Introduction to Magnetism and Magnetic Materials

Jaejun Yu

School of Physics, Seoul National University

jyu@snu.ac.kr

KIAS-SNU Physics Winter Camp

5-18 January 2005

Abstract

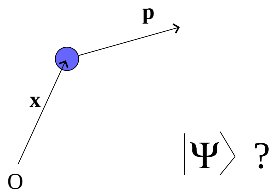
In this lecture,[1] I will give a brief introduction on a quantum mechanical view on magnetism in real materials, especially, consisting of transition metal elements and their compounds, and the physical principles for the applications of magnetic materials as magnetic sensors and memory devices. Further, I will discuss the connection between magnetism and superconductivity in high T_c superconductors as an example.

[1]This lecture is support by KIAS and SNU-CTP.

Contents

1. What is all about condensed matter physics?

... How do we understand the physical properties of single particle systems in a classical or quantum sense? In other words, what do we measure or observe?



... In classical dynamics, the state of a single particle is determined by the observables $\{\mathbf{x}(t), \mathbf{p}(t)\}$. It can be extended to the system with many particles where the state of the system is described by the set of observables $\{\mathbf{x}_i(t), \mathbf{p}_i(t) | i = 1, 2, ..., N\}$. However, when $N \sim 10^{25}$, it is practically impossible to trace the orbits of all, even the part of, the particles. Here it is the point where the statistical physics comes into playing a role. Instead of following each individual particles, we measure a quantity by an (ensemble or time) average of the given quantities adopted in classical dynamics. In addition, now we have to deal with new observables such as entropy, temperature, ...

The same thing applies for the case of quantum systems. The only difference is the dynamics state of the quantum system is determined by a state vector $|\psi(\mathbf{x}, t)\rangle$ for a single particle and $|\Psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N, t)\rangle$.

1.1. Macroscopic vs. microscopic objects

- Observables for the macro object consisting of more than $\sim 10^{20}$ particles:
  - specific heat $c_v \longleftarrow$ entropy, temperature
  - bulk modulus or compressibility $\kappa \longleftarrow$ pressure P
  - polarization $\mathbf{P}$, magnetization $\mathbf{M} \longleftarrow$ electro-magnetic field $\mathbf{E}$, $\mathbf{B}$
  - reflectivity, color, conductivity, ... etc.

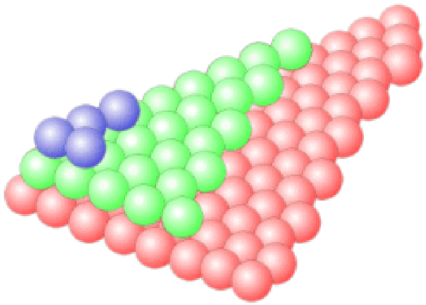
For an example, what physical property of the cube (or disk) makes this happen, i.e., a cube float over a magnet against gravitation?

(Hint: This is the phenomenon called magnetic levitation, which is mainly attributed to the "Meisner effect" of superconductors.)

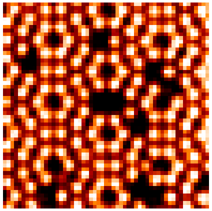
Jaejun Yu, <jyu@snu.ac.kr>

Observables for the micro or nano object of order $\sim 10^2$ particles:

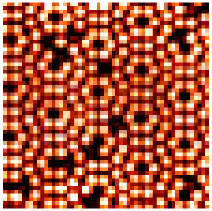


- conductance G / electron tunneling current I
- force $\mathbf{F}$
- magnetic Flux Φ
- charge density distribution, electron cloud (bonding), ... etc.

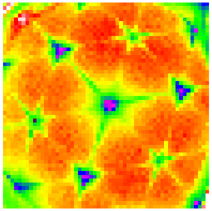
an AFM image



an STM image



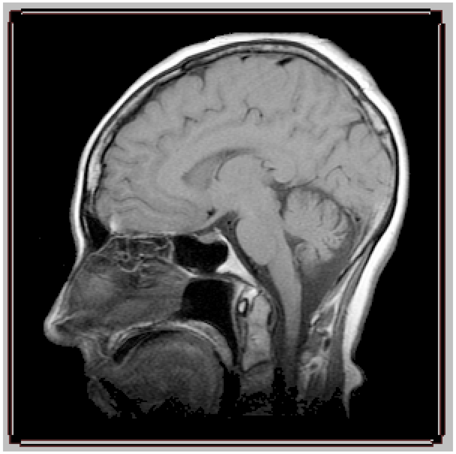
a LEED image



What do we really see in these images?
What physical quantities do they represent?

An example of the SEM System:

MRI Image: What do we really see in this image?
What physical quantity does it represent?



(This is an image of our brain probed by using the technique of the nuclear magnetic resonance.)

1.2. Most condensed matter systems are quantum mechanical by nature!

$$\lambda \sim \frac{\hbar}{p} \sim d$$

- Unfortunately, however, there is no quantum mechanical solution available except for free (i.e., non-interacting) particle systems.

- An example of exactly solvable models:

$$\mathcal{H} = \hbar\omega(a^+ a + \frac{1}{2})$$

$$a^+ a|n\rangle = n|n\rangle$$

$$a|O\rangle = 0$$

1.3. How do we approach the condensed matter system in order to understand the physics of a “black box”?

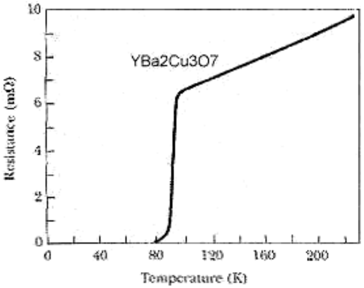
- Experimental Methods:
  By disturbing the black box by phtons, phonons, electrons, and/or neutrons, try to get a hint on elementary excitations in the system.

- Theoretical Methods:
  By guessing possible elementary excitations and working out the QM equation of motions, see if we can predict the physics of the system. If wrong, correct the model for the elementary excitations for the better description.

- How to disturb the “black box”?

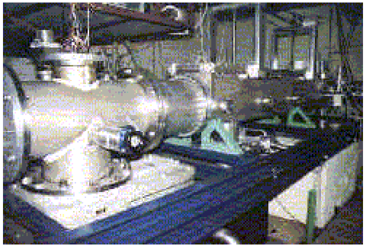
Question: Measuring the dc resistance is a way of disturbing the system? What really happens inside the black box when we apply a bias voltage?

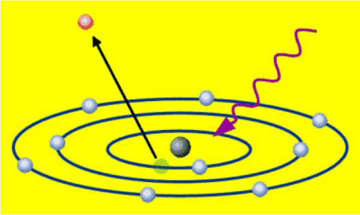
♠ Current-Voltage curve of a YBCO high T_c superconductor



Question: What happens when we shine a light on the matter?

Light scattering experiment: (Photoemission / IR spectroscopy)





Jaejun Yu, <jyu@snu.ac.kr>

1.4. Particle zoo in the condensed matter systems

"elementary excitations in solids"

- quasi-particles: electrons, holes, polarons, excitons, Cooper pairs, ...
- collective excitations: phonons, magnons, zero-sound, plasmons, ...

1.5. Energy scale

The condensed matter system is merely a collection of atoms, where each atom consists of electrons and a nucleus ($m_e \ll m_N$).

From the uncertainty principle $\Delta x \Delta p \sim \hbar$,

$$\Delta p = \sqrt{2m_e E} \approx \sqrt{3mk_B T}$$

Thus, practically, the size of atom $\approx$ the size of electrons.

- atomic unit: $\hbar = e^2 = m_e = 1$

$$\Delta x \approx a_B = \frac{\hbar^2}{me^2} = 0.529177\text{Å (Bohr radius)}$$

$$E_B = -\frac{1}{2}\frac{e^2}{a_B} = -\frac{me^4}{2\hbar^2} = -13.6058\text{eV} = -1\text{Ry}$$

In atomic unit, $a_B = 1$, $E_B = -1/2$, $c = 1/\alpha \approx 137$,
$k_B \approx 3.2 \times 10^{-6}\mathrm{K}^{-1}$
$\mu_B = 2.13 \times 10^{-6}\mathrm{T}^{-1}$, ...

($\alpha = e^2/\hbar c$: fine structure constant)

Jaejun Yu, <jyu@snu.ac.kr>

- energy of an electron in a box of size L:

$$\Delta x \sim L \quad \longrightarrow \quad \Delta p \approx \frac{\hbar}{L}$$

$$E_o = \frac{p^2}{2m} \approx \frac{1}{2L^2}$$

- speed of electrons in a box:

$$v_e \sim \frac{1}{L} \sim \frac{\alpha c}{L}$$

- electrons in solid
  - Fermions: Pauli exclusion principle
  - Degenerate Electrons: lowest possible excitations near the Fermi energy

Jaejun Yu, <jyu@snu.ac.kr>

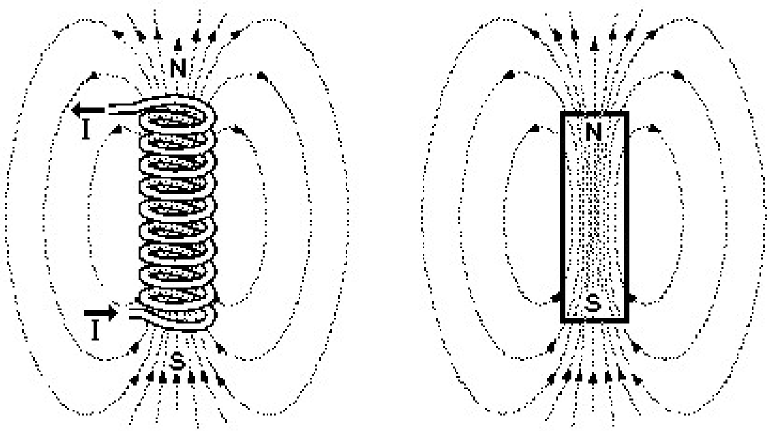
Energy Scale

- Coulomb interaction: $\sim$ eV
- Magnetic ordering temperature T_c: 0.1 meV $\sim$ 50 meV
- Dipole-dipole interaction: $\sim$ 0.1 meV

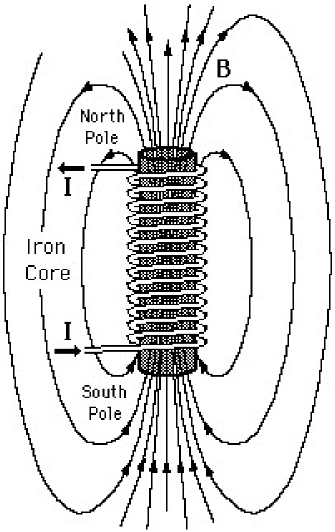
2. Magnetism in Real Materials

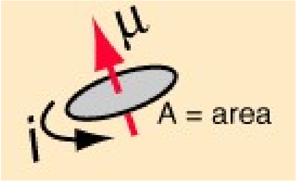
Magnets

Solenoid vs. Bar Magnet



Origin of Magnetic Moments

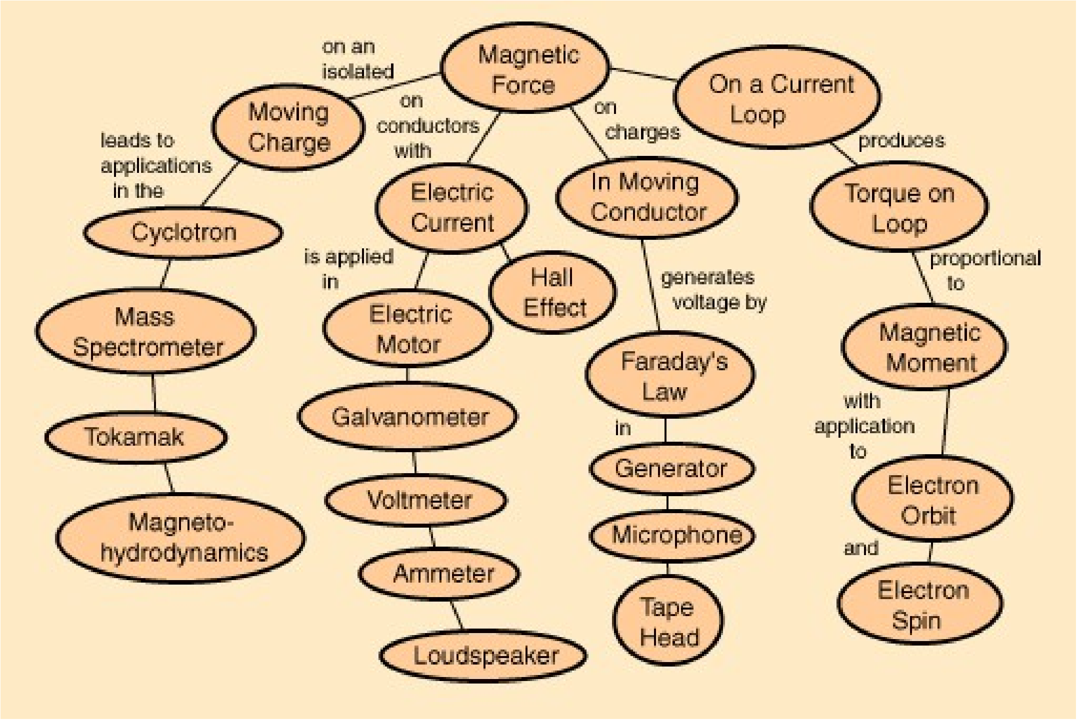




Magnetic permeability and origin of magnetic moments?

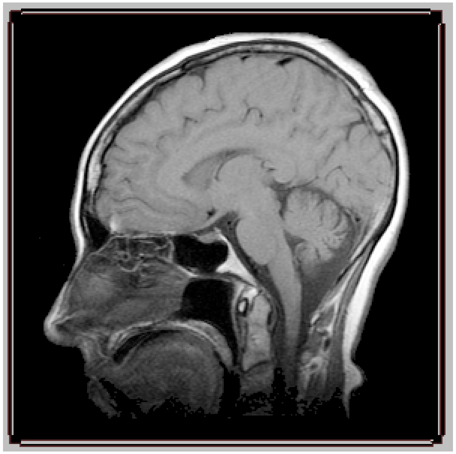
Jaejun Yu, <jyu@snu.ac.kr>

Magnetic Diagram



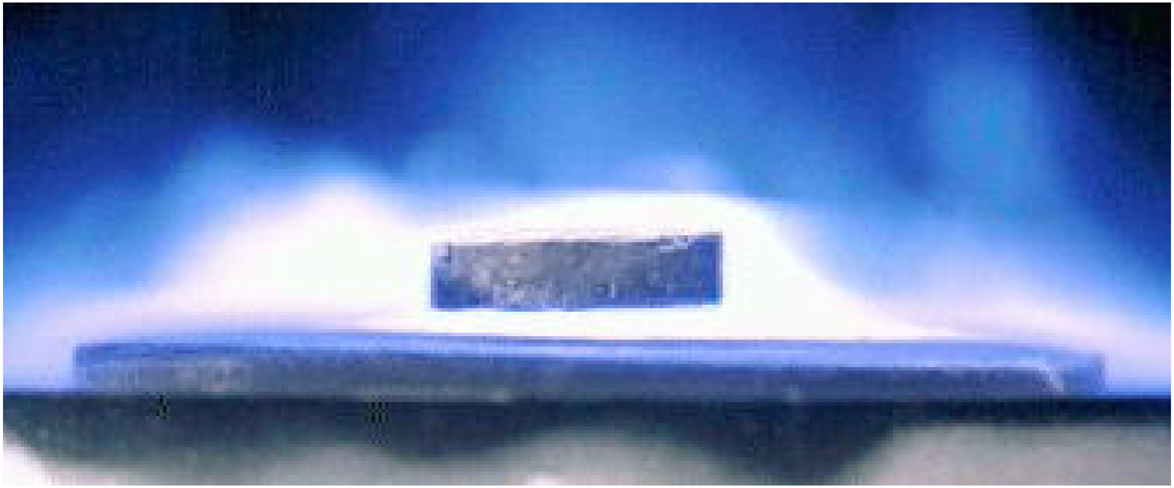
Magnetic Image of Our Brain

MRI (Magnetic Resonance Imaging) using the NMR technique



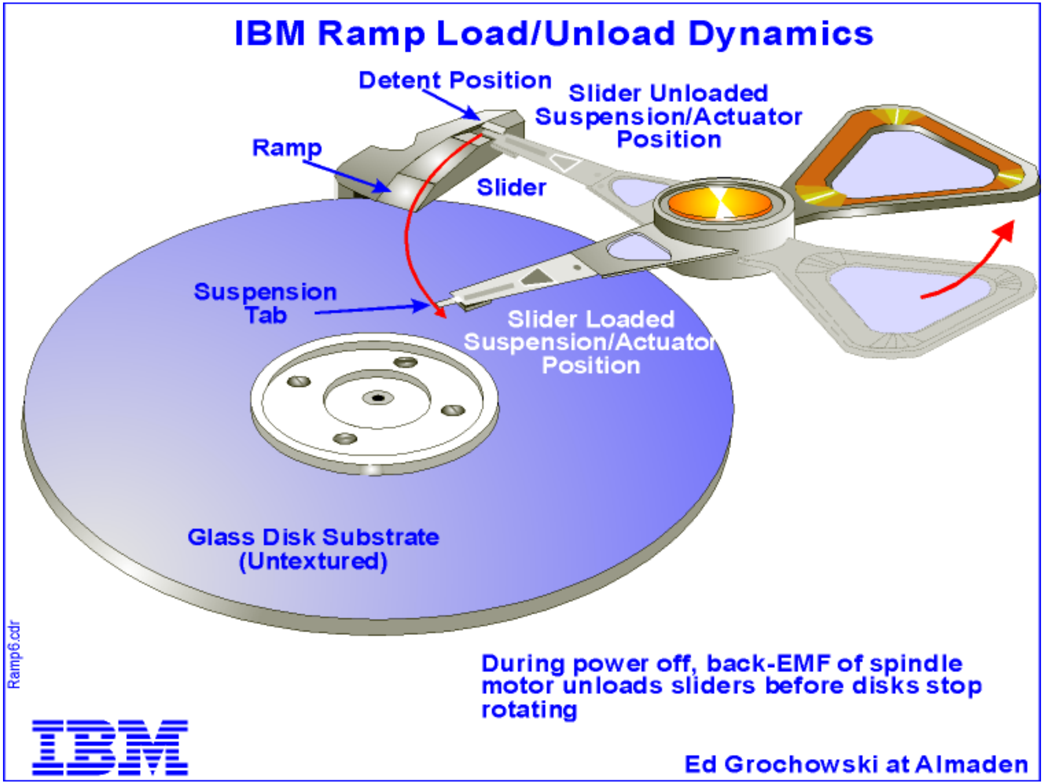
→ **Mapping of Proton Spin Resonance Frequencies**

Levitating magnetic bar on a superconducting bed

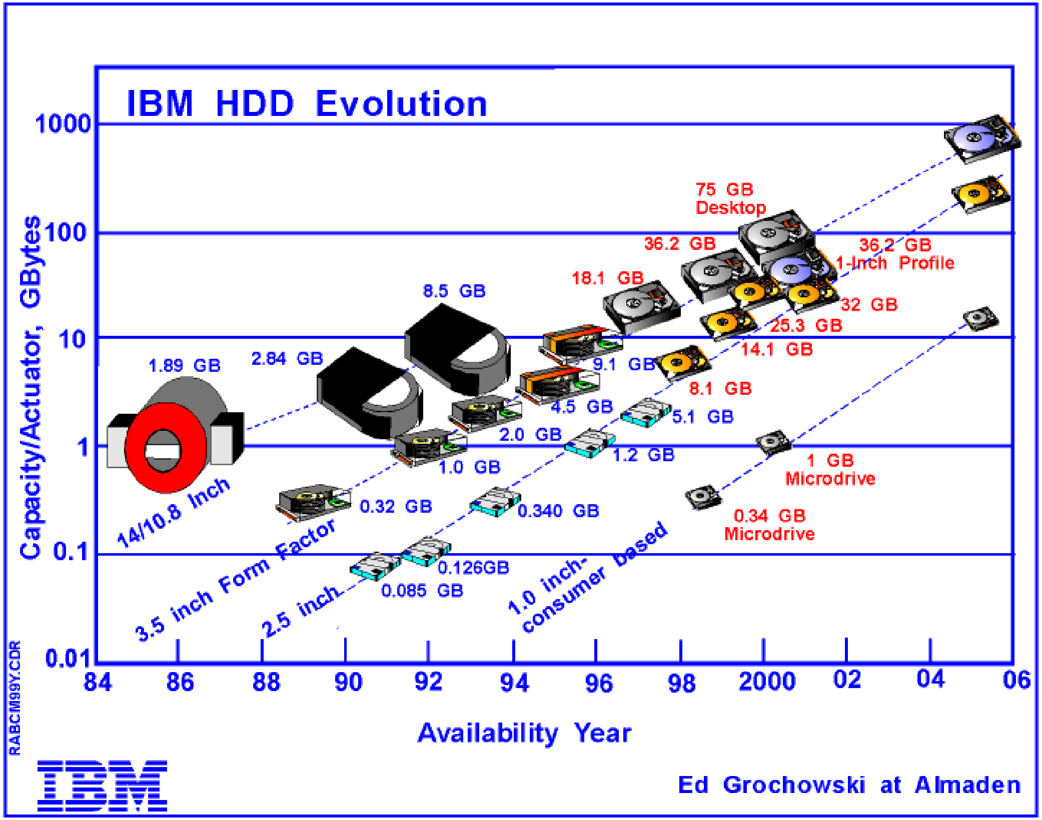


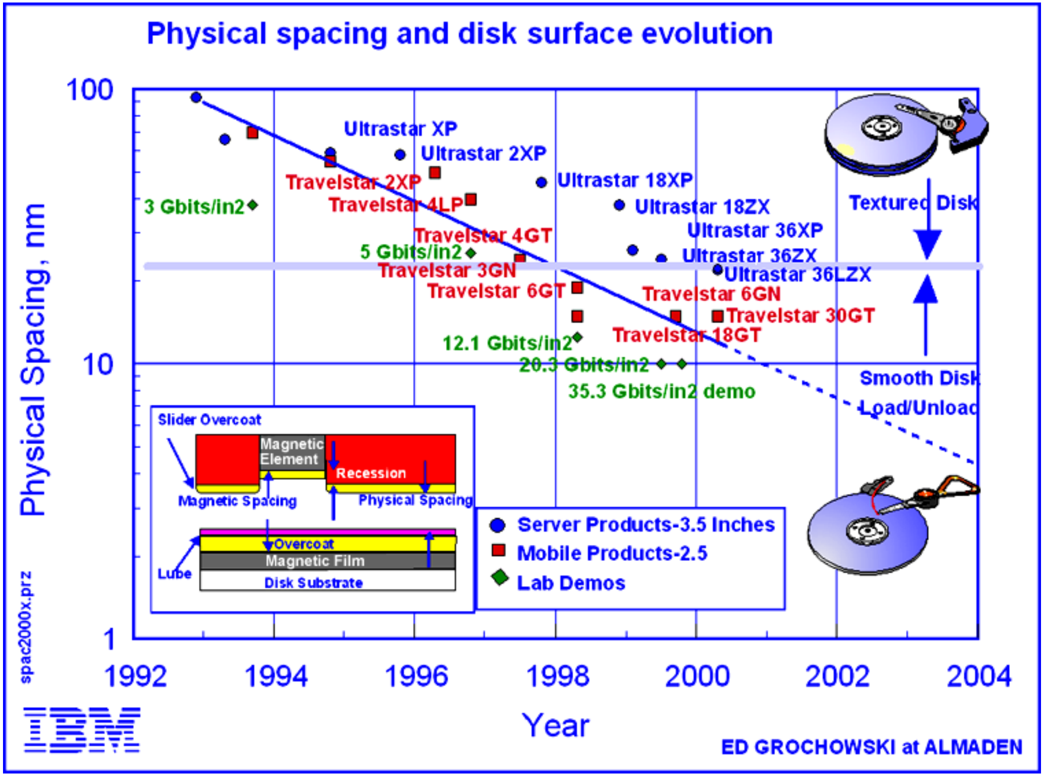
Magnetic shielding by the superconducting current

2.1. Magnetic Storages

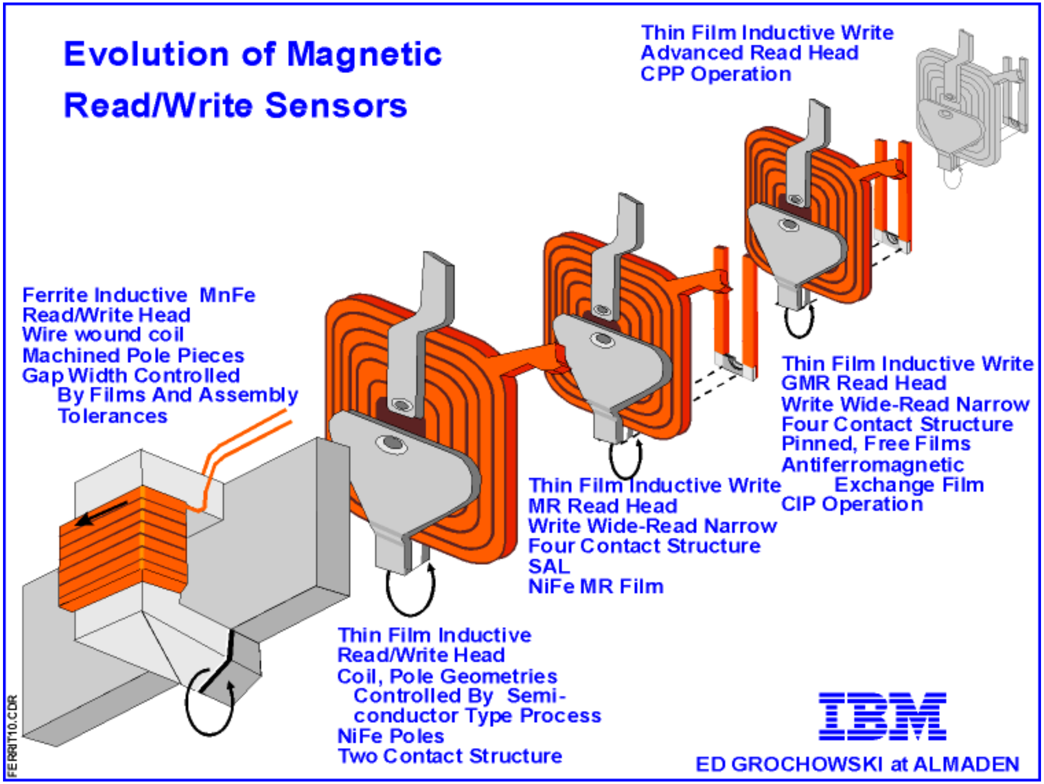


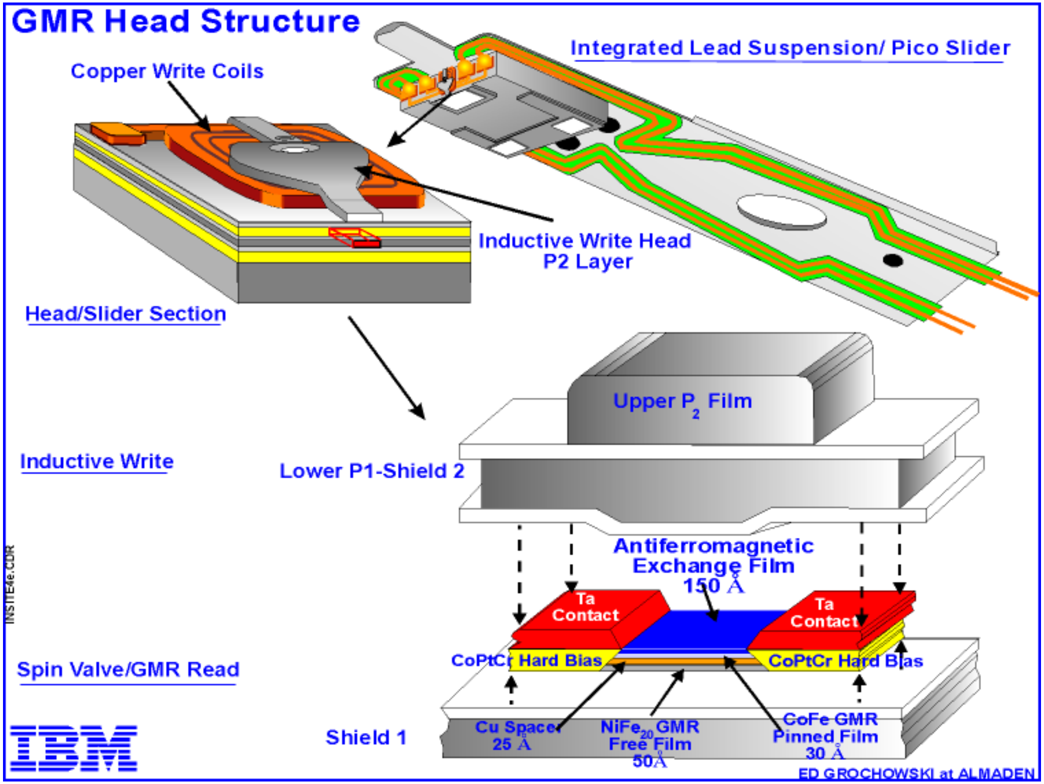
Magnetic thin films

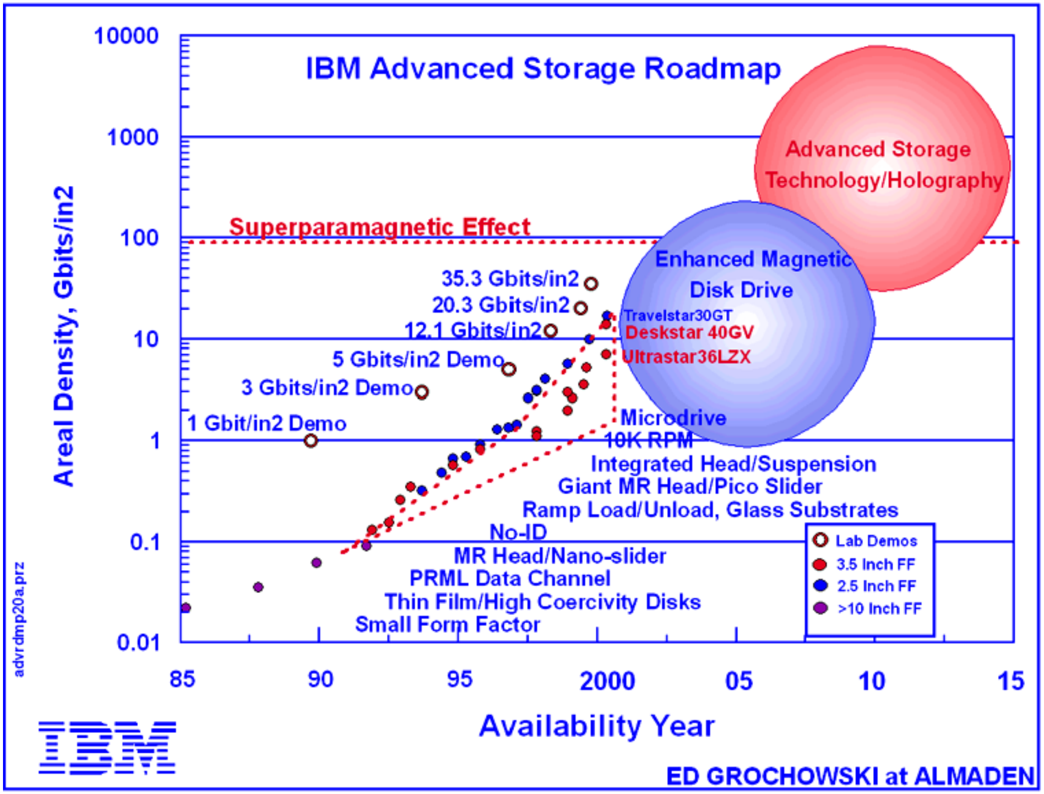

IBM HDD Evolution
Capacity/Actuator, GBytes
1000
100
10
1
0.1
0.01
84
86
88
90
92
94
96
98
2000
02
04
06
Availability Year
1.89 GB
2.84 GB
8.5 GB
18.1 GB
36.2 GB
75 GB
Desktop
36.2 GB
1-Inch Profile
32 GB
25.3 GB
14.1 GB
9.1 GB
8.1 GB
4.5 GB
5.1 GB
2.0 GB
1.2 GB
1.0 GB
0.32 GB
0.340 GB
0.126GB
0.085 GB
1 GB
Microdrive
0.34 GB
Microdrive
14/10.8 Inch
3.5 inch Form Factor
2.5 inch
1.0 inch-
consumer based
RABCM99Y.CDR
IBM
Ed Grochowski at Almaden


Physical spacing and disk surface evolution
100
10
1
Physical Spacing, nm
1992
1994
1996
1998
2000
2002
2004
Year
Ultrastar XP
Ultrastar 2XP
Ultrastar 18XP
Ultrastar 18ZX
Ultrastar 36XP
Ultrastar 36ZX
Ultrastar 36LZX
Travelstar 2XP
Travelstar 4LP
Travelstar 4GT
Travelstar 3GN
Travelstar 6GT
Travelstar 6GN
Travelstar 30GT
Travelstar 18GT
3 Gbits/in2
5 Gbits/in2
12.1 Gbits/in2
20.3 Gbits/in2
35.3 Gbits/in2 demo
Textured Disk
Smooth Disk
Load/Unload
Slider Overcoat
Magnetic Element
Recession
Magnetic Spacing
Physical Spacing
Overcoat
Magnetic Film
Lube
Disk Substrate
Server Products-3.5 Inches
Mobile Products-2.5
Lab Demos
spac2000x.prz
IBM
ED GROCHOWSKI at ALMADEN

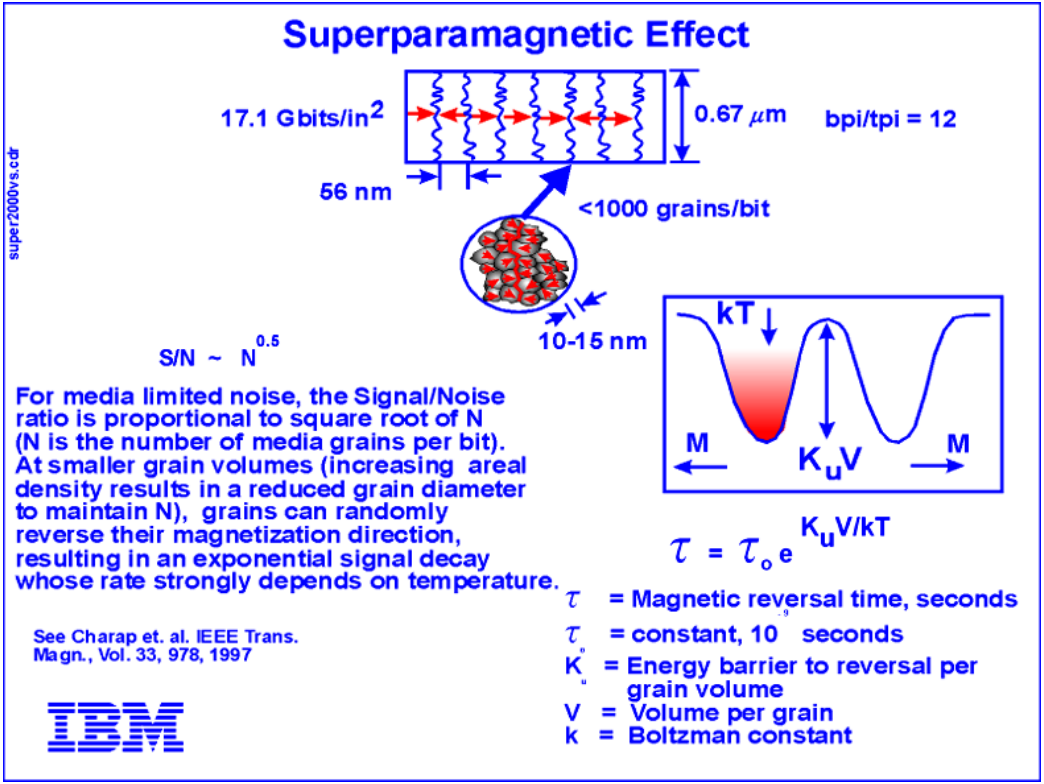
2.2. Magnetic Sensors




GMR Head Structure
Integrated Lead Suspension/ Pico Slider
Copper Write Coils
Inductive Write Head
P2 Layer
Head/Slider Section
Upper P2 Film
Inductive Write
Lower P1-Shield 2
Antiferromagnetic
Exchange Film
150 Å
Ta
Contact
Ta
Contact
CoPtCr Hard Bias
CoPtCr Hard Bias
Spin Valve/GMR Read
Shield 1
Cu Spacer
25 Å
NiFe20 GMR
Free Film
50Å
CoFe GMR
Pinned Film
30 Å
INSITE4e.CDR
ED GROCHOWSKI at ALMADEN



IBM Advanced Storage Roadmap
Areal Density, Gbits/in2
10000
1000
100
10
1
0.1
0.01
Superparamagnetic Effect
Advanced Storage Technology/Holography
Enhanced Magnetic Disk Drive
35.3 Gbits/in2
20.3 Gbits/in2
12.1 Gbits/in2
5 Gbits/in2 Demo
3 Gbits/in2 Demo
1 Gbit/in2 Demo
Travelstar30GT
Deskstar 40GV
Ultrastar36LZX
Microdrive
10K RPM
Integrated Head/Suspension
Giant MR Head/Pico Slider
Ramp Load/Unload, Glass Substrates
No-ID
MR Head/Nano-slider
PRML Data Channel
Thin Film/High Coercivity Disks
Small Form Factor
Lab Demos
3.5 Inch FF
2.5 Inch FF
>10 Inch FF
advrdmp20a.prz
85
90
95
2000
05
10
15
Availability Year
IBM
ED GROCHOWSKI at ALMADEN


Superparamagnetic Effect
17.1 Gbits/in2
0.67 µm
bpi/tpi = 12
56 nm
<1000 grains/bit
10-15 nm
super2000vs.cdr
S/N ~ N0.5
For media limited noise, the Signal/Noise ratio is proportional to square root of N (N is the number of media grains per bit). At smaller grain volumes (increasing areal density results in a reduced grain diameter to maintain N), grains can randomly reverse their magnetization direction, resulting in an exponential signal decay whose rate strongly depends on temperature.
kT
M
KuV
M
τ = τo e KuV/kT
τ = Magnetic reversal time, seconds
τo = constant, 10-9 seconds
Ku = Energy barrier to reversal per grain volume
V = Volume per grain
k = Boltzman constant
See Charap et. al. IEEE Trans. Magn., Vol. 33, 978, 1997
IBM

super2000vt.cdr

Attacking Superparamagnetism

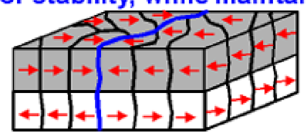
Media

1. Increase media coercivity (increases K_u to compensate for a reduced V)

$$\tau = \tau_o e^{K_u V/kT}$$

Involves new magnetic materials

2. Exchange coupled media (effectively increases V for stability, while maintaining S/N, $Mr\delta$)



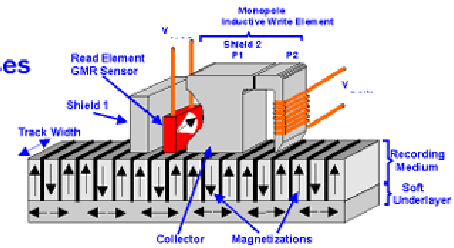
See Doerner et. al. IEEE Intermag Conf. Proceedings, Toronto, April 2000

3. Patterned media

Heads

4. Reduce BAR (Bit aspect ratio) 20 ----> 4

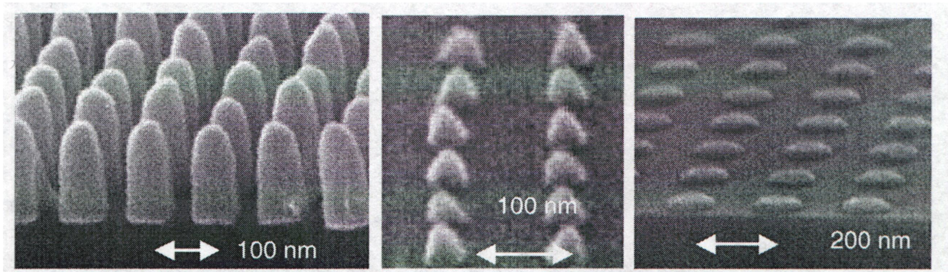
5. Perpendicular recording

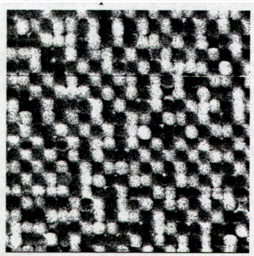


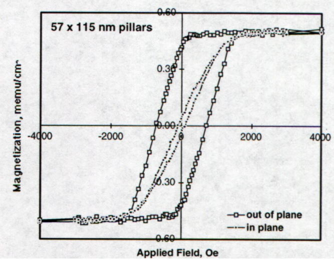
Reduces demagnitizing influence of adjacent bit fields, minimizes transition parameter. Involves new head configuration, return path soft underlayer, NiFe in media.

IBM

MFM (Magnetic Force Microscopy) Image of Nanomagnet Array
(C. A. Ross, MIT)



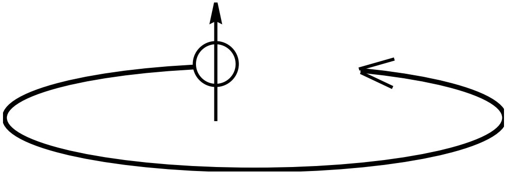




3. A quantum mechanical view of magnets: Pauli exclusion principle and Coulomb interactions

3.1. Sources of Magnetic Moments

- Magnetic moment: $\mathcal{M} = g\mu_B \mathbf{J}$
  proportional to the angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$
  - Spin moment $\mathbf{S}$
  - Orbital moment $\mathbf{L}$



Localized State

- Since the rotational symmetry is preserved, it has the quantum eigenstates $|jm\rangle$:

$$\mathbf{J}^2|jm\rangle = j(j+1)|jm\rangle$$

where

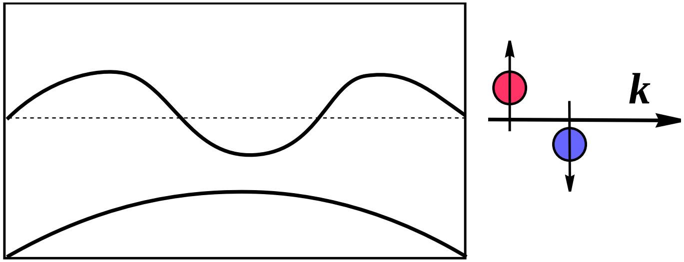
$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

- If the spherical symmetry is broken, e.g., inside a lattice, the orbital moment can be quenched due to the lack of rotational symmetry, i.e.,

$$\langle \mathbf{L} \rangle = 0$$

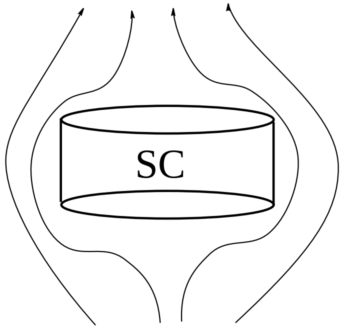
Delocalized State

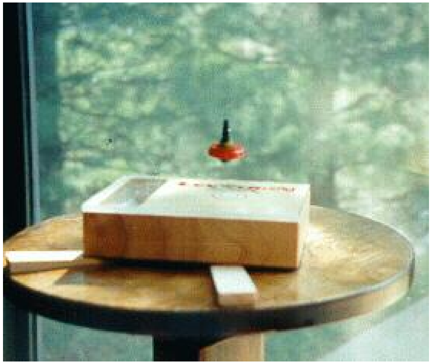
- A free electron state such as $|\mathbf{k}\rangle$ may not be an eigenstate of the angular momentum operator $\mathbf{L}$.
- Only $|sm_s\rangle$ may contribute to the magnetic moment.



- Exception: Diamagnetic shielding current in a superconducting state.

Perfect Diamagnetism: Superconductivity





- Inside the superconductor:

$$\mathbf{B} = 0$$

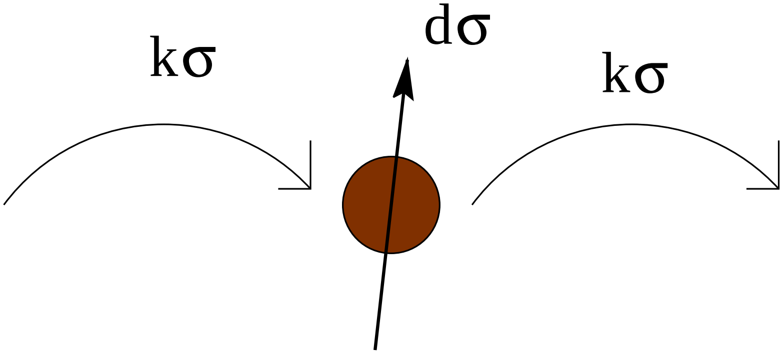
- Supercurrent induced by the current of Cooper pair electrons:

$$\mathbf{J}_s(\mathbf{r}) = \Lambda \cdot \mathbf{A}(\mathbf{r})$$

Jaejun Yu, <jyu@snu.ac.kr>

A Localized State Coupled to Delocalized States?

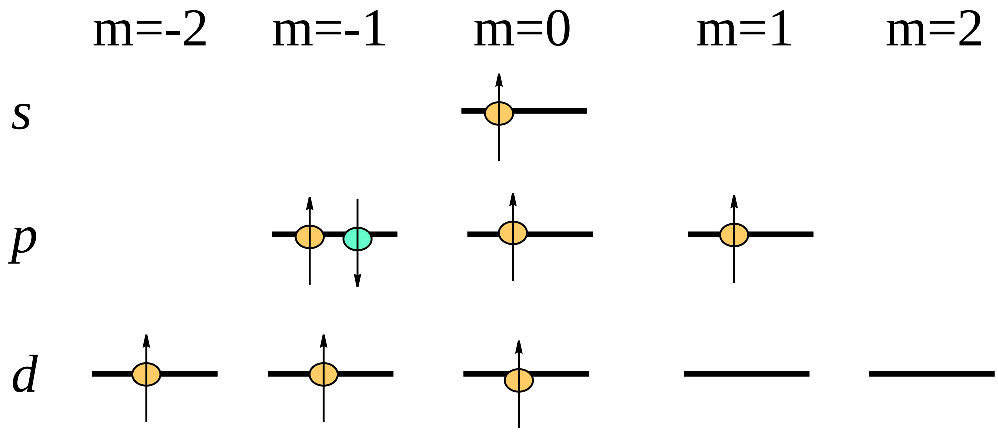
⇔ An impurity atom in a metal



Formation of a Local Moment ⇒ Broken Symmetry State!

Anderson Impurity Model

3.2. Magnetic Moment of an Atom



Hund's Rule

1. Maximum total $S = \max S_z$ with $S_z = \sum_i m_{si}$
   Obeying the Pauli exclusion principle
2. Maximum total $L = \max L_z$ with $L_z = \sum_i m_{li}$
   Minimizing the Coulomb interaction energy
3. Spin-orbit interaction:

$$J = \begin{cases} |L+S| & \text{if less than half-filled} \\ |L-S| & \text{if more than half-filled} \end{cases}$$

Jaejun Yu, <jyu@snu.ac.kr>

Exchange Energy

- Pauli exclusion principle: anti-symmetric two-particle wavefunction

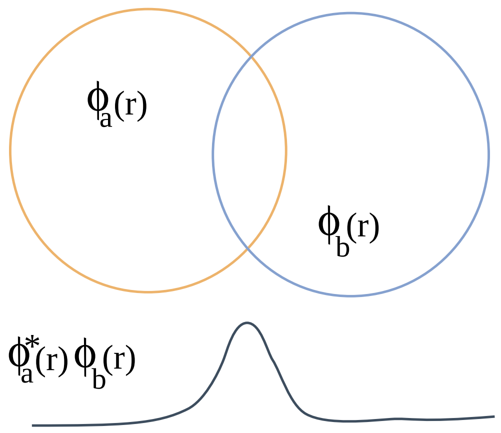
$$|\Psi(\mathbf{r}_1 \uparrow; \mathbf{r}_2 \uparrow)\rangle = \frac{1}{\sqrt{2}} [\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) - \phi_b(\mathbf{r}_1)\phi_a(\mathbf{r}_2)] \,|\uparrow\rangle |\uparrow\rangle$$

- Coulomb interaction

$$V_C(\mathbf{r}_1 - \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$\begin{aligned} E_{C2} &= \; < \Psi(1,2)|V_C|\Psi(1,2)\rangle \\ &= \int d\mathbf{r}_1 d\mathbf{r}_2 V_C(\mathbf{r}_1 - \mathbf{r}_2)|\phi_a(\mathbf{r}_1)|^2|\phi_b(\mathbf{r}_2)|^2 - \\ & \quad \int d\mathbf{r}_1 d\mathbf{r}_2 V_C(\mathbf{r}_1 - \mathbf{r}_2)\phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1) \\ &= U_{ab} - J_{ab} \end{aligned}$$

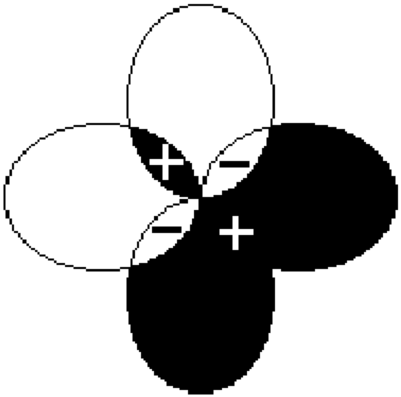
Exchange Density



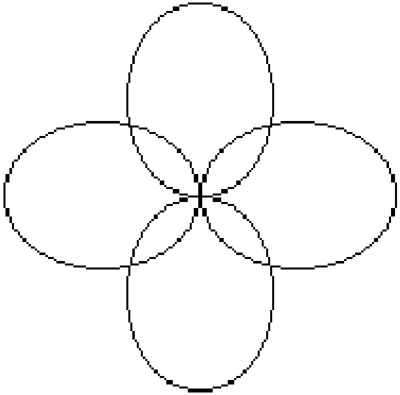
$\Rightarrow$ Gaining more (negative) exchange energy by aligning spins:

Hund's 1st rule

Overlap and Exchange Integrals of the atomic p-orbitals



$S_{ab} = 0$



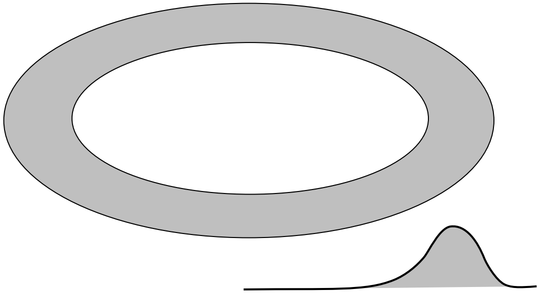
$K_{ab} > 0$

Jaejun Yu, <jyu@snu.ac.kr>

Minimization of Coulomb Energy Term U_{ab}

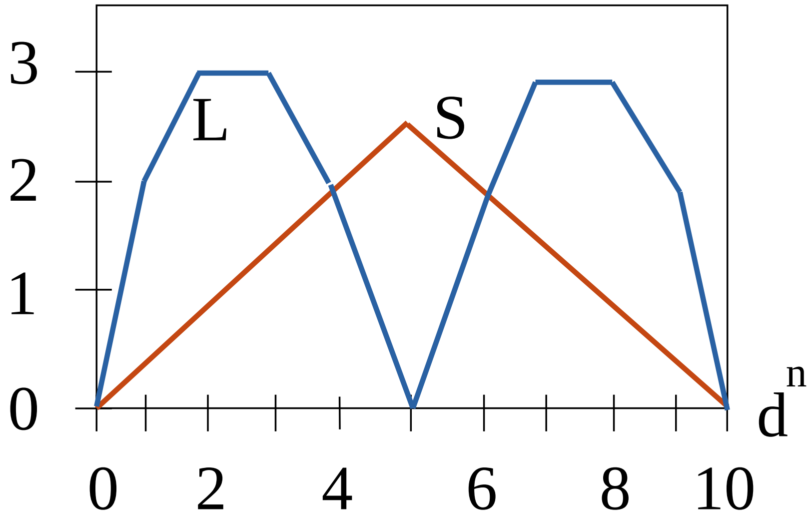
$\Rightarrow$ by letting $\rho(\mathbf{r})$ be separated: Hund's 2nd rule

$$Y_{lm}(\theta, \phi) = (-1)^m Y^*_{l-m}(\theta, \phi)$$



Jaejun Yu, <jyu@snu.ac.kr>

Configuration of 3d Transition Metal Ions



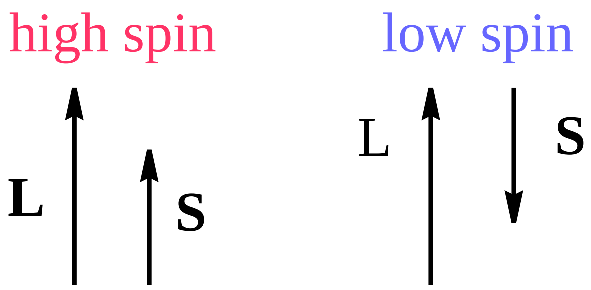
Spin-Orbit Coupling

$\Rightarrow$ determined by the sign of the coupling constant

$$\lambda \mathbf{L} \cdot \mathbf{S}$$

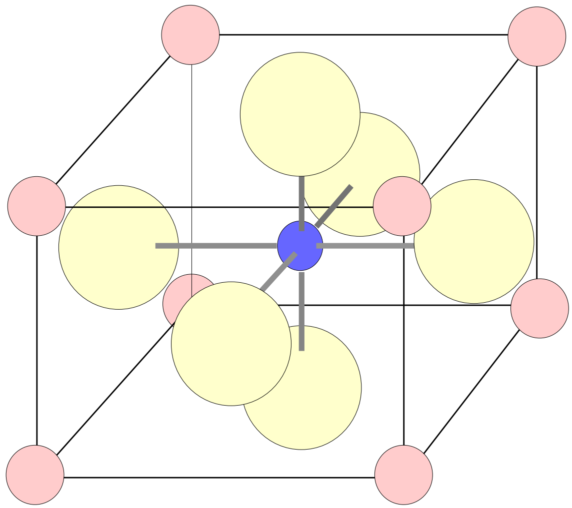
where

$$\lambda \sim -\frac{dV(r)}{dr}$$



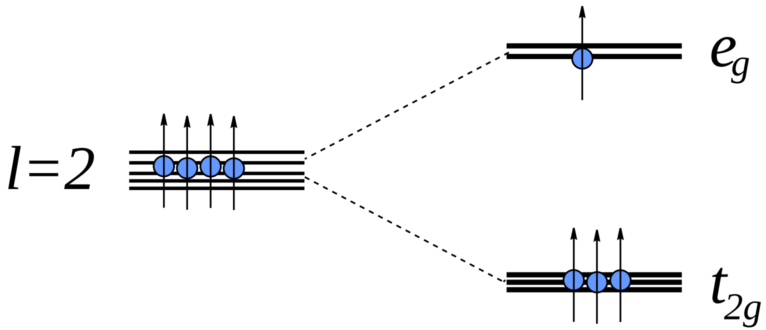
Jaejun Yu, <jyu@snu.ac.kr>

3.3. Magnetic Moments in Solids



Cubic Lattice Symmetry: Broken Spherical Symmetry

$\Rightarrow$ Crystal Field Splitting:



$$|e_g\rangle = \{|x^2 - y^2\rangle, |z^2 - r^2/3\rangle\}$$

$$|t_{2g}\rangle = \{|xy\rangle, |yz\rangle, |zx\rangle\}$$

Kinetic Energy vs. Coulomb Energy

- Uncertainty Principle:

$$\Delta p \approx \frac{\hbar}{\Delta x}$$

- Kinetic Energy:

$$E_K = \frac{p^2}{2m} \approx \frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}$$

- Coulomb Exchange Energy:

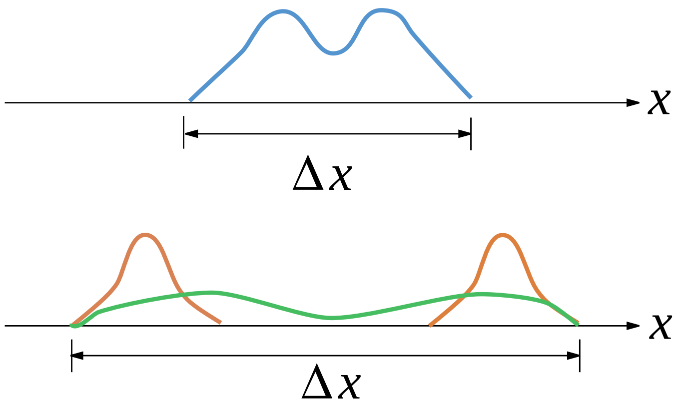
$$E_C \approx -A\frac{e^2}{\Delta x}$$

  where $A \sim 0.1$, an order of magnitude smaller than the direct Coulomb interaction energy.

When $\Delta x \gg 1$, the Coulomb energy dominates over the kinetic energy.

$\Rightarrow$ **Wigner solid: frozen localized electrons**

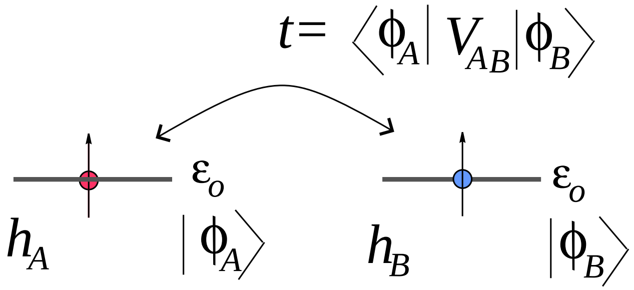
Wigner Crystal: Metal-Insulator Transition



Result of the competition between kinetic and Coulomb energy!

♠ Here we dropped the interaction term between electrons and background positive charge. What is it?

Delocalized State: Molecular / Band State

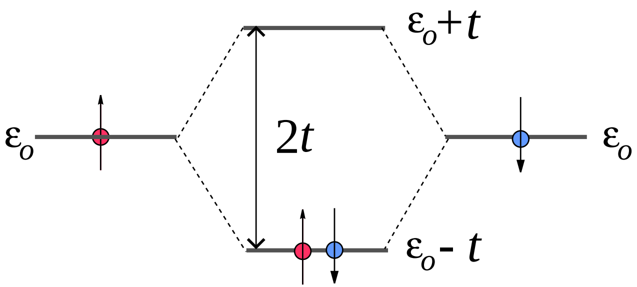


$$\mathcal{H}_o = h_A + h_B + V_{AB}$$

$$\mathcal{H}_o = \begin{pmatrix} \varepsilon_o & t \\ t & \varepsilon_o \end{pmatrix}$$

Single-particle eigenstates and eigenvalues:

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\phi_A\rangle \pm |\phi_B\rangle\right) \qquad \varepsilon_\pm = \varepsilon_o \pm t$$

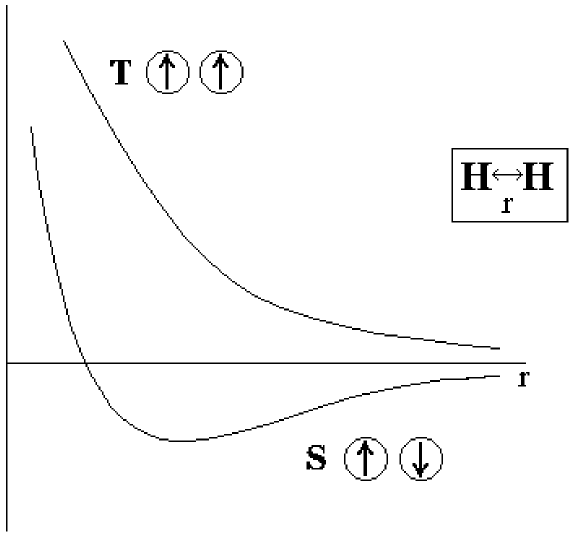


Corresponding two-particle state:

$$\Psi_2\rangle = \frac{1}{\sqrt{2}}\left[|\psi_+,\uparrow\rangle|\psi_+,\downarrow\rangle - |\psi_+,\downarrow\rangle|\psi_+,\uparrow\rangle\right]$$

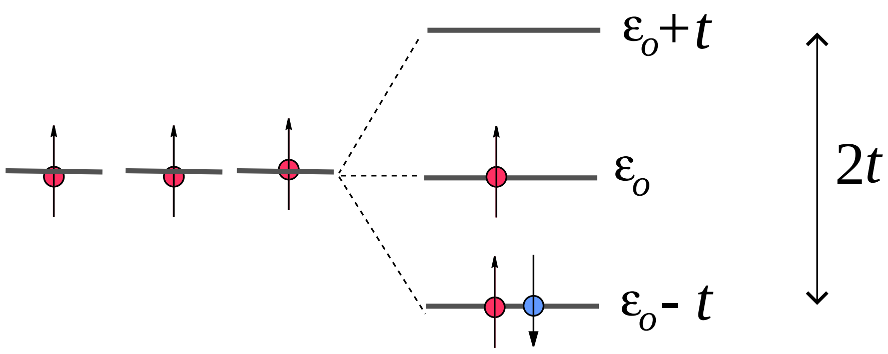
$\Rightarrow$ Spin-singlet ground state with single-particle molecular states $|\psi_\pm\rangle$

Energy Curve for a Hydrogen Molecule

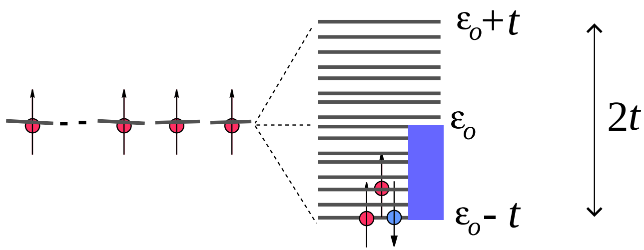


Consider two hydrogen atoms separated by a distance d. What are the ground states of this system in the limits of $d \to 0$ and $d \to \infty$? What is the dominating factor in each limit? Try to make a qualitative argument in describing the physics.
What about a lattice of hydrogen atoms with a lattice constant d? Discuss the possible physical properties of the lattice with varying d from ∞ to 0.

Three-Sites Molecular States



N-Sites States: Tight-Binding Energy Band



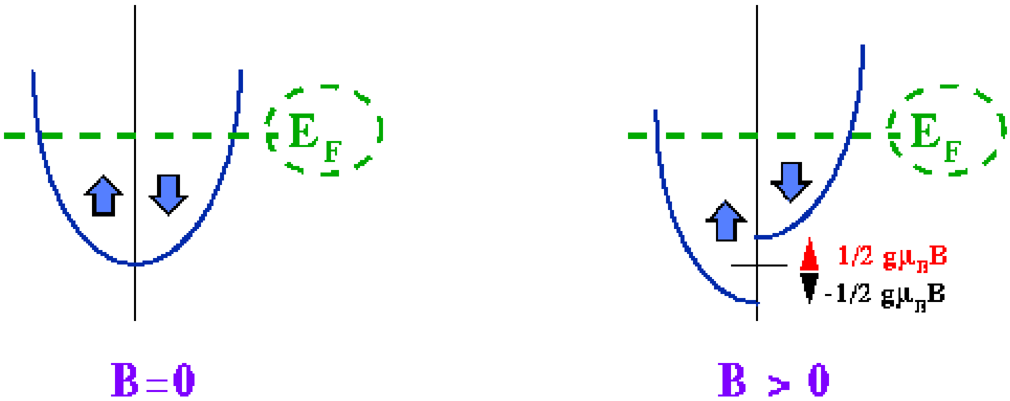
These delocalized molecular state is stable when the Coulomb interaction energy U is **smaller** than the kinetic energy gain $W = 2t$.

$$U = \langle \Psi_2 | V_C(1,2) | \Psi_2 \rangle \approx \int d\mathbf{r}_1 d\mathbf{r}_2 V_C(\mathbf{r}_1 - \mathbf{r}_2) \rho_A(\mathbf{r}_1) \rho_A(\mathbf{r}_2)$$

: on-site Coulomb interaction energy

Jaejun Yu, <jyu@snu.ac.kr>

Pauli Paramagnetism



♠ the change of the Density-of-states due to the Zeeman coupling:

$$D(\varepsilon) = \frac{dN(\varepsilon)}{d\varepsilon}$$

Pauli Paramagnetic Susceptibility

$$\Delta N_\uparrow = \int_{-\mu_B B}^{E_F} \frac{1}{2} D(E+\mu_B B)dE - \int_0^{E_F} \frac{1}{2} D(E)dE = \frac{1}{2}\mu_B B D(E_F)$$

$$\Delta N_\downarrow = \int_{\mu_B B}^{E_F} \frac{1}{2} D(E-\mu_B B)dE - \int_0^{E_F} \frac{1}{2} D(E)dE = -\frac{1}{2}\mu_B B D(E_F)$$

$$M = \mu_B(\Delta N_\uparrow - \Delta N_\downarrow) = \mu_B^2 D(E_F) B = \frac{3N\mu_B^2}{2k_B T_F} B \implies \chi_s = \frac{3N\mu_B^2}{2k_B T_F}$$

Substracting the Landau diamagnetic contribution $\chi_L = -\frac{N\mu_B^2}{2k_B T_F}$, we have the Pauli Paramagnetic Susceptibility:

$$\chi_P = \frac{N\mu_B^2}{k_B T_F}$$

3.4. A Model for the Exchange Interactions in Solids

When $U \gg W$, the localized states of $|\Psi_o\rangle$ becomes stable relative to the band (molecular) state $|\Psi_2\rangle$:

$$|\Psi_o\rangle = \frac{1}{\sqrt{2}} \left[|\phi_\alpha, s_1\rangle |\phi_\beta, s_2\rangle - |\phi_\beta, s_2\rangle |\phi_\alpha, s_1\rangle \right]$$

which is a combination of the localized orbitals $|\phi_{A,B}\rangle$ instead of the molecular states $|\psi_\pm\rangle$.

Here the starting Hamiltonian $\mathcal{H}_o$ include the interaction term of $\hat{U}$:

$$\mathcal{H}_o = h_A + h_B + \hat{U}$$

and the hopping term V_{AB} should be considered as a perturbation.

Jaejun Yu, <jyu@snu.ac.kr>

Many-Particle Excited States

Two-particle excited states:

$$|\Psi_o(s_1, s_2)\rangle = |\phi_A, s_1\rangle|\phi_B, s_2\rangle$$

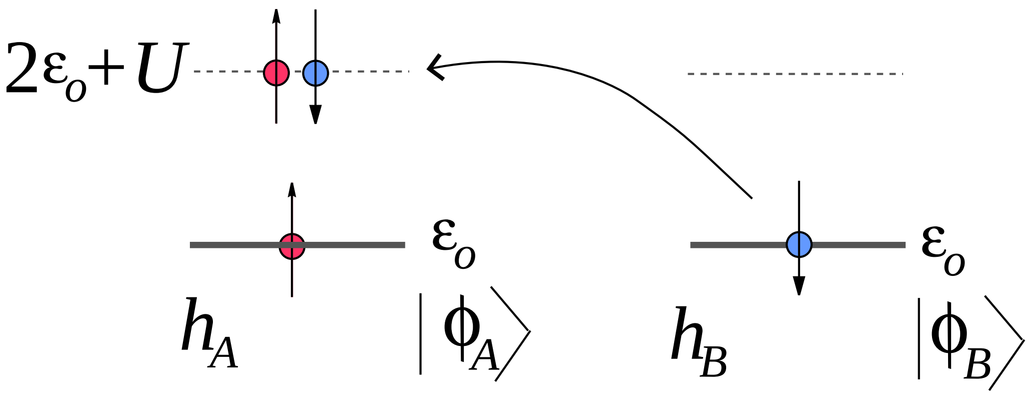
$$|\Psi_A(\uparrow, \downarrow)\rangle = |\phi_A, \uparrow\rangle|\phi_A, \downarrow\rangle$$

$$|\Psi_B(\uparrow, \downarrow)\rangle = |\phi_B, \uparrow\rangle|\phi_B, \downarrow\rangle$$

$$\mathcal{H}_o|\Phi_o\rangle = 2\varepsilon_o|\Psi_o\rangle$$

$$\mathcal{H}_o|\Phi_A\rangle = (2\varepsilon_o + U)|\Psi_A\rangle$$

$$\mathcal{H}_o|\Phi_B\rangle = (2\varepsilon_o + U)|\Psi_B\rangle$$


$2\varepsilon_o+U$
ε_o
ε_o
h_A
$|\phi_A\rangle$
h_B
$|\phi_B\rangle$

Only remaining degrees of freedom of the ground state $|\Psi_o\rangle$ are

spins!

$$|\Psi_p(s_1, s_2)\rangle = |s_1, s_2\rangle$$

Energy Correction via the Perturbation Theory with $\mathcal{H}_1 = V_{AB}$

- First-order correction:

$$\langle s_1, s_2|\mathcal{H}_1|s_1, s_2\rangle = 0$$

Pauli exclusion prohibits the double occupancy at the same site:

$$|\phi_A, \uparrow\rangle|\phi_A, \uparrow\rangle = 0$$

That is,

$$|\phi_A, s_1\rangle|\phi_A, s_1\rangle = 0$$

- Second-order correction:

$$\langle \uparrow, \downarrow |\mathcal{H}_1|\Phi_A\rangle = \langle \uparrow, \downarrow |\mathcal{H}_1|\Phi_B\rangle = t$$

$$\langle \uparrow, \uparrow |\mathcal{H}_1|\Phi_A\rangle = \langle \uparrow, \uparrow |\mathcal{H}_1|\Phi_B\rangle = 0$$

$$E^{(2)}_{\uparrow,\uparrow} = -\sum_n{}' \frac{|\langle \uparrow, \uparrow |\mathcal{H}_1|\Phi_n\rangle|^2}{E_n - E_o} = 0$$

$$E^{(2)}_{\uparrow,\downarrow} = -\sum_n{}' \frac{|\langle \uparrow, \downarrow |\mathcal{H}_1|\Phi_n\rangle|^2}{E_n - E_o} = -\frac{2t^2}{U} = -J_{\mathrm{AF}}$$

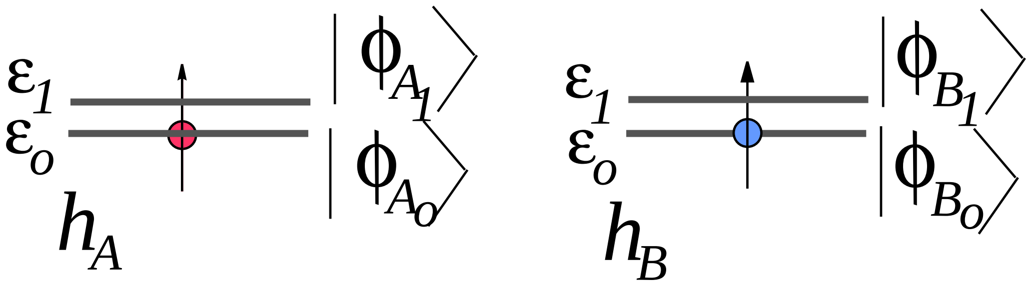
Anti-Ferromagnetic Superexchange Interactions

$$\mathcal{H}_{\mathrm{eff}} = +J_{\mathrm{AF}}\vec{\sigma}_A \cdot \vec{\sigma}_B$$

Jaejun Yu, <jyu@snu.ac.kr>

Ferromagnetic Exchange Interactions

What happens if additional degenerate (or almost degenerate) states exist at each atom while $U \gg W$?



Now additional excited states become available:

$$|\Phi_A(\uparrow,\uparrow)\rangle = |\phi_{A_o},\uparrow\rangle|\phi_{A_1},\uparrow\rangle$$

and

$$\langle\Phi_o(\uparrow,\uparrow)|\mathcal{H}_1|\Phi_A(\uparrow,\uparrow)\rangle \neq 0$$

$$\mathcal{H}_o|\Phi_A(\uparrow,\uparrow)\rangle = (\varepsilon_o+\varepsilon_1+U-J)|\Phi_A(\uparrow,\uparrow)\rangle = E_A(\uparrow,\uparrow)|\Phi_A(\uparrow,\uparrow)\rangle$$

If the exchange energy is larger than the difference $|\varepsilon_o-\varepsilon_1|$, i.e.,

$$J > |\varepsilon_o-\varepsilon_1|$$

we have

$$E_A(\uparrow,\uparrow) < E_A(\uparrow,\downarrow)$$

Therefore,

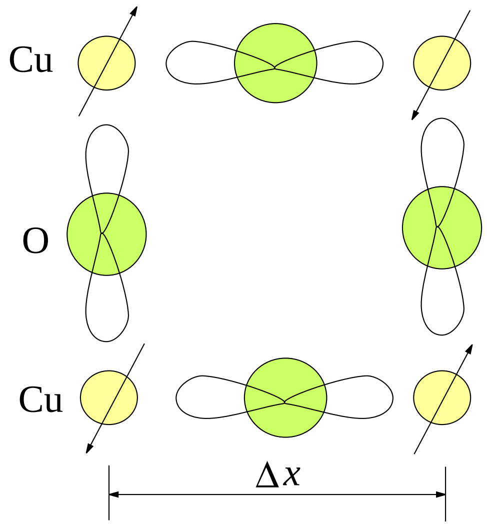
$$E^{(2)}_{\uparrow,\uparrow} = -{\sum_n}' \frac{|\langle\uparrow,\uparrow|\mathcal{H}_1|\Phi_n\rangle|^2}{E_n-E_o} \approx -\frac{2t^2}{U-J} < E^{(2)}_{\uparrow,\downarrow} = -\frac{2t^2}{U}$$

Ferromagnetic Exchange Interaction

$$\mathcal{H}_{\rm eff} = -|J_{FM}|\vec{\sigma}_A \cdot \vec{\sigma}_B$$

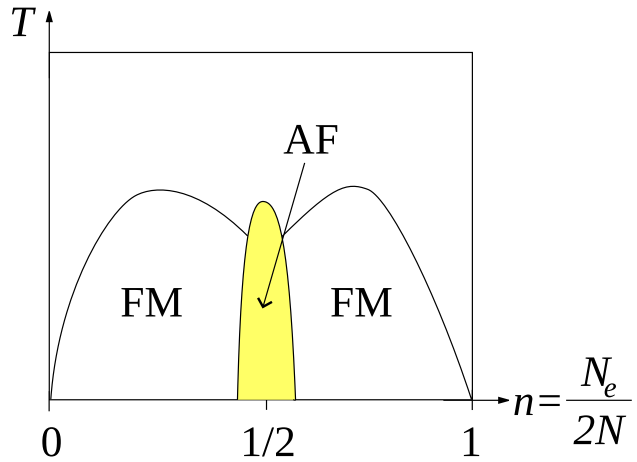
Jaejun Yu, <jyu@snu.ac.kr>

3.5. Transition Metal Oxides



The larger Δx, the smaller t, i.e., $W \implies$ more localized!

FM Metal and AF Insulator

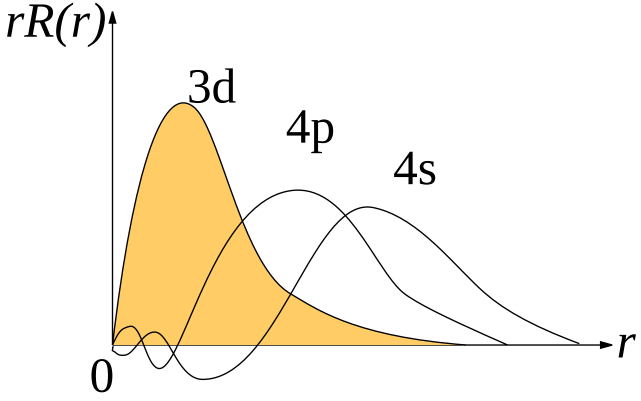


Band-filling controlled by band degeneracy or by doping

Question: Why should the half-filled state be an insulator? What can one imagine to happen when an additional electron or hole is introduced in a half-filled system?

Jaejun Yu, <jyu@snu.ac.kr>

Why Transition Metals (TM) and TM Compounds



⇒ both 3d and 4f electron wavefunctions are extremely localized:
no node in radial wavefunctions

Question:

Let us consider the transition-metal fluoride MnF_2, which is observed to be antiferromagnetic at low temperatures. In this system, the fluorine F becomes F^- being fully ionized so that the manganese Mn becomes Mn^{2+}.

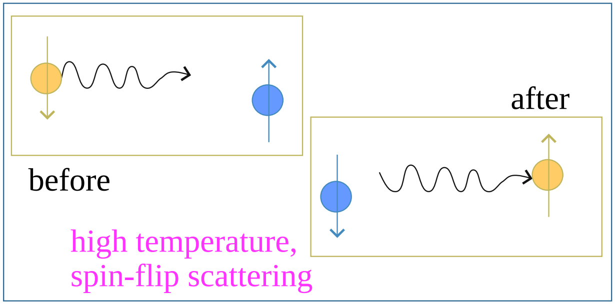
(a) Based on the Hund's rule, discuss the possible spin and orbital configuration of Mn^{2+} ions. (Note that Mn^{2+} has a $3d^5$ configuration.)

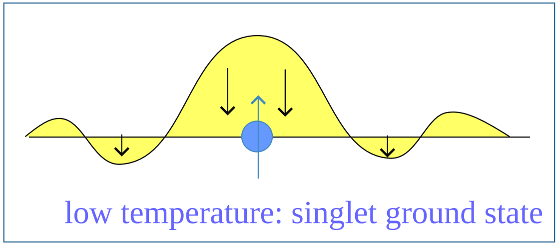
(b) Considering that the Mn ions of MnF_2 form a bcc lattice, guess the magnetic configuration of the ground state of MnF_2.

(c) What difference would it make if we replace F^- ions by O^{2-} ions, that is, the ground state of MnO_2? (Hint: Consider the crystal field effect in a cubic lattice.)

Now consider the long-range magnetic order in metals. We know that Cu is a good paramagnetic metal while Fe is a ferromagnetic metal. Explain the difference and similarity of the two systems. Why Fe is not anti-ferromagnetic instead of being ferromagnetic? (Note that Fe has a configuration of $3d^6 4s^2$ and Cu has $3d^{10} 4s^1$.)

3.6. Magnetic Impurity in a Metal



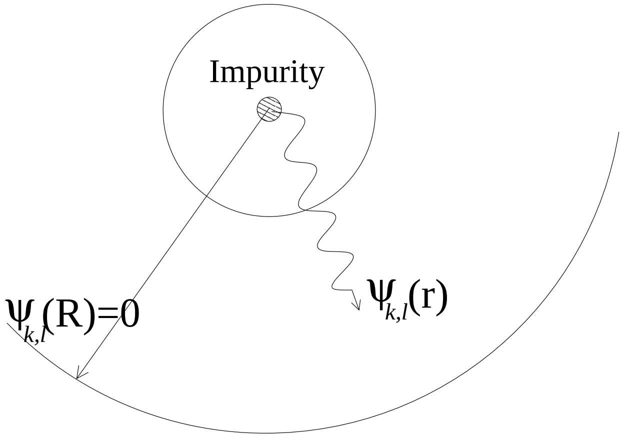


Kondo Effect

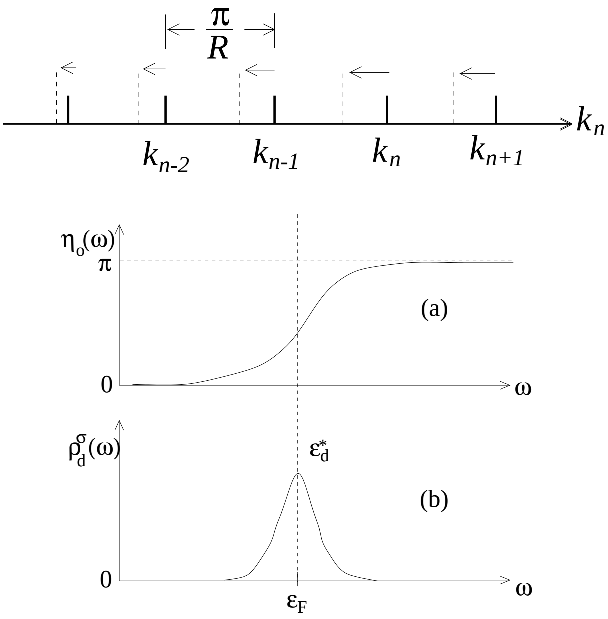
- Spin-flip scattering between the free electrons of a metal and the local moment of a magnetic impurity $\Longrightarrow$ the Kondo effect.
- Highly correlated ground state where the conduction electrons form a spin-polarized "cloud" around the magnetic impurity.
- Below "Kondo temperature", $\Longrightarrow$ a narrow resonance at the Fermi energy: Kondo resonance.

Friedel Sum Rule

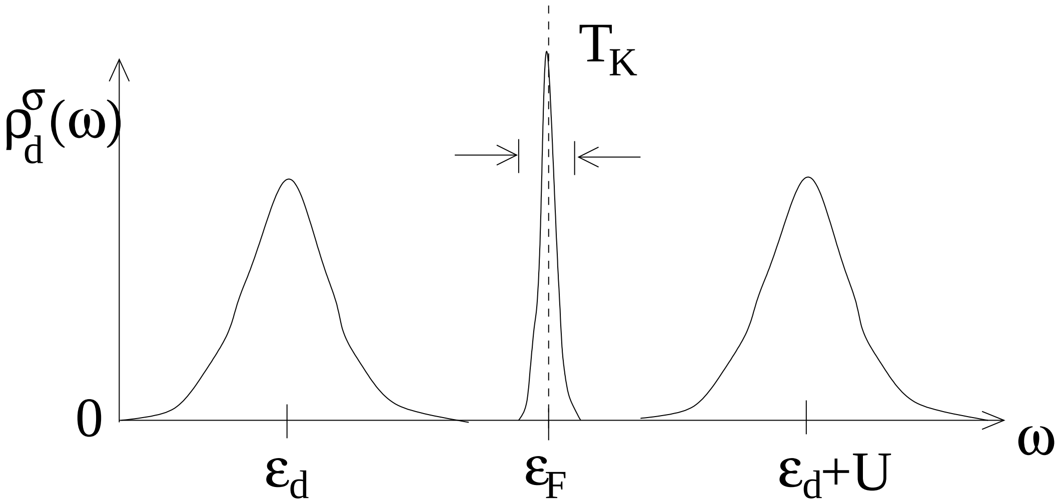
$$\Delta N_{\text{tot}} = \frac{1}{\pi}\sum_{lm\sigma}\eta_{lm,k_F} = \frac{2}{\pi}\sum_{l}(2l+1)\eta_{l,k_F}$$



Scattering Phase Shift and Change of Density-of-State



Kondo Resonance



4. Effective Hamiltonian and Phenomenological Theory

4.1. Heisenberg Model: Mean Field Solution

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + g\mu_B \mathbf{H} \cdot \sum_i \mathbf{S}_i$$

Introducing an effective field $\mathbf{H}_{\text{eff}}$,

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + g\mu_B \mathbf{H} \cdot \sum_i \mathbf{S}_i = g\mu_B \sum_i \mathbf{S}_i \cdot \mathbf{H}_{\text{eff}}$$

where the effective mean field

$$\mathbf{H}_{\text{eff}} = \mathbf{H} - \frac{1}{g\mu_B} \sum_j J_{ij} \mathbf{S}_j$$

and the average magnetization

$$\langle \mathbf{S}_i \rangle = \frac{V}{N} \frac{\mathbf{M}}{g\mu_B}$$

$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \lambda \mathbf{M}$$

$$\lambda = \frac{V}{N} \frac{J_o}{(g\mu_B)^2}$$

$$M = -\frac{N}{V} \frac{\partial F}{\partial H} = M_o\left(\frac{H_{\text{eff}}}{T}\right)$$

- For the case of $H = 0$,
  one can fine the magnetization M by solving the equation:

$$M(T) = M_o(\frac{\lambda M}{T})$$

$$\chi_o(T) = \left(\frac{\partial M_o}{\partial H}\right)_{H=0} = \frac{M_o'(0)}{T}$$

  where the Curie's constant is determined to be $C_o = M_o'(0)$.

- For the case of $H \neq 0$,

$$\chi = \frac{\partial M}{\partial H} = \frac{\partial M_o}{\partial H_{\text{eff}}}\frac{\partial H_{\text{eff}}}{\partial H} = \chi_o(1 + \lambda\chi)$$

$$\chi = \frac{\chi_o}{1 - \lambda\chi_o} = \frac{C_o}{T - T_c}$$

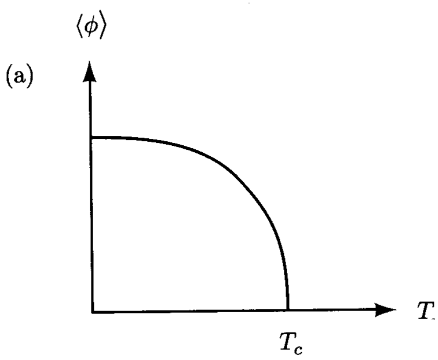
  where the critical temperature T_c becomes

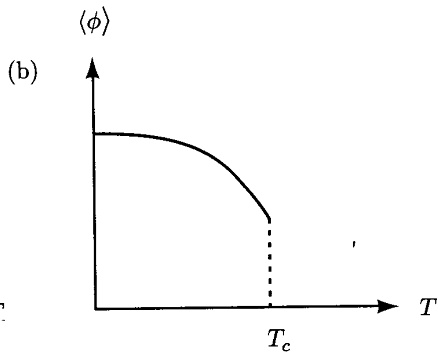
$$T_c = \frac{N}{V}\frac{(g\mu_B)^2}{3k_B}S(S+1)\lambda = \frac{S(S+1)}{3k_B}J_o$$

4.2. Order Parameters: Description of Phase Transition

	$T > T_c$	$T < T_c$	Symmetry
Supercondutor	$\psi_s(\mathbf{r}) = 0$	$\psi_s(\mathbf{r}) \neq 0$	$U(1)$
Magnets	$\mathbf{M}_s(\mathbf{r}) = 0$	$\mathbf{M}_s(\mathbf{r}) \neq 0$	$O(3)$
Ferroelectrics	$\mathbf{P}_s(\mathbf{r}) = 0$	$\mathbf{P}_s(\mathbf{r}) \neq 0$	$O(3)$
Liquid/Gas-Solid	$\rho(\mathbf{G}) = 0$ for $\mathbf{G} \neq 0$	$\rho(\mathbf{G}) \neq 0$ for $\mathbf{G} \neq 0$	$\mathcal{T}_{\mathbf{R}}$
Order-disorder	$\eta = 0$	$\eta \neq 0$	Z_2

$$\eta = \langle n_A \rangle_A - \langle n_B \rangle_A$$





Jaejun Yu, <jyu@snu.ac.kr>

4.3. Bragg-Williams Theory

Consider the Ising model with the spin $\sigma = |\uparrow\rangle$ or $|\downarrow\rangle$. The order parameter $m = \langle\sigma\rangle$ is the average of the spin:

$$m = (N_\uparrow - N_\downarrow)/N$$

- Entropy S:

$$S = \ln C^N_{N_\uparrow} = \ln C^N_{N(1+m)/2}$$

$$\frac{S}{N} = s(m) = \ln 2 - \frac{1}{2}(1+m)\ln(1+m) - \frac{1}{2}(1-m)\ln(1-m)$$

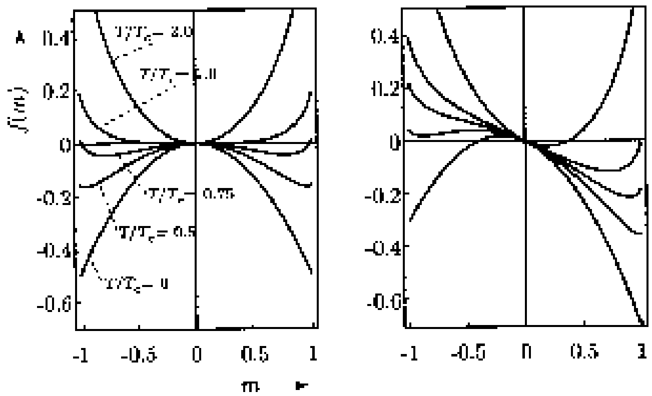
- Average Energy E:

$$E = -J\sum_{\langle ij\rangle} m^2 = -\frac{1}{2}JNzm^2$$

  where z is the number of nearest neighbor sites.

- Bragg-Williams free energy $f(T,m)$:

$$f(T,m) = (E-TS)/N = -\frac{1}{2}Jzm^2 + \frac{1}{2}T[(1+m)\ln(1+m) + (1-m)\ln(1-m)] - T\ln 2$$



(a) $h=0$ (b) $h>0$

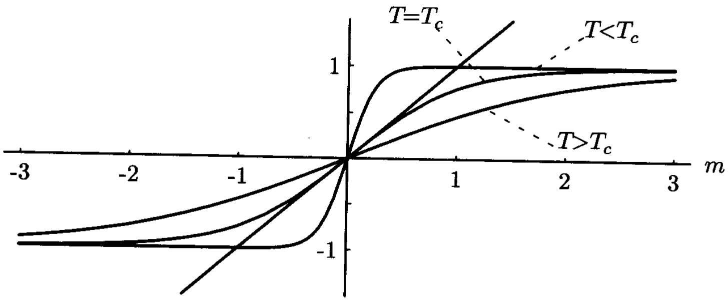
- The equation of state under an external field h:

$$\frac{\partial f}{\partial m} = -zJm + \frac{1}{2}T\ln[(1+m)/(1-m)] = h$$

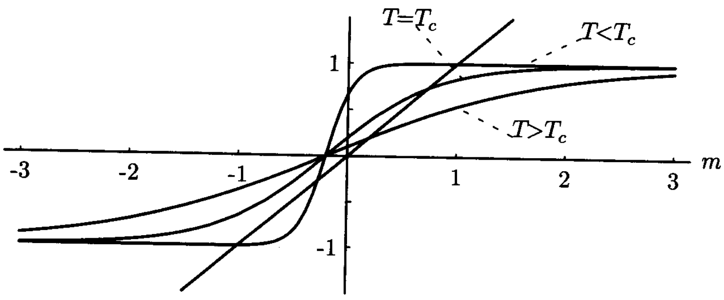
$$-zJm + T\tanh^{-1} m = h$$

$$\therefore m = \tanh[(h + T_c m)/T]$$

Note that $h_{\rm eff} = h + T_c m$.



(a)



(b)

- Mean field solutions for $h = 0$:
  - near $T \approx 0$:

$$m = \tanh(T_c m/T) \approx 1 - 2e^{-2zJ/T}$$

◦ near $T \to T_c^-$:

$$m \approx (T_c/T)m - \frac{1}{3}(T_c/T)^3 m^3 \approx (T_c/T)m - \frac{1}{3}m^3$$

$$m = \pm[3(T_c - T)/T]^{1/2}$$

4.4. Ginzburg-Landau Functional

Free energy near T_c

$$s(m) = \ln 2 - \frac{1}{2}m^2 - \frac{1}{12}m^4 + ...$$

$$f(m) = \frac{1}{2}(T - T_c)m^2 + \frac{1}{12}m^4 - T\ln 2 + ...$$

where $T_c = zJ$

Assuming $\phi(\mathbf{r})$ as a local order parameter,

$$F = \int d\mathbf{r} f(T, \phi(\mathbf{r})) + \int d\mathbf{r} \frac{1}{2} c\, |\nabla\phi(\mathbf{r})|^2$$

where f can be expanded by

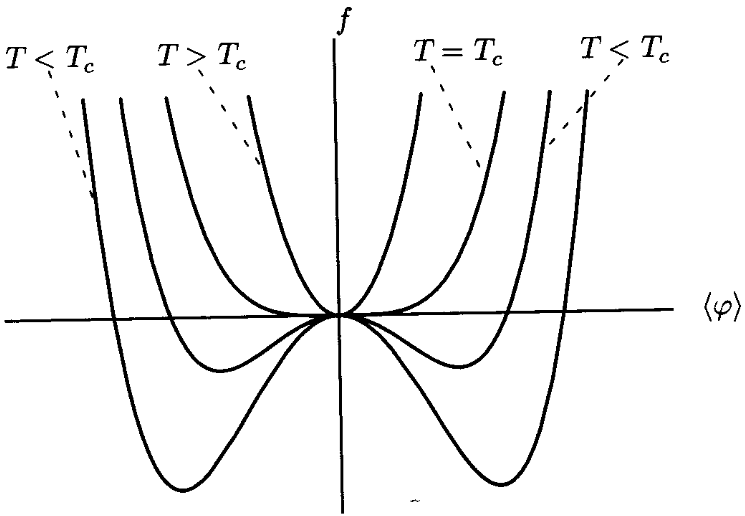
$$f(T, \phi) = \frac{1}{2}r\phi^2 - w\phi^3 + u\phi^4 + ...$$

where $r = a(T - T_c)$

Symmetry properties of the free energy functional F!

4.5. Second-Order Phase Transition

$$f(T,\phi) = \frac{1}{2}r\phi^2 + u\phi^4$$



The equation of state:

$$r\phi + 4u\phi^3 = h$$

- For $h = 0$,

$$\phi = \begin{cases} 0 & \text{if} \quad T > T_c \\ \pm(-r/4u)^{1/2} & \text{if} \quad T < T_c \end{cases}$$

$$\phi \sim (T_c - T)^{\beta}$$

where $\beta = 1/2$.

- Susceptibility χ

$$[r + 12u\phi^2]\frac{\partial \phi}{\partial h} = 1$$

$$\chi = \frac{\partial \phi}{\partial h} = \begin{cases} 1/r & \text{if} T > T_c \\ 1/(2|r|) & \text{if} T < T_c \end{cases}$$

$$\chi \sim |T - T_c|^{-\gamma}$$

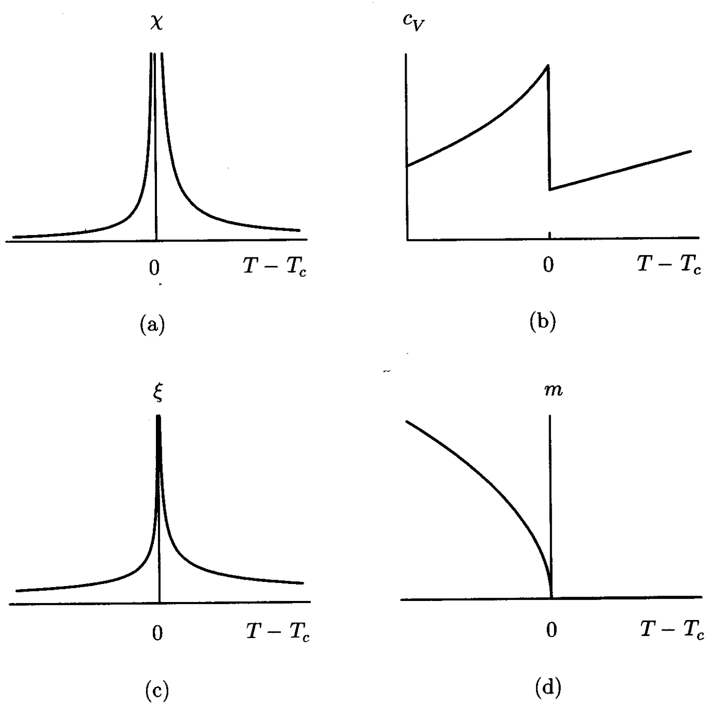
with $\gamma = 1$.

- Free energy density f

$$f = \begin{cases} 0 & \text{if} T > T_c \\ -r^2/(16u) & \text{if} T < T_c \end{cases}$$

- Specific heat c_v

$$c_v = -T\frac{\partial^2 f}{\partial T^2} = \begin{cases} 0 & \text{if} T > T_c \\ Ta^2/(8u) & \text{if} T < T_c \end{cases}$$



χ
0
$T - T_c$
(a)
c_V
0
$T - T_c$
(b)
ξ
0
$T - T_c$
(c)
m
0
$T - T_c$
(d)

4.6. correlation length

$$\chi^{-1}(\mathbf{r},\mathbf{r}') = \frac{\delta^2 F}{\delta\phi(\mathbf{r})\delta\phi(\mathbf{r}')} = (r + 12u\phi^2 - c\nabla^2)\delta(\mathbf{r}-\mathbf{r}')$$

$$\chi(\mathbf{q}) = \frac{1}{r + 12u\phi^2 + cq^2}$$

$$\chi(\mathbf{q}) = \frac{\chi}{1+(q\xi)^2} = \frac{1}{c}\frac{\xi^2}{1+(q\xi)^2}$$

where

$$\xi = c^{1/2}[r + 12u\phi^2]^{-1/2} = \begin{cases} (c/r)^{1/2} & \text{if} T > T_c \\ c^{1/2}/(-2r)^{1/2} & \text{if} T < T_c \end{cases}$$

and the correlation length $\xi \sim |T - T_c|^{-\nu}$ with $\nu = 1/2$.

$$\xi_0 = \left(\frac{c}{r(T=0)}\right)^{1/2} = \left(\frac{c}{aT_c}\right)^{1/2}$$

Jaejun Yu, <jyu@snu.ac.kr>

5. Giant magnetoresistance (GMR) and magnetic sensors

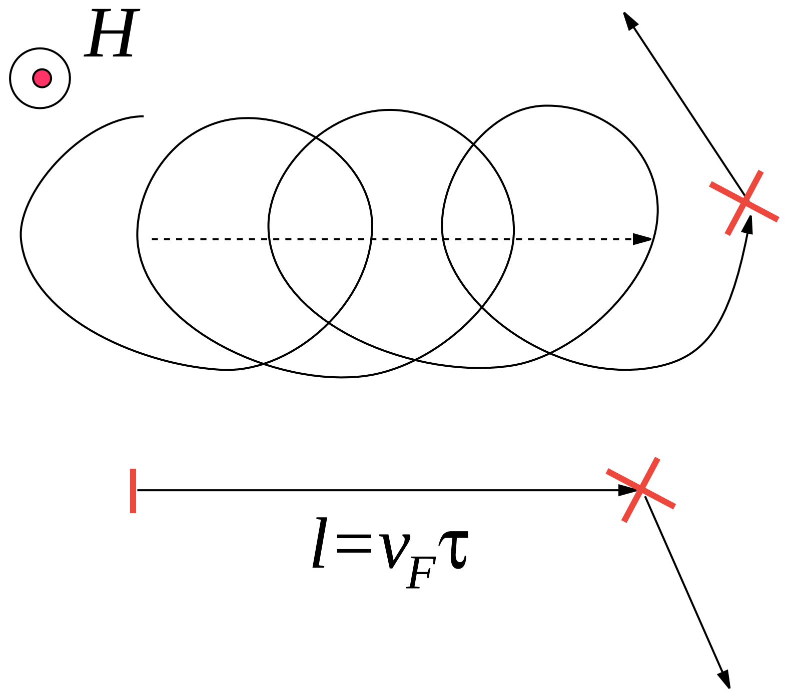
What is Magnetoresistance?

In the free electron system, the conductivity is often described by the Drude model:

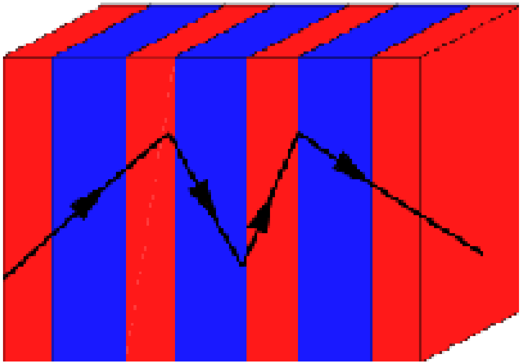
$$\sigma = \frac{ne^2}{m}\tau$$

Unless H (magnetic field) is too large, the mean scattering time τ does not depend on H:

$$\frac{\partial \rho(H)}{\partial H} = 0 + o(H^2)$$


H
$l=v_F\tau$

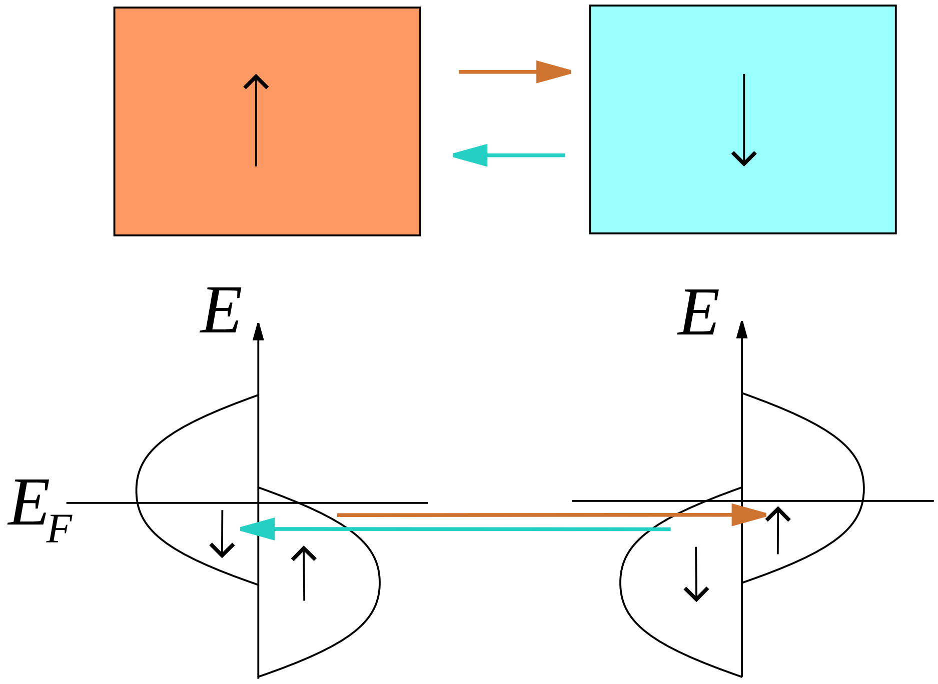
Magnetic Multilayer Structure



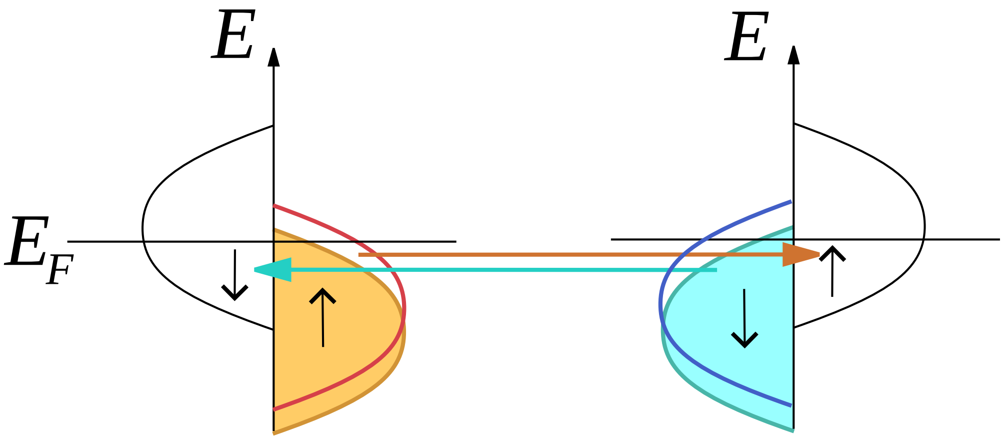
Spin-dependent Density-of-State at ε_F: $D_s(\varepsilon_F)$

$$\Longrightarrow \; \sigma_s = \frac{e^2\tau}{m} n_s(H)$$

$$n_s(H) \propto D_s(\varepsilon_F)$$


↑
↓
E
E
E_F
↓
↑
↑
↓

Change of $D_s(\varepsilon)$ with an external magnetic field H



$\Rightarrow \sigma_s$ increases by the application of H, i.e., $\partial\sigma/\partial H > 0$

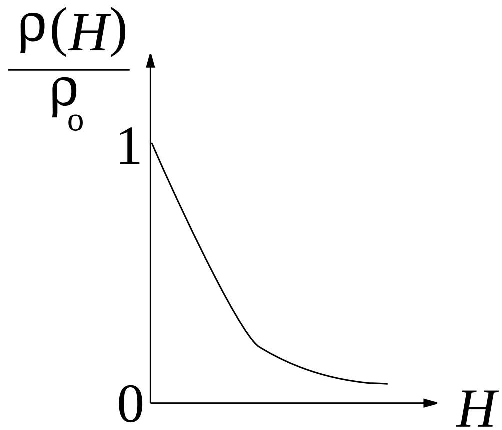
Giant magnetoresistance effect (GMR)

- Giant magnetoresistance effect (GMR) in a junction between two magnetic electrodes
- Electrons undergo quantum tunneling through a thin insulating layer
- Conductance Γ_s across the junction

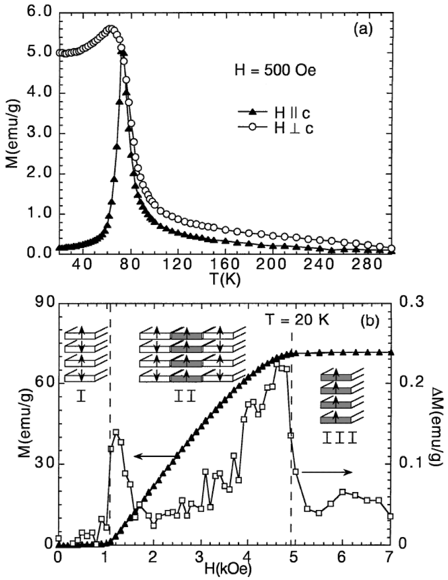
$$\Gamma_s = \frac{4e^2}{hN_{\parallel}} D_s^L(\varepsilon_F) D_s^R(\varepsilon_F)$$

Jaejun Yu, <jyu@snu.ac.kr>

Tunneling Magnetoresistance (TMR)



TMR in Layered Manganites: $La_{1+x}Sr_{2-x}Mn_2O_7$ (x=0.4)

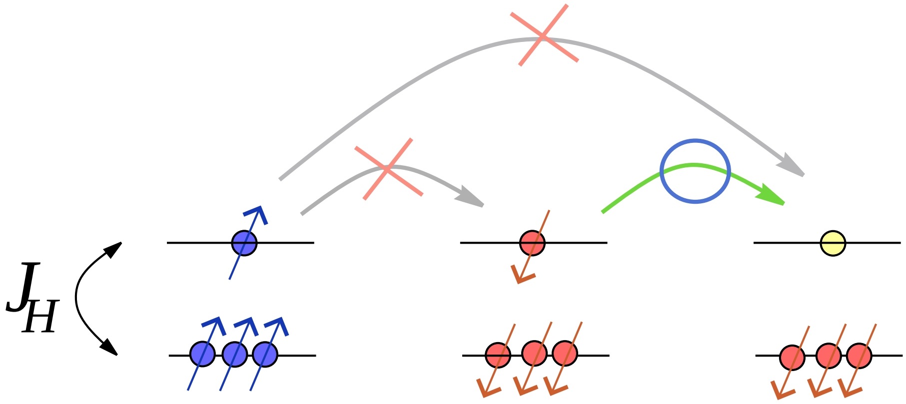


$La_{1.4}Sr_{1.6}Mn_2O_7$ (Welp *et al.*, PRL 83)

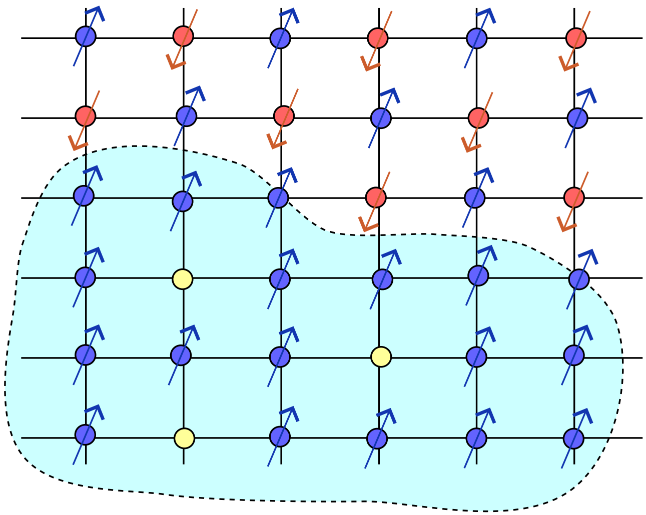
Effective Model Hamiltonians for Doped Manganites

Double Exchange Model with Superexchange Interactions

$$H = -\sum_{\langle ij\rangle,\sigma}^{L}\left(t_{ij}c^{+}_{i\sigma}c_{j\sigma} + \mathrm{h.c.}\right) - J_H\sum_{i,ab}^{L}\vec{S}_i\cdot\vec{\sigma}_{ab}c^{+}_{ia}c_{ib} + J_{AF}\sum_{i,j}^{L}\vec{S}_i\cdot\vec{S}_j,$$

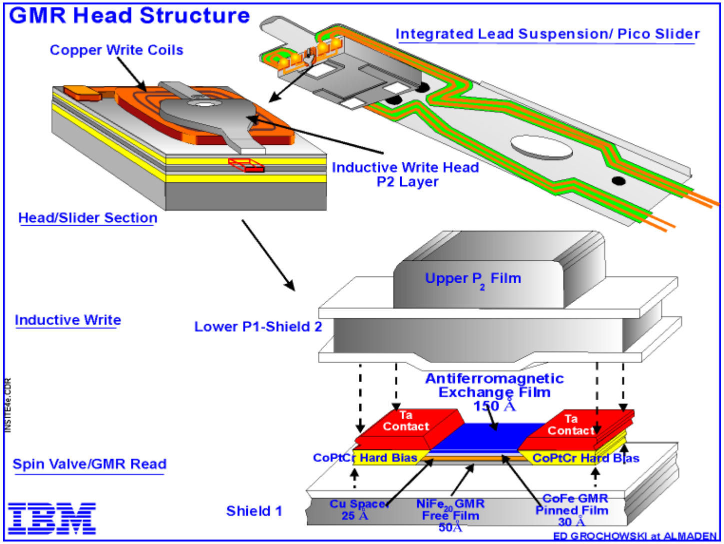


Formation of Ferromagnetic Domain:
Kinetic Energy Gain by the Double Exchange Mechanism



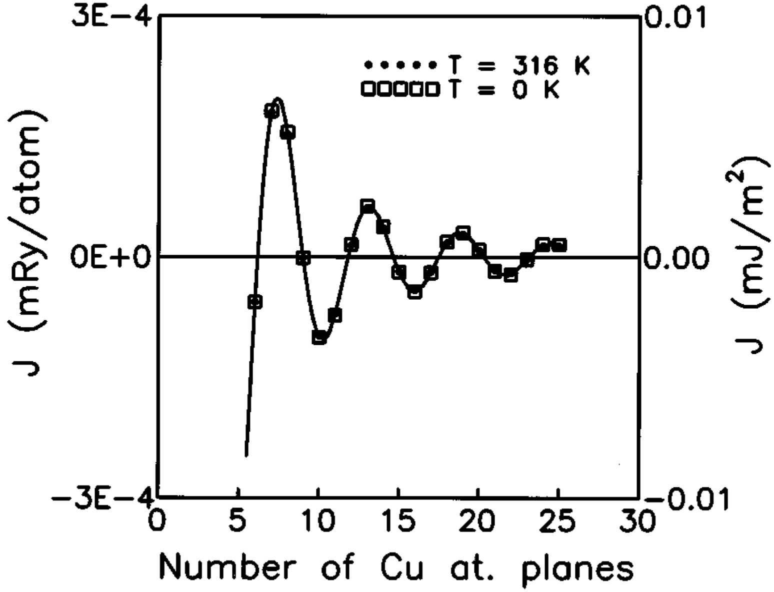
Jaejun Yu, <jyu@snu.ac.kr>

Application of a GMR Device



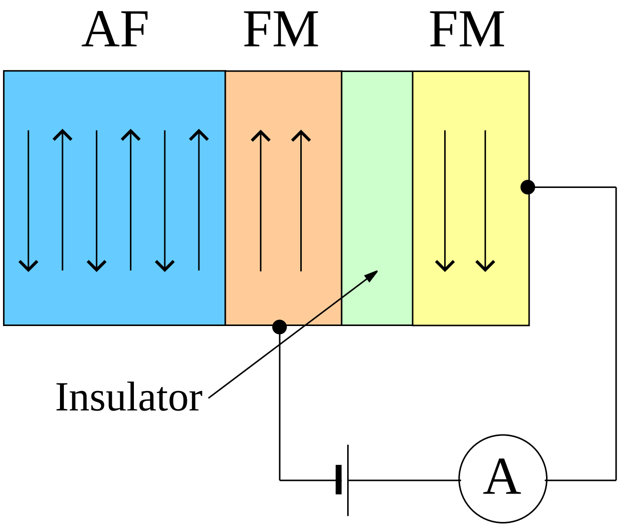
Exchange Coupling in Magnetic Multilayers

- The magnetic coupling of two magnetic layers depends on the thickness of the intervening non-magnetic spacer layer.
- Oscillatory exchange coupling: observable quantum interference effects.
- Confinement of electrons in a quantum well formed in the nonmagnetic layer by the spin-dependent potentials of the magnetic layers.

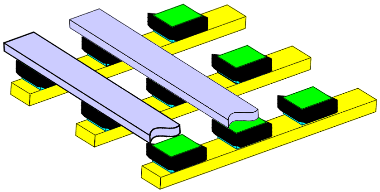


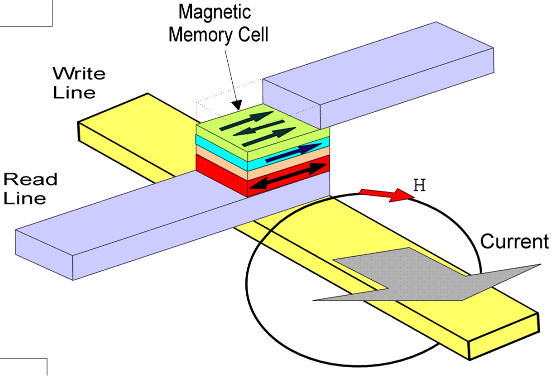
(Mathon *et al.*)

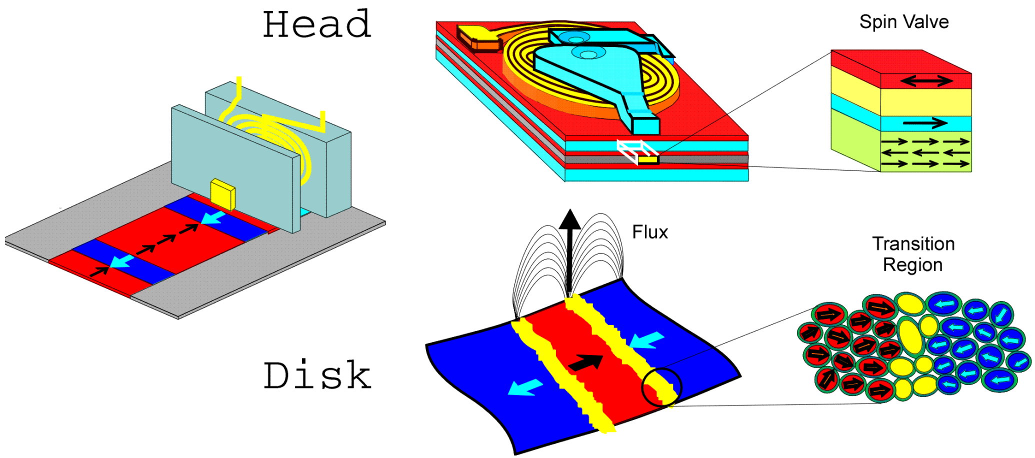
MRAM (magnetic random access memory)


AF
FM
FM
Insulator
A

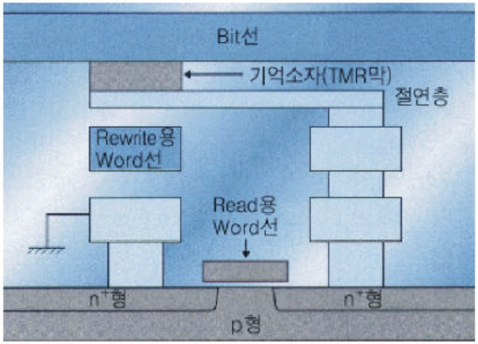
Memory



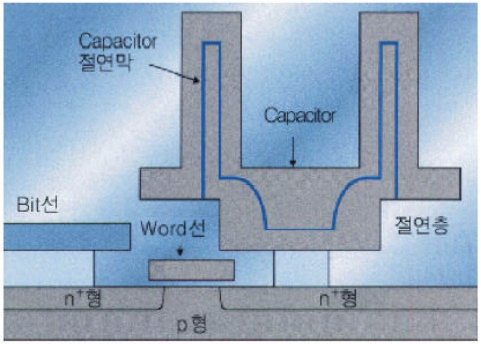


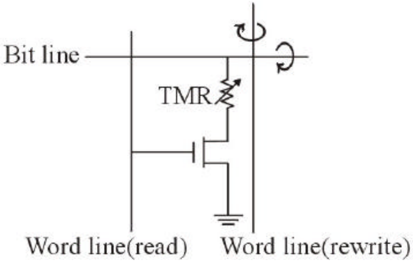

Head
Spin Valve
Flux
Transition
Region
Disk

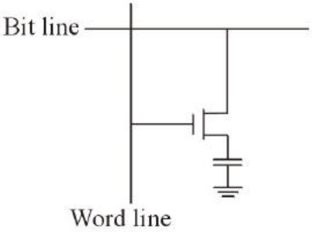
(A) MRAM



(B) DRAM (stack structure)

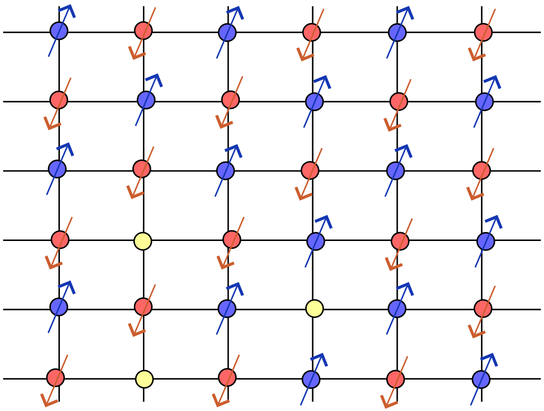




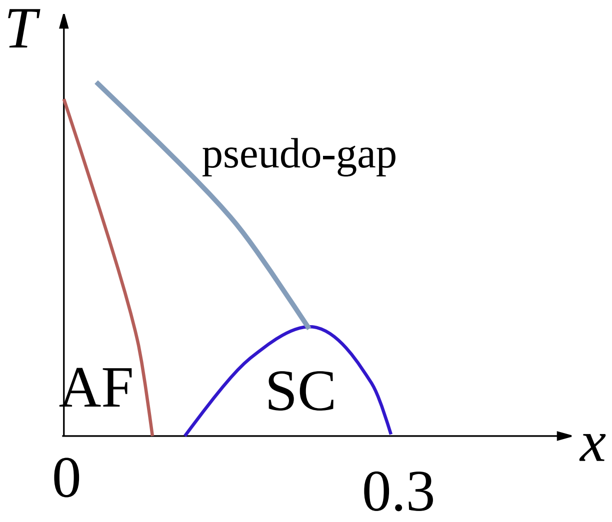


6. Magnetism and superconducitivity: High T_c superconductivity

What happens when the half-filled AF insulator is being doped?



Phase Diagram of High T_c Superconductors: Doped Cu-oxides Systems



Anti-Ferromagnetic Spin Correlation vs. BCS State

- Spin-order Ground State of an Anti-Ferromagnet:

$$|\Psi_{\mathrm{AF}}\rangle = \prod_i c^+_{(2i)\uparrow} c^+_{(2i+1)\downarrow} |O\rangle$$

- BCS State of a Superconductor:

$$|\Psi_{\mathrm{BCS}}\rangle = \prod_k (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow}) |O\rangle$$

- t-J Model for the High T_c Superconductivity:

$$\mathcal{H}_{\mathrm{eff}} = -\sum_{\langle ij\rangle\sigma} c^+_{i\sigma} c_{j\sigma} + J \sum_{\langle ij\rangle} \mathbf{s}_i \cdot \mathbf{s}_j$$

7. References

- Basic Quantum Mechanics:

  1. S. Gasiorowicz, “Quantum Physics”, ‘(John Wiley & Sons, 1996).
  2. C. Cohen-Tannoudji, B. Diu, and F. Laloë, “Quantum Mechanics”, (Hermann, 1977).

- Magnetism:

  1. R. M. White, “Quantum Theory of Magnetism”, (Springer, 1983)
  2. D. C. Mattis, “The Theory of Magnetism”, (Spinger, 1981)

- Correlated Electron Systems:

  1. P. Fulde, “Electron Correlations in Molecules and Solids”, (Springer, 1995).
  2. M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).