Advanced Nanotechnology (Nanoscience)

Optical Electrical Thermal Properties of Top-down Bottom-up Magnetic

Nanomaterials and structures

Magnetism to Spintronics Dr. Shang-Fan Lee Institute of Physics, Academia Sinica Introduction to Solid State Physics Kittel 8th ed Chap. 11-13,

Solid State Physics Ashcroft and Mermin Chap. 31-33,

Condensed Matter Physics Marder 2nd ed Chap. 24-26, Why do most broken permanent magnets repel each other?





Cooperative phenomena

- Elementary excitations in solids describe the response of a solid to a perturbation
 - Quasiparticles
 - usually fermions, resemble the particles that make the system, e.g. quasi-electrons
 - Collective excitations
 - usually bosons, describe collective motions
 - use second quantization with Fermi-Dirac or Bose-Einstein statistics

Magnetism

• the Bohr–van Leeuwen theorem

when statistical mechanics and <u>classical mechanics</u> are applied consistently, the thermal average of the magnetization is always zero.

- Magnetism in solids is solely a <u>quantum mechanical</u> effect
- Origin of the magnetic moment:
 - Electron spin \vec{S}
 - Electron orbital momentum \vec{L}
- From (macroscopic) response to external magnetic field \vec{H}
 - Diamagnetism $\chi < 0, \chi \sim 1 \times 10^{-6}$, insensitive to temperature
 - Paramagnetism $\chi > 0$, $\chi = \frac{C}{T}$ Curie law $\chi = \frac{C}{T+\Delta}$ Curie-Weiss law
 - Ferromagnetism exchange interaction (quantum)

Magnetism



逆磁性 diamagnetism







Family Tree of Magnetism



Why do most broken permanent magnets repel each other?



- Classical and quantum theory for diamagnetism Calculate $\langle r^2 \rangle$
- Classical and quantum theory for paramagnetism
 - Superparamagnetism, Langevin function
 - Hund's rules
 - Magnetic state ${}^{2S+1}L_I$
 - Crystal field
 - Quenching of orbital angular momentum L_z
 - Angular momentum operator
 - Spherical harmonics
 - Jahn-Teller effect
 - Paramagnetic susceptibility of conduction electrons

- Ferromagnetism
 - Microscopic ferro, antiferro, ferri magnetism
 - Exchange interaction
 - Exchange splitting source of magnetization two-electron system spin-independent
 Schrodinger equation
 - Type of exchange: direct exchange, super exchange, indirect exchange, itinerant exchange
 - Spin Hamiltonian and Heisenberg model
 - Molecular-field (mean-field) approximation

Ferromagnetic elements: 鐵 Fe, 鈷 Co, 鎳 Ni, 釓 Gd, 鏑 Dy, 錳 Mn, 鈀 Pd ??

Elements with ferromagnetic properties

合金, alloys 錳氧化物 MnOx,



58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	\mathbf{Pm}	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
90	- 91	92	93	- 94	95	96	97	- 98	- 99	100	101	102	103
Th	Pa	U	Np	Pu	\mathbf{Am}	Cm	Bk	Cf	Es	\mathbf{Fm}	Md	No	Lr

Platonic solid

From Wikipedia

In geometry, a Platonic solid is a <u>convex polyhedron</u> that is <u>regular</u>, in the sense of a <u>regular polygon</u>. Specifically, the faces of a Platonic solid are <u>congruent</u> regular polygons, with the same number of faces meeting at each <u>vertex</u>; thus, all its edges are congruent, as are its vertices and angles. There are precisely five Platonic solids (shown below):

The name of each figure is derived from its number of faces: respectively 4, 6, 8, 12, and 20.

<u>The aesthetic beauty and symmetry of the Platonic solids have made them a</u> <u>favorite subject of geometers</u> for thousands of years. They are named for the <u>ancient Greek philosopher Plato who theorized that the classical elements were</u> <u>constructed from the regular solids.</u>





Electronic orbit





s, p electron orbits



Orbital viewer

Resonance

Onedimensional

dimensional

Two-



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Threedimensional

Hydrogen atom

3d transition metals: Mn atom has 5 d ↑ electrons Bulk Mn is NOT magnetic

s, p electron orbital



Bulk Co is magnetic.

Orbital viewer

d orbitals







Stern-Gerlach Experiment



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There are two kinds of electrons: spin-up and spin-down.

Stern and Gerlach: How a Bad Cigar Helped Reorient Atomic Physics

Physics Today 56, 53 (2003) 10.1063/1.1650229

Stoner criterion for ferromagnetism:

I N(E_F) > 1, I is the **Stoner exchange parameter** and N(E_F) is the density of states at the Fermi energy.





For the non-magnetic state there are identical density of states for the two spins. For a ferromagnetic state, $N \uparrow > N \downarrow$. The polarization is indicated by the thick blue arrow.

Schematic plot for the energy band structure of 3d transition metals.

Teodorescu and Lungu, <u>"Band ferromagnetism in systems of variable dimensionality"</u>. J Optoelectronics and Adv. Mat. **10**, 3058–3068 (2008).

Stoner band ferromagnetism

Teodorescu, C. M.; Lungu, G. A. (November 2008). <u>"Band ferromagnetism in systems</u> of variable dimensionality". *Journal of Optoelectronics and Advanced Materials* **10** (11): 3058–3068.

$$\mathcal{E} = \int_0^{\mathcal{E}_F - \Delta} d\mathcal{E}' D(\mathcal{E}') \mathcal{E}' + \frac{1}{2} \int_{\mathcal{E}_F - \Delta}^{\mathcal{E}_F + \Delta} d\mathcal{E}' D(\mathcal{E}') \mathcal{E}' - \frac{1}{2} n J \langle S \rangle^2$$
$$\langle S \rangle = \frac{1}{2n} \int_{\mathcal{E}_F - \Delta}^{\mathcal{E}_F + \Delta} d\mathcal{E}' \frac{1}{2} D(\mathcal{E}') = \frac{1}{2n} D(\mathcal{E}_F) \Delta$$

$$\frac{\partial \mathcal{E}}{\partial \Delta}\Big|_{\mathcal{E}_F} = \Delta D(\mathcal{E}_F) - \frac{J}{4n} D(\mathcal{E}_F)^2 \Delta$$
$$\frac{\partial \mathcal{E}}{\partial \Delta}\Big|_{\mathcal{E}_F} = 0 \Rightarrow \frac{J}{n} D(\mathcal{E}_F) = 4$$

Exchange interaction



Although in the hydrogen molecule the exchange integral, Eq. (6), is negative. Heisenberg first suggested that it changes sign at some critical ratio of internuclear distance to

🔍 100% 🛛 👻

Double exchange interaction

Super exchange interaction



In superexchange, a ferromagnetic or antiferromagnetic alignment occurs between two atoms with the same <u>valence</u> (number of electrons) or differs by two, and the electrons are localized;

while in double-exchange, the interaction occurs only when one atom has an extra electron compared to the other, the electrons are itinerant (delocalized); this results in the material displaying magnetic exchange coupling, as well as metallic conductivity.

Berry Phase

Aharonov-Bohm Effect



Electrons traveling around a flux tube suffer a phase change and can interfere with themselves even if they only travel through regions where B = 0. (B) An open flux tube is not experimentally realizable, but a small toroidal magnet with no flux leakage can be constructed instead.

$$\Phi = \int d^2 r B_z = \oint d\vec{r} \cdot \vec{A}$$
$$A_{\phi} = \frac{\Phi}{2\pi r}$$





Electron hologram showing interference fringes of electrons passing through small toroidal magnet. The magnetic flux passing through the torus is quantized so as to produce an integer multiple of π phase change in the electron wave functions. The electron is completely screened from the magnetic induction in the magnet. In (A) the phase change is 0, while in (B) the phase change is π . [Source: Tonomura (1993), p. 67.]



Parallel transport of a vector along a closed path on the sphere S₂ leads to a geometric phase between initial and final state.

Real-space Berry phases: Skyrmion soccer (invited) Karin Everschor-Sitte and Matthias Sitte Journal of Applied Physics **115**, 172602 (2014); doi: 10.1063/1.4870695

Berry phase formalism for From Prof. Guo Guang-Yu Berry phase Hall effects

[Berry, Proc. Roy. Soc. London A 392, 451 (1984)]

Parameter dependent system:

$$\{ \varepsilon_n(\lambda), \psi_n(\lambda) \}$$

Adiabatic theorem:

$$\Psi(t) = \Psi_n(\lambda(t)) e^{-i\int_0^t dt \,\varepsilon_n/\hbar} e^{-i\gamma_n(t)/\hbar}$$

_t

Geometric phase:

$$\gamma_n = \int_{\lambda_0}^{\lambda_t} d\lambda \left\langle \Psi_n \right| i \frac{\partial}{\partial \lambda} \left| \Psi_n \right\rangle$$

 \mathcal{E}_n *t*) λ_{2} λ_{0} 24 Well defined for a closed path

From Prof. Guo Guang-Yu

$$\gamma_n = \oint_C d\lambda \left\langle \Psi_n \left| i \frac{\partial}{\partial \lambda} \right| \Psi_n \right\rangle$$

Stokes theorem

$$\gamma_n = \iint d\lambda_1 d\lambda_2 \ \Omega$$



Berry Curvature

$$\Omega = i \frac{\partial}{\partial \lambda_1} \langle \psi | \frac{\partial}{\partial \lambda_2} | \psi \rangle - i \frac{\partial}{\partial \lambda_2} \langle \psi | \frac{\partial}{\partial \lambda_1} | \psi \rangle$$

Analogies

From Prof. Guo Guang-Yu

Berry curvature

 $\Omega(\vec{\lambda})$

Berry connection

$$\left\langle \psi \right| i \frac{\partial}{\partial \lambda} \left| \psi \right\rangle$$

Geometric phase

$$\oint d\lambda \left\langle \psi \right| i \frac{\partial}{\partial \lambda} \left| \psi \right\rangle = \iint d^2 \lambda \ \Omega(\vec{\lambda})$$

Chern number

$$\oint d^2 \lambda \ \Omega(\vec{\lambda}) = \text{integer}$$

Magnetic field

 $B(\vec{r})$

Vector pot $A(\vec{r})$

Aharonov-Bohm phase

$$\oint dr \ A(\vec{r}) = \iint d^2 r \ B(\vec{r})$$

Dirac monopole

$$\oint d^2 r \ B(\vec{r}) = \text{integer } h / e$$

Semiclassical dynamics of Bloch electrons

$$Olc \dot{\mathbf{x}}_{c} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_{n}(\mathbf{k})}{\partial \mathbf{k}},$$

$$\dot{\mathbf{k}} = -\frac{e}{\hbar} \mathbf{E} - \frac{e}{\hbar} \dot{\mathbf{x}}_{c} \times \mathbf{B} = \frac{e}{\hbar} \frac{\partial \varphi(\mathbf{r})}{\partial \mathbf{r}} - \frac{e}{\hbar} \dot{\mathbf{x}}_{c} \times \mathbf{B}$$

$$(976)$$

New version [Marder, 2000]

Berry phase correction [Chang & Niu, PRL (1995), PRB

$$\dot{\mathbf{x}}_{c} = \frac{1}{\hbar} \frac{\partial \varepsilon_{n}(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}_{n}(\mathbf{k}),$$
$$\dot{\mathbf{k}} = \frac{e}{\hbar} \frac{\partial \varphi(\mathbf{r})}{\partial \mathbf{r}} - \frac{e}{\hbar} \dot{\mathbf{x}}_{c} \times \mathbf{B},$$
$$\mathbf{\Omega}_{n}(\mathbf{k}) = -\operatorname{Im} \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} | \times | \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right\rangle$$

(Berry curvature)

From Prof. Guo Guang-Yu

Demagnetization factor D

can be solved analytically in some cases, numerically in others

Oblate Spheroid (pancake shape) c/a = r < 1; a = b

 $D_c = \frac{4\pi}{1 - r^2} \left[1 - \frac{r}{\sqrt{1 - r^2}} \cos^{-1} r \right] \qquad D_a = D_b = \frac{4\pi - D_c}{2}$

For an ellipsoid $D_x + D_y + D_z = 1$ (SI units) $D_x + D_y + D_z = 4\pi$ (cgs units) Solution for Spheroid $a = b \neq c$

1. Prolate spheroid (football shape) c/a = r > 1; a = b, In cgs units

$$D_{c} = \frac{4\pi}{r^{2}-1} \left[\frac{r}{\sqrt{r^{2}-1}} \ln\left(r + \sqrt{r^{2}-1}\right) - 1 \right]$$

$$D_{a} = D_{b} = \frac{4\pi - D_{c}}{2}$$

Limiting case r >> 1 (long rod)

$$D_c = \frac{4\pi}{r^2} \left[\ln(2r) - 1 \right] \ll 1$$
$$D_a = D_b = 2\pi$$

Note: you measure $2\pi M$ without knowing the sample

—□— In-plane H —△— Perpendicular H



Limiting case r >> 1 (flat disk)

2.

$$D_c = 4\pi$$
$$D_a = D_b = \pi^2 r \ll 1$$

Note: you measure $4\pi M$ without knowing the sample

Surface anisotropy

 $E = E_{exchange} + E_{Zeeman} + E_{mag} + E_{anisotropy} + \cdots$

- $E_{ex}: \sum 2J\overrightarrow{S_i} \cdot \overrightarrow{S_j}$
- $E_{Zeeman}: \vec{M} \cdot \vec{H}$
- $E_{mag}: \frac{1}{8\pi} \int B^2 dV$
- Eanisotropy



For hcp Co= $K'_1 \sin^2 \theta + K_2' \sin^4 \theta$ For bcc Fe = $K_1(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2) + K_2(\alpha_1^2 \alpha_2^2 \alpha_3^2)$ α_i : directional cosines

Surface anisotropy
$$K_{\text{eff}} = \frac{2K_S}{t} + K_V \rightarrow K_{\text{eff}} \cdot t = 2K_S + K_V \cdot t$$

Stoner–Wohlfarth model

A widely used model for the magnetization of singledomain ferromagnets. It is a simple example of <u>magnetic</u> <u>hysteresis</u> and is useful for modeling small magnetic particles





 $E = K_u V \sin^2 (\phi - \theta) - \mu_0 M_s V H \cos \phi,$

where K_u is the uniaxial anisotropy parameter, V is the volume of the magnet, M_s is the saturation magnetization.

Ferromagnetic domains

- competition between exchange, anisotropy, and magnetic energies.
- Bloch wall: rotation out of the plane of the two spins
- Neel wall: rotation within the plane of the two spins

For a 180° Bloch wall rotated in N+1 atomic planes $N\Delta E_{ex} = N(JS^2 \left(\frac{\pi}{N}\right)^2)$ Wall energy density $\sigma_w = \sigma_{ex} + \sigma_{anis} \approx JS^2 \pi^2 / (Na^2) + KNa$ a: lattice constant $\partial \sigma_w / \partial N \equiv 0$, $N = \sqrt{[JS^2\pi^2/(Ka^3)]} \approx 300$ in Fe $\sigma_w = 2\pi \sqrt{KJS^2/a} \approx 1 \text{ erg/cm}^2$ in Fe Wall width $Na = \pi \sqrt{JS^2/Ka} \equiv \pi \sqrt{\frac{A}{K}}$, $A = JS^2/a$ Exchange stiffness constant

Domain wall energy γ versus thickness D of Ni₈₀Fe₂₀ thin films



 $\gamma_{\rm N} < \gamma_{\rm B} \sim 50 {\rm nm}$

Thick films have Bloch walls Thin films have Neel walls

Cross-tie walls show up in between.

A=10⁻⁶ erg/cm

K=1500 erg/cm³

Further reference: Antonio DeSimone, Hans Knupfer, and Felix Otto, Calculus of Variations 27, 233–253 (2006) 2-d stability of the Neel wall

Magnetic Resonance

- Nuclear Magnetic Resonance (NMR)
 - Line width
 - Hyperfine Splitting, Knight Shift
 - Nuclear Quadrupole Resonance (NQR)
- Ferromagnetic Resonance (FMR)
 - Shape Effect
 - Spin Wave resonance (SWR)
- Antiferromagnetic Resonance (AFMR)
- Electron Paramagnetic Resonance (EPR or ESR)
 - Exchange narrowing
 - Zero-field Splitting
- Maser

What we can learn:

- From absorption fine structure → electronic structure of single defects
- From changes in linewidth → relative motion of the spin to the surroundings
- From resonance frequency → internal magnetic field
- Collective spin excitations

FMR

Equation of motion of a magnetic moment μ in an external field B_0

$$\frac{\hbar dI}{dt} = \mu \times B \qquad \mu = \gamma \hbar I \qquad \frac{d\mu}{dt} = \gamma \mu \times B \qquad \frac{dM}{dt} = \gamma M \times B$$
Shape effect:
internal magnetic field
$$B_x^i = B_x^0 - N_x M_x \qquad B_y^i = B_y^0 - N_y M_y \qquad B_z^i = B_z^0 - N_z M_z$$

$$\frac{dM_x}{dt} = \gamma (M_y B_z^i - M_z B_y^i) = \gamma [B_0 + (N_y - N_z)M] M_y$$

$$\frac{dM_y}{dt} = \gamma [M(-N_x M_x) - M_x (B_0 - N_z M)] = -\gamma [B_0 + (N_x - N_z)M] M_x$$
To first order
$$\frac{dM_z}{dt} = 0 \qquad M_z = M$$

$$\begin{vmatrix} i\omega & \gamma [B_0 + (N_y - N_z)M] \\ -\gamma [B_0 + (N_x - N_z)M] & i\omega \end{vmatrix} = 0$$

$$\omega_0^2 = \gamma^2 [B_0 + (N_y - N_z)M] [B_0 + (N_x - N_z)M] \qquad \text{Uniform mode}$$

Uniform mode



$$\begin{split} N_x &= N_y = N_z & N_x = N_y = 0 \quad N_z = 4\pi & N_x = N_z = 0 \quad N_y = 4\pi \\ \omega_0 &= \gamma B_0 & \omega_0 = \gamma \left(B_0 - 4\pi M\right) & \omega_0 = \gamma \left[B_0 (B_0 + 4\pi M)\right]^{1/2} \end{split}$$

Spin wave resonance; Magnons

Consider a one-dimensional spin chain with only nearest-neighbor interactions.

$$U = -2J \sum \vec{S_i} \cdot \vec{S_j}$$
 We can derive $\hbar \omega = 4JS(1 - \cos ka)$

When $ka \ll 1$ $\hbar\omega \cong (2JSa^2)k^2$

flat plate with perpendicular field $\omega_0 = \gamma (B_0 - 4\pi M) + Dk^2$

Quantization of (uniform mode) spin waves, then consider the thermal excitation of Mannons, leads to Bloch T^{3/2} law. $\Delta M/M(0) \propto T^{3/2}$

AFMR

Spin wave resonance; Antiferromagnetic Magnons

Consider a one-dimensional antiferromangetic spin chain with only nearest-neighbor interactions. Treat sublattice A with up spin S and sublattice B with down spin –S, J<0.

$$U = -2J \sum_{i} \vec{S_i} \cdot \vec{S_j} \qquad \text{We can derive} \qquad \hbar\omega = -4JS |\sin ka|$$

When $ka << 1 \qquad \hbar\omega \cong (-4JS)|ka|$

AFMR

exchange plus anisotropy fields on the two sublattices

$$\begin{split} B_1 &= -\lambda M_2 + B_A \hat{z} \quad \text{on } \mathbf{M}_1 \qquad B_2 = -\lambda M_1 - B_A \hat{z} \quad \text{on } \mathbf{M}_2 \\ M_1^z &\equiv M \qquad M_2^z \equiv -M \qquad M_1^+ \equiv M_1^x + iM_1^y \qquad M_2^+ \equiv M_2^x + iM_2^y \qquad B_E \equiv \lambda M \\ \frac{dM_1^+}{dt} &= -i\gamma [M_1^+ (B_A + B_E) + M_2^+ B_E] \\ \frac{dM_2^+}{dt} &= -i\gamma [M_2^+ (B_A + B_E) + M_1^+ B_E] \\ \left| \begin{array}{c} \gamma (B_A + B_E) - \omega \qquad \gamma B_E \\ B_E \qquad \gamma (B_A + B_E) + \omega \end{array} \right| = 0 \\ \omega_0^2 &= \gamma^2 B_A (B_A + 2B_E) \qquad \text{Uniform mode} \end{split}$$

Spintronics

Electronics with electron spin as an extra degree of freedom Generate, inject, process, and detect spin currents

- Generation: ferromagnetic materials, spin Hall effect, spin pumping effect etc.
- Injection: interfaces, heterogeneous structures, tunnel junctions
- Process: spin transfer torque
- Detection: Giant Magnetoresistance, Tunneling MR
- Historically, from magnetic coupling to transport phenomena

important materials: CoFe, CoFeB, Cu, Ru, IrMn, PtMn, MgO, Al2O3, Pt, Ta

Spin Transfer Torque



The transverse spin component is lost by the conduction electrons, transferred to the global spin of Sthe

$$\dot{\boldsymbol{S}}_{1,2} = (\boldsymbol{I}_{e} \boldsymbol{g}/\boldsymbol{e}) \, \boldsymbol{\hat{s}}_{1,2} \times (\boldsymbol{\hat{s}}_{1} \times \boldsymbol{\hat{s}}_{2})$$

Slonczewski JMMM 159, L1 (1996)

Modified Landau-Lifshitz-Gilbert (LLG) equation



FIG. 1. The point contact dV/dI(V) spectra for a series of magnetic fields (2, 3, 5, 6, 7, and 8 T) revealing an upward step and a corresponding peak in dV/dI at a certain negative bias voltage $V^*(H)$. The inset shows that $V^*(H)$ increases linearly with the applied magnetic field H.

Tsoi et al. PRL 61, 2472 (1998)

$$\frac{dm}{dt} = -\gamma m \times H_{eff} + \alpha m \times \frac{dm}{dt} + \frac{\gamma \hbar PI}{2e\mu_0 M_S V} (m \times \sigma \times m)$$

Experimantally determined current density ~10¹⁰-10¹²A/m² 38





In a trilayer, current direction determines the relative orientation of F_1 and F_2 when H = 0

Spin Transfer Torque

Landau-Lifshitz-Gilbert equation with Spin Transfer Torque terms

Current induced domain wall motion

Passing spin polarized current from Domain A to Domain $B \Rightarrow B$ switches



Spin Transfer Torque

Landau-Lifshitz-Gilbert equation with Spin Transfer Torque terms



Industrial applications

Read head in hard drives











Magnetic skyrmions



• Neel

• Bloch

- How to generate
- To detect
- To manipulate

- Magnetic field
- Electric current
- Spin current, spin wave