Lecture 30

Thursday, February 3, 2022 2:34 PM

NV centers and NV magnetometry

Nitrogen vacancy (NV) center in diamond

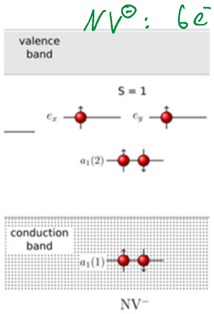
• substitutional **nitrogen** and a nearest neighbor **lattice vacancy**

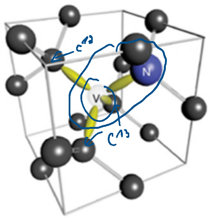
• pointdefect, ***C₃v*** ymmetry

- S = 1 (when negatively charged)

NV^0 : $5e^-$

NV^- : $6e^-$





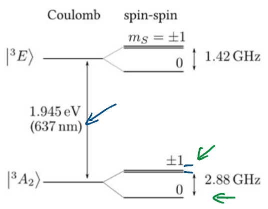
ground-state spin Hamiltonian:

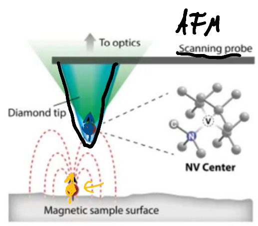
$$\mathcal{H} = \overbrace{hD_{\parallel}S_z^2 + g\mu_B B_{NV} S_z}^{\text{axial } \mathcal{H}_{\parallel}}$$

c

$$\nu_{\pm} = D_{\parallel} \pm \frac{g\mu_B}{h} B_{NV}$$

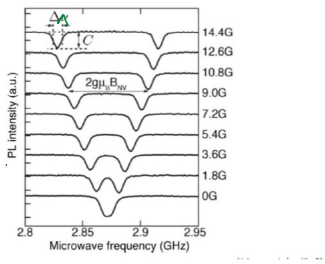
NV centers and NV magnetometry





Spin readout

- spin detection via **fluorescence intensity**
  - $m_s = 0$ ⇨ **bright**
  - $m_s = \pm 1$ ➡ **dark**
  - ➡ contrast up to **30%**, for GS and ES
- opticall detected magnetic resonance (**ODMR**)



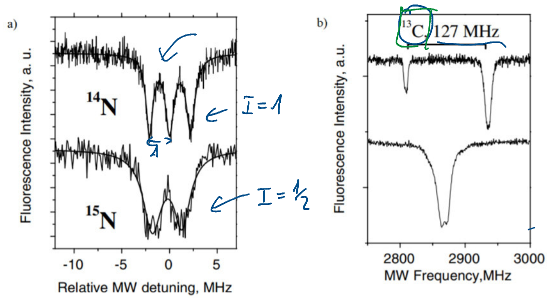
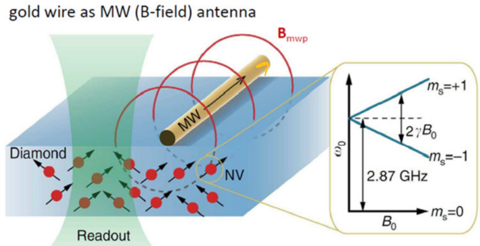
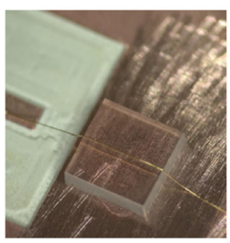


Fig. 10 ODMR spectra with resolved ^{14}N and ^{15}N hyperfine structure (a) and ^{13}C hyperfine structure (b). The spectra have been acquired at room temperature without the application of an external magnetic field.

gold wire as MW (B-field) antenna





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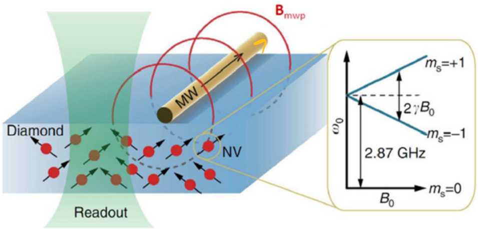
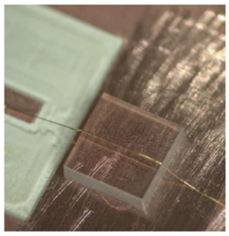
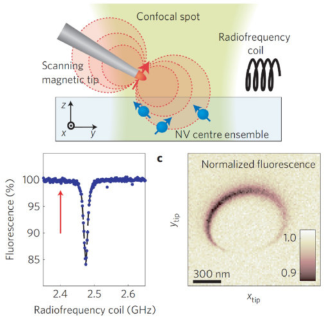




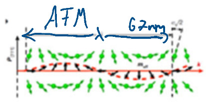
20 µm gold wire above 2x2x0.5 mm³ SC bulk diamond (N < 1ppm)

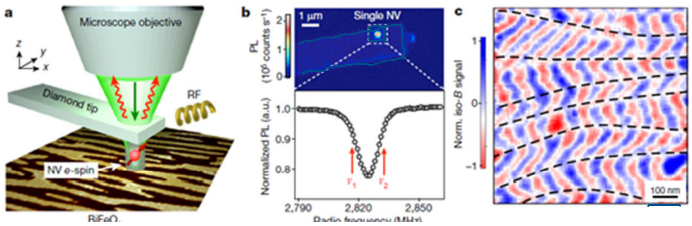


Grinolds et al., *Nat. Phys.* **7** (2011).

NV centers and NV magnetometry

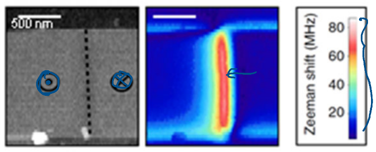
Ferroelectric and magnetic order in BiFeO₃





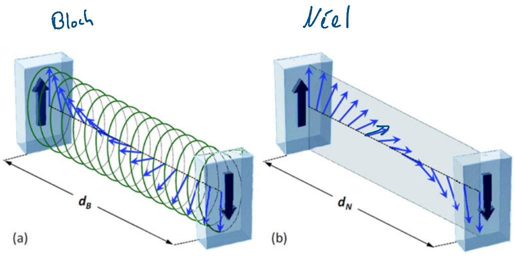
Nature **549** 252–256 (2017)

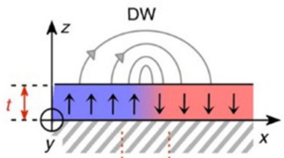
Bloch DWs in a Ta/CoFeB/MgO wire



AFM NV image

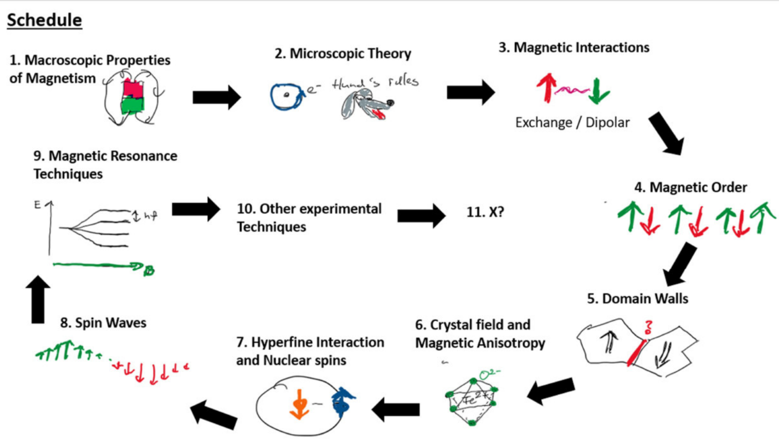
Nat. Commun 6 6733 (2015)





Magnetism –

In a Nutshell



- Books:
  - Gross + Marx: Chapter 12
  - Blundell: Magnetism in Condensed Matter
  - Abragam + Bleaney: Electron Paramagnetic Resonance of Transition ions

Microscopic Theory

- Consider a system of atoms; non-interacting

$$H = \underbrace{\frac{1}{2m}\left[\vec{p} + e\vec{A}\right]^2}_{\text{kinetic part } T} + V(\vec{r})$$

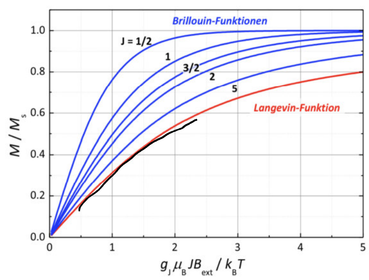
$V(\vec{r})$: electrostatic potential "crystal"

$$\Delta E_n = \langle n | \Delta H | n \rangle + \sum_{n \neq n'} \frac{|\langle n | \Delta H | n' \rangle|^2}{E_n - E_{n'}} + \dots$$

$$= \frac{\mu_B \cdot B_z}{\hbar} \langle n | L_z + g_s S_z | n \rangle \quad \text{(1) Atomic paramagnetism (Langevin)}$$

$$+ \frac{e^2 B_z^2}{8m} \langle n | \sum_i (x_i^2 + y_i^2) | n \rangle \quad \text{(2) Larmor diamagnetism (no spin!)}$$

$$+ \frac{\mu_B^2 B_z^2}{\hbar^2} \sum_{n \neq n'} \frac{|\langle n | L_z + g_s S_z | n' \rangle|^2}{E_n - E_{n'}} \quad \text{(3) Van-Vleck paramagnetism}$$

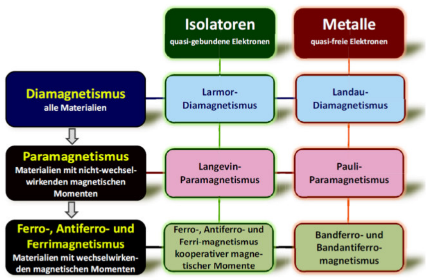


Susceptibility

$$\chi = \frac{C}{T} \quad \text{Curie-law}$$

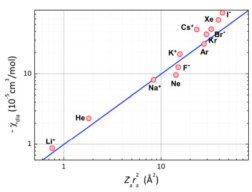
$$C = \frac{\mu_0 \cdot \mu_B^2 \cdot n \cdot J(J+1) \cdot g_J^2}{3 k_B}$$

Curie constant



Larmor Diamagnetism

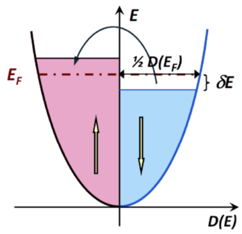
$$\chi_{Dia} \approx -\mu_0 \frac{e^2}{6m} \rho \cdot Z_a \cdot r_a^2$$



Pauli Paramagnetism

$$\chi_p = \mu_0 \cdot \left(\frac{\partial M}{\partial B}\right) = \mu_0 \cdot \mu_B^2 \frac{D(E_F)}{V} = n \cdot \frac{3}{2} \cdot \frac{\mu_0 \cdot \mu_B^2}{k_B \cdot T_F}$$

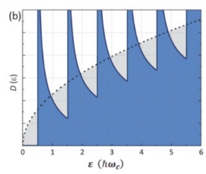
Metall	n (10^{22} cm^{-3})	E_F (eV)	T_F (K)	k_F (10^8 cm^{-1})	v_F (10^8 cm/s)
Li	4.70	4.72	54 800	1.11	1.27
Na	2.54	3.16	36 700	0.91	1.05
Rb	1.15	1.85	21 500	0.69	0.79
Cu	8.45	7.00	81 200	1.35	1.55
Au	5.90	5.51	63 900	1.20	1.38
Ag	5.86	5.49	63 700	1.20	1.39
Be	24.2	14.14	164 100	1.92	2.21
Zn	13.10	9.39	109 000	1.56	1.79
Al	18.06	11.63	134 900	1.74	2.00
Pb	13.20	9.37	108 700	1.57	1.81



Landau Diamagnetism

for a free e^- gas: $\chi_L = -\frac{1}{3} \chi_p$

for a real crystal: $\chi_L = -\frac{1}{3} \chi_p \cdot \left(\frac{m}{m^*}\right)^2$



Review: Hund's rule

- Answers the question: What are **S, L and J** for the many particle ground state

S + L = J

1. Rule
Max $S = \sum_i s_i$
- Pauli exclusion
- Coulomb repulsion

$\Delta E > 1eV$

2. Rule
Max $L = \sum_i l_i$
- 1 Rule
- Coulomb repulsion (evenly distributed charges)

$\Delta E \lessapprox 1eV$

3. Rule
Couple L+S to J

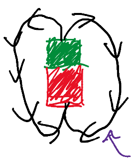
Optimize the spin-orbit interaction

$\lambda \cdot \vec{L} \cdot \vec{S}$ $\Delta E \leq 1eV$

$$J = \begin{cases} |L-S| & \text{for } n \leq (2l+1) \quad \lambda > 0 \\ |L+S| & \text{for } n > (2l+1) \quad \lambda < 0 \end{cases}$$

Magnetic Interaction

3.1. Magnetic dipolar Interaction



$$E_D = \frac{\mu_0}{4\pi} \cdot \frac{1}{r^3} \underbrace{\left[\vec{m}_1 \cdot \vec{m}_2 - 3\left(\vec{m}_1 \cdot \hat{r}\right)\left(\vec{m}_2 \cdot \hat{r}\right)\right]}_{\text{MDI is anisotropic}}$$

$g_e \cdot \mu_B \cdot \vec{S}_2$

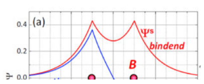
Connecting vector

3.2. Magnetic Exchange Interaction

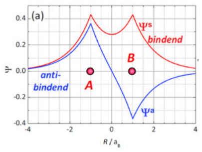
$$\chi_{asym} = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$$

r_1 r_2 r_1 r_2

$$\underbrace{\chi_{sym} = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{cases}}_{\text{triplet}}$$



triplet

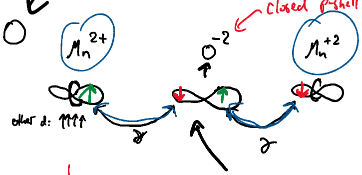


$J(r)$

Heisenberg model $\quad H_{ex} = -\frac{J}{\hbar^2} \cdot \vec{S}_1 \cdot \vec{S}_2$

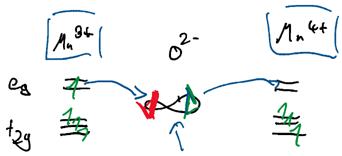
- Direct exchange
- Super exchange:

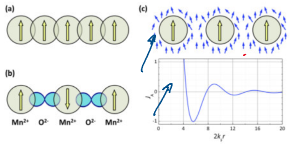
MnO



- Double exchange:

In "mixed-valence compounds"





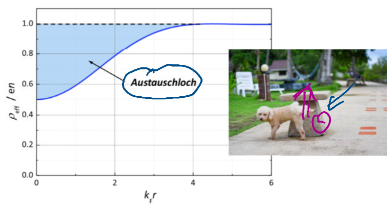
- RKKY - Interaction (Ruderman - Kittel - Kasuya - Yosida)

$$J_{RKKY} \propto \frac{\cos(2 \cdot k_F \cdot r)}{(2 \cdot k_F \cdot r)^3}$$

- Antisymmetric Exchange (Dzyaloshinskii - Moriya interaction) DM

$$H_{DM} = D_{ij} \cdot (\vec{S}_i \times \vec{S}_j)$$

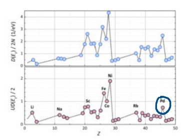
Exchange Interaction between itinerant (mobile) electrons



--> e^- less shielded by any other e^-
↳ sees more positive cores
↳ Higher binding energy
⇒ good for Coulomb
↳ But: trapped in a hole
→ Higher kin energy

Stoner Criterion

$$\boxed{\frac{1}{2} U \cdot D(E_F) > 1}$$



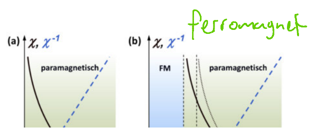
$$\boxed{\chi = I \cdot \chi_p}$$

χ_p: Pauli - susceptibility

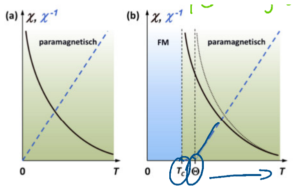
$$I = \frac{1}{1 - \frac{1}{2} U \cdot D(E_F)}$$

$\uparrow \lambda$

4. Magnetic Order

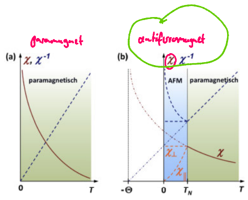


$$\boxed{T_C = \gamma \cdot C}$$



$$\boxed{T_c = \gamma \cdot C}$$

$$\boxed{\chi = \frac{C}{T - T_c}}$$ Curie-Weiss-law



$$\boxed{T_N = |\gamma_{AB} - \gamma_{AA}| \cdot C}$$ ← only for 1 sublattice (otherwise $\frac{1}{2}$)

T_N: Néel

$$\boxed{\chi = \frac{2C}{T + \Theta} \quad (\text{above } T_N) \qquad \Theta = |\gamma_{AB} + \gamma_{AA}| \cdot C}$$

(paramagnetic Néel temperature)

5. Crystal field and magnetic anisotropy

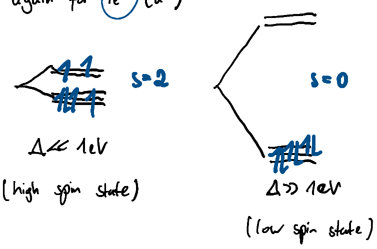
electric field induced by neighboring ions

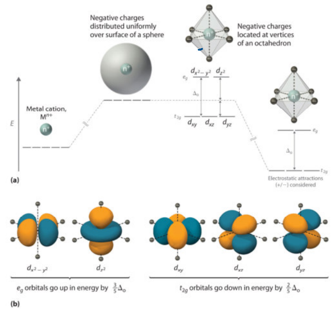
⇒ Crystal field
- break spherical symmetry
- ≈ 1 eV for 3d
- stronger than spin-orbit interaction $\lambda \cdot \vec{S} \cdot \vec{L}$

↳ Violation for 3rd Hunds' rule (J is not a good quantum number anymore)

Tetrahedral

again for Fe^{2+} (d^6)





Orbital quenching

$g_J(J(J+1))^{1/2}$ $\quad$ $g_S(S(S+1))^{1/2}$

$L = 0$

$\uparrow$

$\lambda \ll \Delta$

ion	shell	S	L	J	term	p_1	p_{exp}	p_2
Ti^{3+}, V^{4+}	$3d^1$	$\frac{1}{2}$	2	$\frac{3}{2}$	$^2D_{3/2}$	1.55	1.70	1.73
V^{3+}	$3d^2$	1	3	2	$^3F_2$	1.63	2.61	2.83
Cr^{3+}, V^{2+}	$3d^3$	$\frac{3}{2}$	3	$\frac{3}{2}$	$^4F_{3/2}$	0.77	3.85	3.87
Mn^{3+}, Cr^{2+}	$3d^4$	2	2	0	$^5D_0$	0	4.82	4.90
Fe^{3+}, Mn^{2+}	$3d^5$	$\frac{5}{2}$	0	$\frac{5}{2}$	$^6S_{5/2}$	5.92	5.82	5.92
Fe^{2+}	$3d^6$	2	2	4	$^5D_4$	6.70	5.36	4.90
Co^{2+}	$3d^7$	$\frac{3}{2}$	3	$\frac{9}{2}$	$^4F_{9/2}$	6.63	4.90	3.87
Ni^{2+}	$3d^8$	1	3	4	$^3F_4$	5.59	3.12	2.83
Cu^{2+}	$3d^9$	$\frac{1}{2}$	2	$\frac{5}{2}$	$^2D_{5/2}$	3.55	1.83	1.73
Zn^{2+}	$3d^{10}$	0	0	0	$^1S_0$	0	0	0

Forms of anisotropy

$$E_{ani} = E_{MC} + E_{shape} + E_{ind}$$

E_{MC}: Magnetocrystalline

E_{ind}: Induced

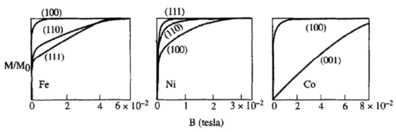


Fig. 6.22 Magnetization in Fe, Co and Ni for applied fields in different directions showing anisotropy. After Honda and Kaya 1926, Kaya 1928.

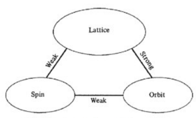


Fig. 7.8 Spin–lattice–orbit interactions.

6. Nuclear spins and Hyperfine interaction

$$\mu_B \approx 58 \frac{\mu eV}{T} \hat{=} 14 \frac{GHz}{T}$$

$/h$

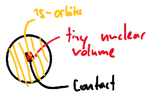
$$\mu_N \approx 31 \frac{neV}{T} \hat{=} 7.6 \frac{MHz}{T}$$

Nucleus	Z	N	I	μ/μ_N	g_I	ν (in MHz for $B = 1$ T)
n	0	1	$\frac{1}{2}$	−1.913	−3.826	29.17
p=^{1}H	1	0	$\frac{1}{2}$	2.793	5.586	42.58
d=^{2}H	1	1	1	0.857	0.857	6.536
t=^{3}H	1	2	$\frac{1}{2}$	−2.128	4.255	32.43
^{12}C	6	6	0	0	0	0
^{13}C	6	7	$\frac{1}{2}$	0.702	1.404	10.71
^{14}N	7	7	1	0.404	0.404	3.076
^{16}O	8	8	0	0	0	0
^{17}O	8	9	$\frac{5}{2}$	−1.893	−0.757	5.772
^{19}F	9	10	$\frac{1}{2}$	2.628	5.257	40.05
^{31}P	15	16	$\frac{1}{2}$	1.132	2.263	17.24
^{33}S	16	17	$\frac{3}{2}$	0.643	0.429	3.266

Hyperfine Interaction

$$H_{HFI} = A \cdot \vec{I} \cdot \vec{J}$$

1 Fermi-contact interaction (isotropic)



$$H_{Contact} = \left(\frac{2}{3}\mu_0\right) g_e \mu_B \cdot g_I \cdot \mu_N \cdot |\Psi(0)|^2 \cdot \vec{I} \cdot \vec{J}$$

probability for e^- to be at the nucleus

(more precisely: density of unpaired s-electrons at the nucleus)

2 magnetic dipolar interaction (anisotropic)

$$H_{Dip} = \frac{\mu_0 g_e g_I \cdot \mu_B \cdot \mu_N}{4\pi r^3} \cdot \left[\vec{I} \cdot \vec{S} - 3 (\vec{I} \cdot \hat{r}) \cdot (\vec{S} \cdot \hat{r})\right]$$

So far: magnetic moments were far apart from each other → treat as point sources

for hyperfine

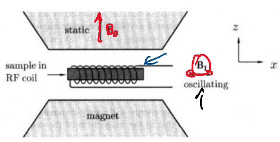
e.g. $d_{x^2-y^2}$

↳ integration required

↳ strong anisotropy of A (-tensor)

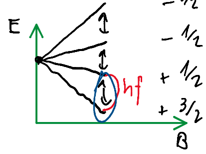
7. Magnetic Resonance Techniques [Experimental Probes of Magnetism]

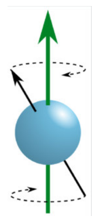
NMR



Nuclear spins in an external magnetic field

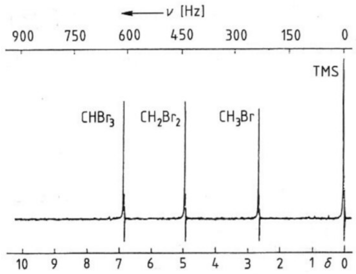
$I = 3/2$





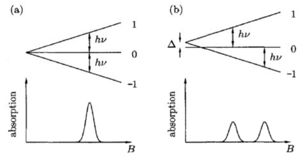
$$E = - g_N \cdot \mu_N \cdot m_I \cdot B$$

$$\Delta E = h \cdot f = g_N \cdot \mu_N \cdot B \cdot \Delta m_I$$



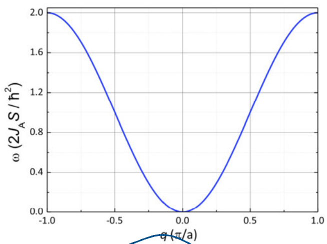
- Works @ Room temperature
- Chemical sensitivity via
  1. Chemical shift
  2. Spin-Spin coupling

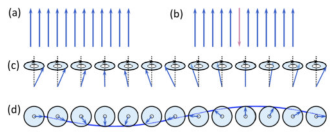
ESR:



- Can probe:
  - g-factor
  - crystal field
  - spin-spin coupling (J or D)
  - hyperfine coupling (A)

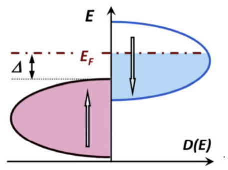
8. Spin waves



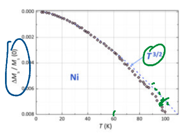


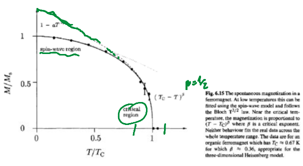
Bloch $T^{3/2}$-law

$$\boxed{\frac{\Delta M}{M_s(T=0)} \propto \left(\frac{k_B T}{J_A\, S/\hbar}\right)^{3/2} \quad \text{Bloch } T^{3/2} \text{ law}}$$



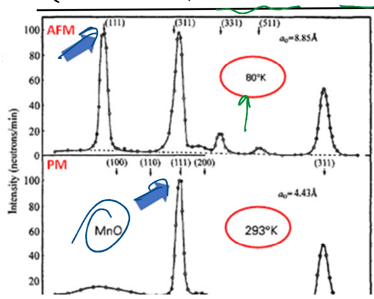
- Describes the LT-dependence of a ferromagnet well





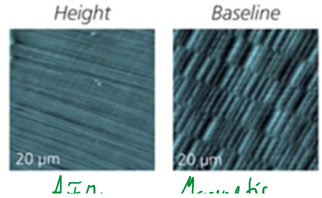
Experimental Probes of Magnetism

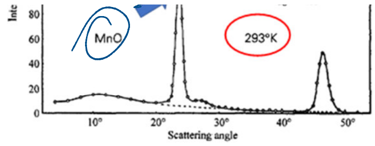
(inelastic) neutron scattering

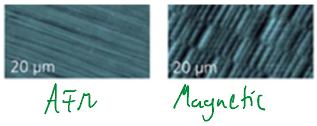


SPM

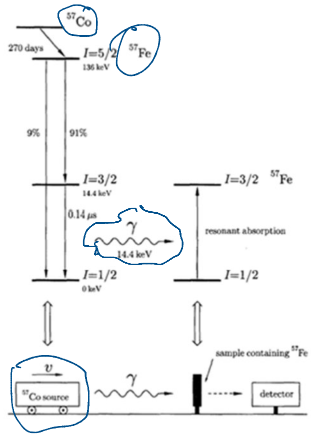
Topography and magnetic structure of a hard disc



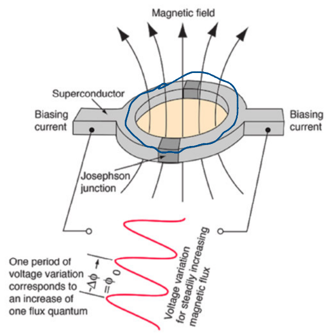




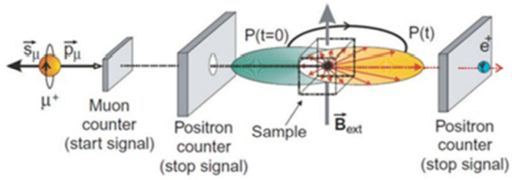
Mößbauer



SQUID



Muon Spin Rotation

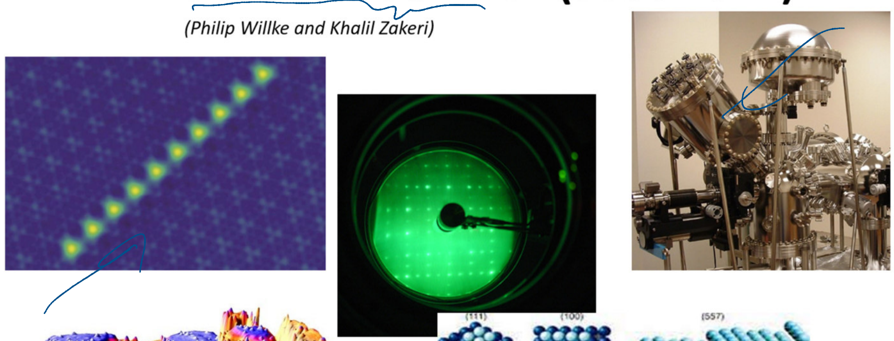


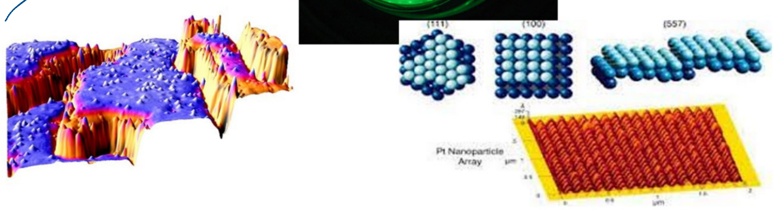
Modulkatalog

Ziel der Vorlesung ist es, die Studenten mit einigen der am häufigsten verwendeten **experimentellen Methoden zur Untersuchung der elektronischen Eigenschaften von kondensierter Materie vertraut zu machen**. Ausgehend von den experimentellen Fakten und modernen Beispielen aus der Erforschung kondensierter Materie werden **Grundbegriffe der Fermiologie** (z.B. Bandstruktur und Fermi-Fläche) und der **experimentellen Methoden (Transport, Thermodynamik, Spektroskopie)** zu deren Untersuchung vorgestellt und ausführlich behandelt. Grundlegende Werkzeuge zur Untersuchung und zum **Verständnis von Phasenübergängen** werden gegeben **(Landau-Theorie, kritische Exponenten)**. Eine detaillierte Einführung in den Magnetismus (**Ursprung des Magnetismus, magnetische Wechselwirkungen, magnetische Struktur und magnetische Messungen**) wird gegeben.

SURFACE SCIENCE (SoSe 2022)

(Philip Willke and Khalil Zakeri)



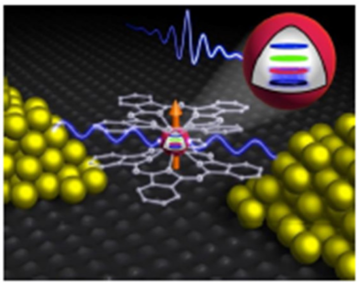


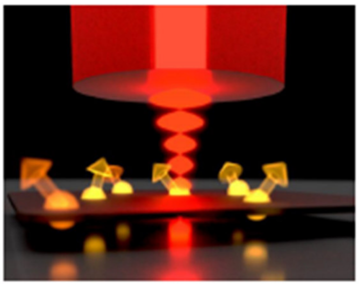
Physikalisches Institut

Prof. Dr. Wolfgang Wernsdorfer, Prof. Dr. David Hunger,
~~Dr. Thomas Reisinger~~, Dr. Philip Willke , MLT

Hauptseminar Sommersemester 2022

Aktuelle Experimente in der Quantenphysik



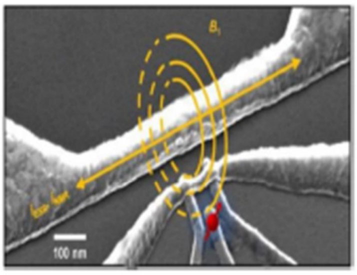


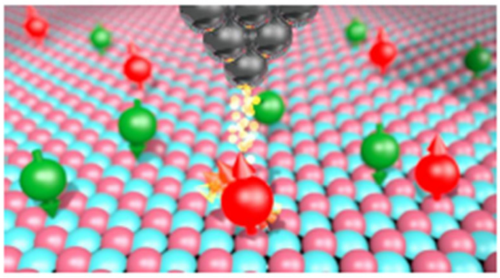
- How to build a qubit
- Quantum Computing
- Techniken zur kohärenten Einzelspinkontrolle (Rabi, Ramsey, Echo)
- Supraleitende Transmon Qubits
- Flux Qubits und das Fluxonium
- Molekulare Einzelmagnete als Spin Qubits
- NV Zentren in Diamant & opt. Spinauslese
- Quantensensing mit NV Zentren
- Quantennetzwerke mit NV Zentren
- Elektronenspinresonanz mit atomaren Einzelmagneten auf Oberflächen
- Magnetometrie auf der atomaren Skala
- Kohärente Spinkontrolle von einzelnen Atomen mit einem Rastertunnelmikroskop

Interessierte können sich ab sofort über Ilias, **anmelden.**

Eine Liste möglicher Themen entnehmen Sie diesem Aushang.

Die **Vorbesprechung** und Einteilung der Vorträge findet am **15.04.2021 um 14:00** Uhr über **Zoom** statt. Der entsprechende Link wird über Ilias bekannt gegeben.





Elektronische Eigenschaften von Festkörpern II

A. Ustinov

superconductivity

Superconductivity