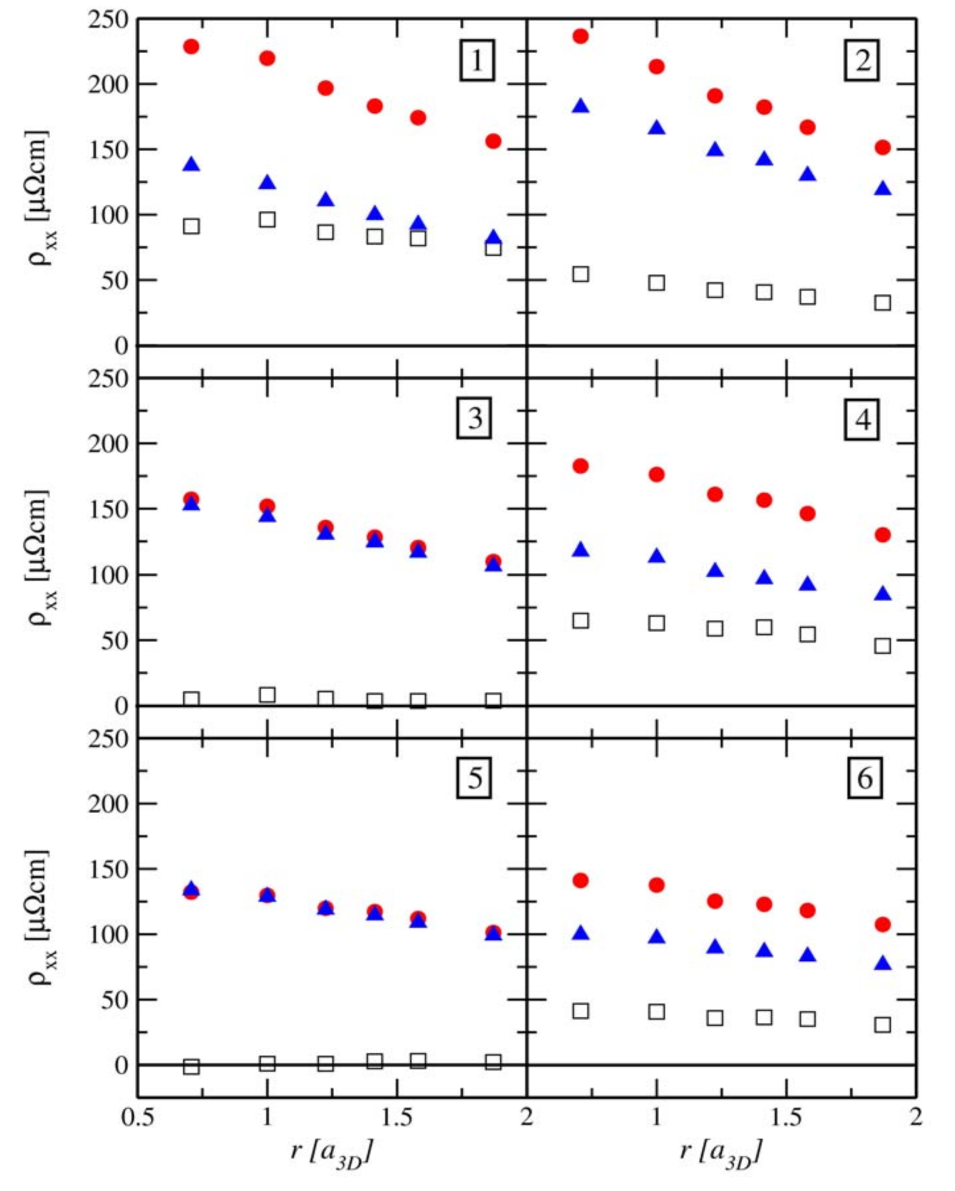
Fe$_n$/Cu(100)



Fe$_n$ /Cu(111)

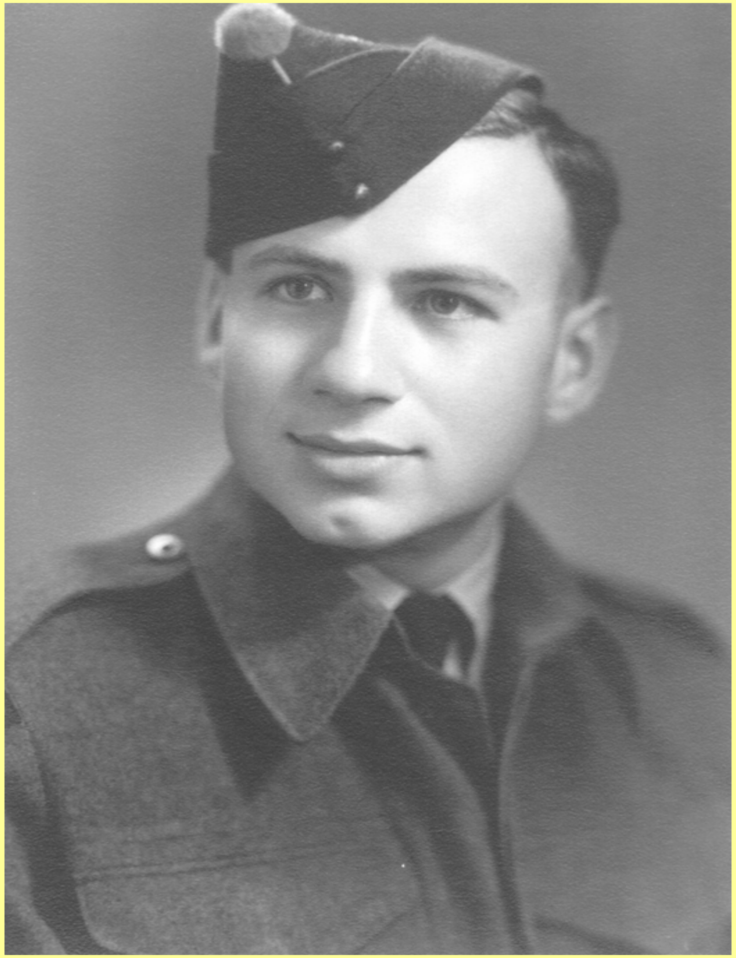


Electric properties of nanostructures



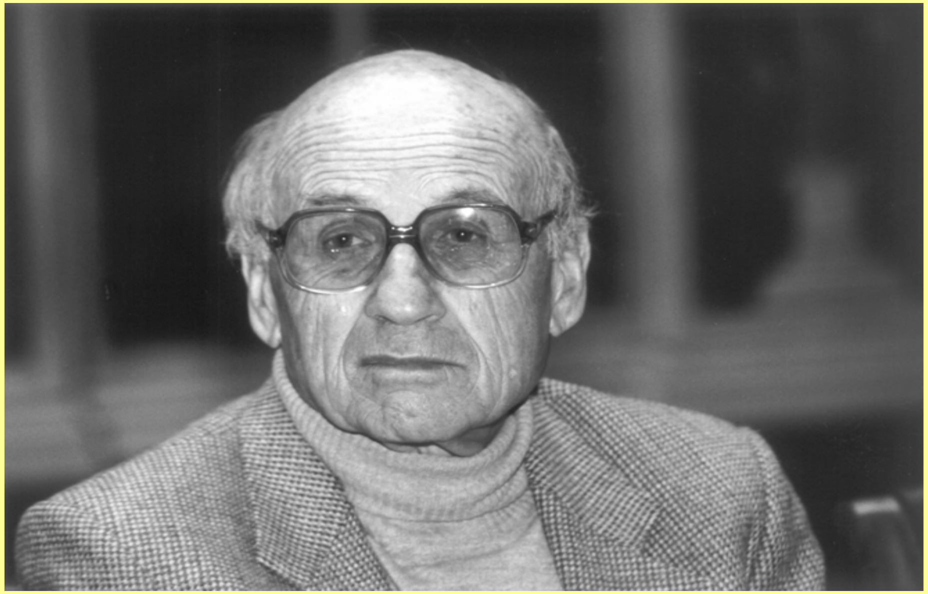
Residual resistivities of finite chains of Fe (circles) and Co (triangles) atoms embedded in the surface plane of Ag(100). Open squares refer to the difference between the Fe and the Ni residual resistivity. The length of the chains is shown explicitly.

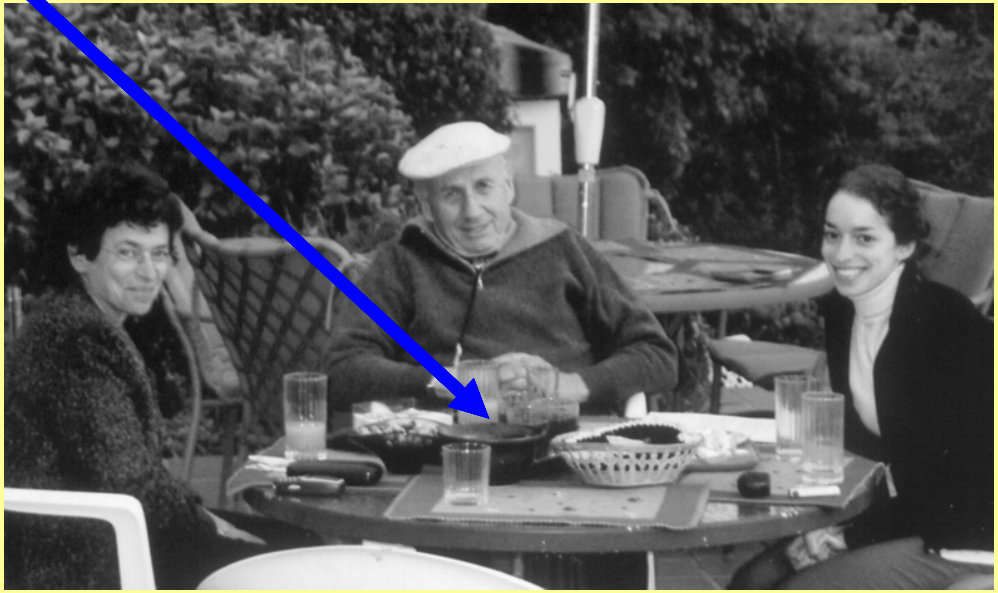
Time-dependent DFT-1



Time-dependent DFT-2

The famous WK-guacamole





- 5

- 1/2

t, [a]