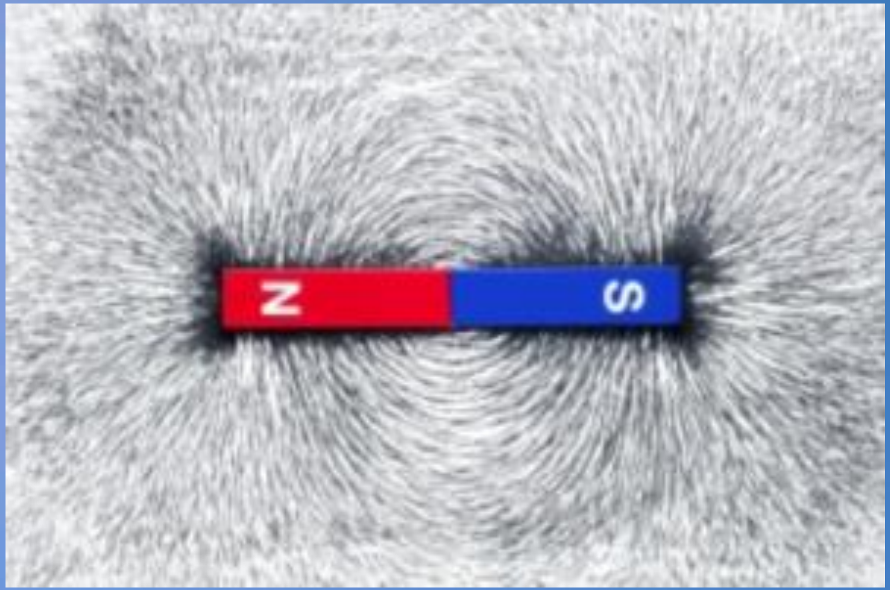
2022.4.6 Lecture 1

10:25 – 11:55

Lecture on

Magnetic Properties of Materials

磁性 (Magnetism)



Institute for Solid State Physics, University of Tokyo

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Syllabus

1. Phenomenology of magnetism. Magnetization process
2. Spin magnetic moments in solids
3. Mutual interaction between spins
4. Ordered states of spins. Phase transitions
5. Magnetism in insulators
6. Magnetism of itinerant electrons
7. Some advanced topics (?)

How the lecture will go on?

- The lecture notes (in Japanese, English) will be uploaded in the site
  https://kats.issp.u-tokyo.ac.jp/kats/magnetism/
  by the end of the lecture week.

- Attendance will be taken. That contributes to the achievement.

- Small amount of problems for your exercise at home will be given in the last of the lecture in every two weeks. Submission deadline of the solutions is two weeks later. In order to submit your answer, you need to register yourself from the web page that will be prepared by the next week.

- In the very last of the lecture in July, the problems for your report will be given. The deadline for the submission of the report will be notified then.

Contents Wed. 6th April 2022

Chapter 1 Basic Notions of Magnetism

1. Electromagnetic fields in the vacuum, and those with materials
2. Experimental methods to measure magnetization
3. Magnetism in classical pictures
4. Spins of electrons and their magnetic moment

Electromagnetic fields in the vacuum

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0},$$

Maxwell equations for electromagnetic fields in the vacuum

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t},$$

Electromagnetic induction

$$\nabla \cdot \boldsymbol{B} = 0,$$

No magnetic monopole

$$\nabla \times \boldsymbol{B} = \mu_0 \left(\boldsymbol{j} + \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} \right).$$

Electric current can create magnetic field

E: Electric field, ***B***: Magnetic flux density (Magnetic field)

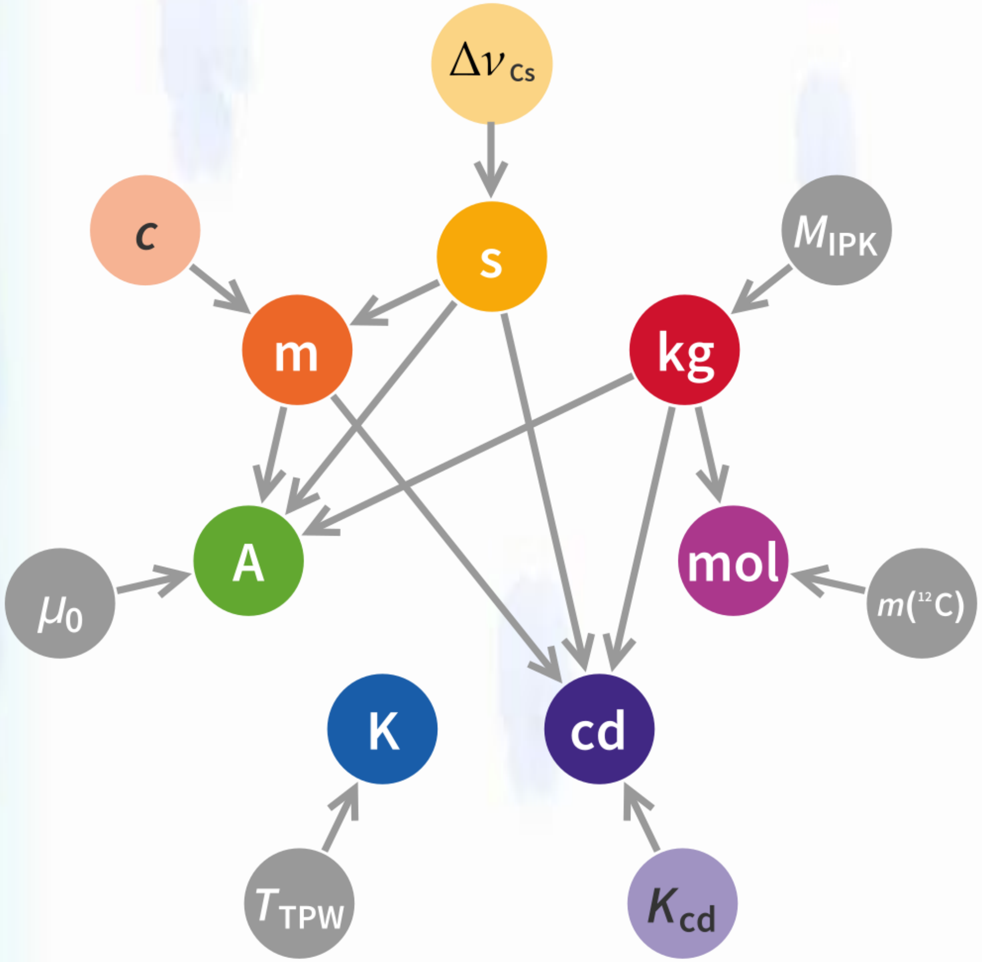
Problem of “Unit”

No 4π factor appears in the above Maxwell equations: rationalized system of units

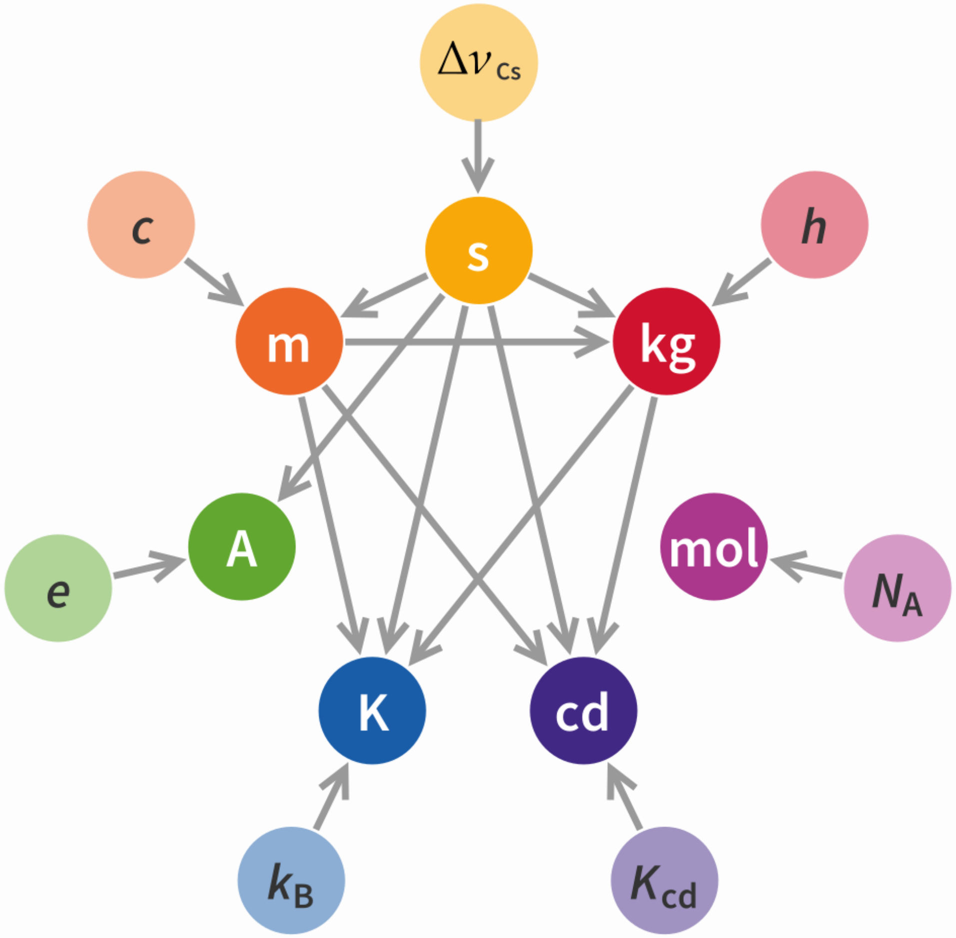
E-B formulation, E-H formulation : Difference in the unit of magnetization!

2019 Redefinition of the SI base units

Old SI



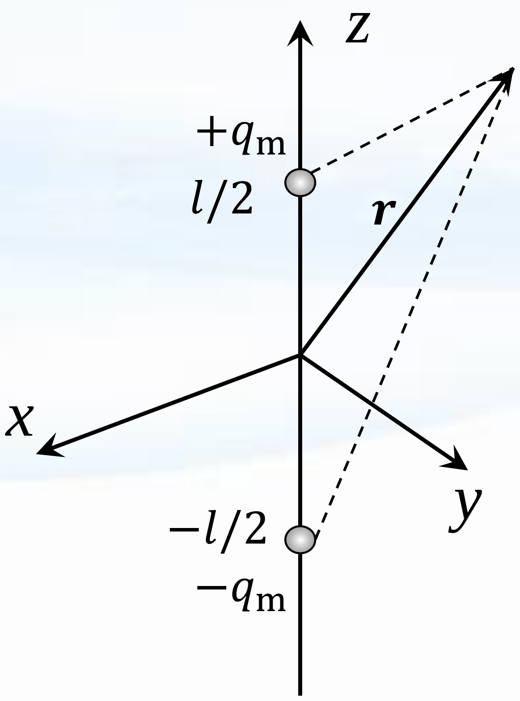
Redefined in 2019



Magnetic dipole: a source of magnetic field

Two ways to introduce magnetic dipole:

1. Introduction of magnetic charge
2. Magnetic dipole as the shrink limit of circular current



Introduction of magnetic charge

There is no magnetic monopole but still we can consider pairs of fictitious magnetic charge with the total charge of zero.

$$\phi_{\mathrm{m}}(\boldsymbol{r}) = \frac{1}{4\pi\mu_0}\left(\frac{q_{\mathrm{m}}}{|\boldsymbol{r}-\boldsymbol{l}/2|} - \frac{q_{\mathrm{m}}}{|\boldsymbol{r}+\boldsymbol{l}/2|}\right)$$

Magnetic potential

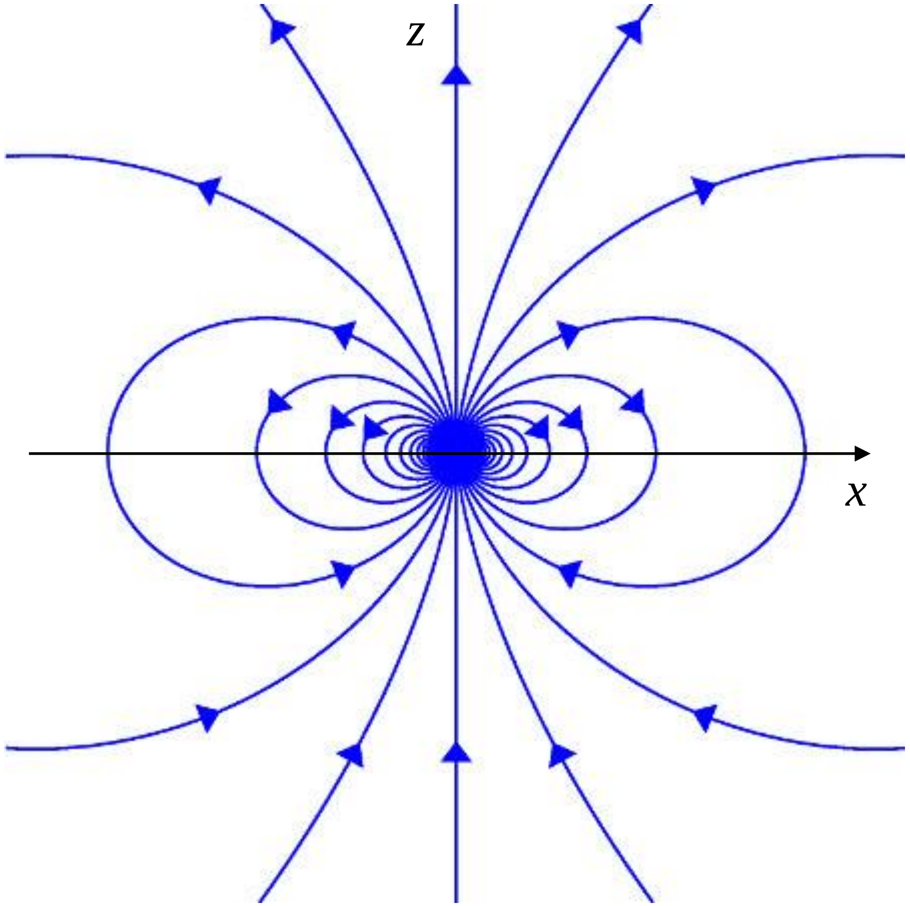
$$\boldsymbol{B} = -\frac{1}{4\pi\mu_0}\nabla\left(\frac{\boldsymbol{\mu}\cdot\boldsymbol{r}}{r^3}\right)$$

Dipole field

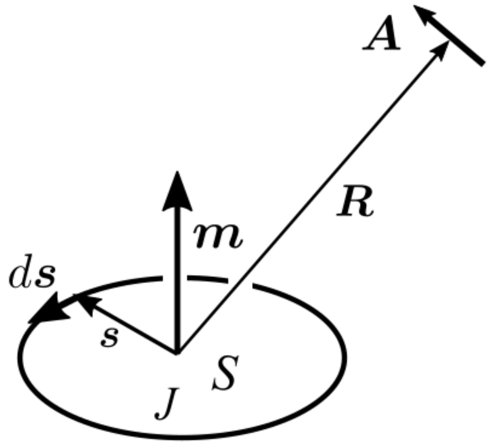
$$B_r = \frac{|\boldsymbol{\mu}|}{4\pi\mu_0}\frac{2\cos\theta}{r^3}, \quad B_\theta = \frac{|\boldsymbol{\mu}|}{4\pi\mu_0}\frac{\sin\theta}{r^3}$$

Expression in polar coordinate

Magnetic dipole: a source of magnetic field (2)



Magnetic dipole as the shrink limit of circular current



Vector potential

$$\boldsymbol{A} \simeq \frac{\mu_0 J}{4\pi} \frac{1}{R^3} \oint (\boldsymbol{R} \cdot \boldsymbol{s}) d\boldsymbol{s}$$

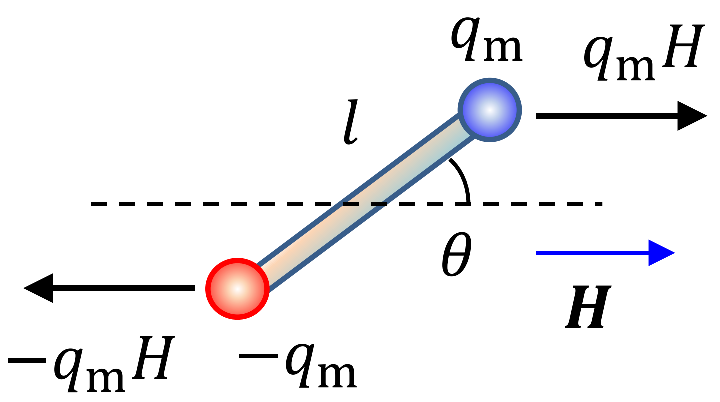
Magnetic moment (see the next)

$$\boldsymbol{\mu} = J \left(\frac{1}{2} \oint \boldsymbol{s} \times d\boldsymbol{s} \right)$$

Magnetic field: $\boldsymbol{B} = -\frac{\mu_0}{4\pi} \nabla \frac{\boldsymbol{\mu} \cdot \boldsymbol{r}}{r^3}$

A circular current can serve as a magnetic dipole.

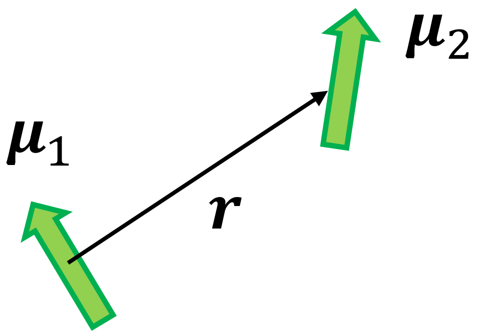
Magnetic moment



Couple of force moment: $L = -q_\mathrm{m} l H \sin\theta = -\dfrac{q_\mathrm{m} l}{\mu_0} B \sin\theta$

Magnetic moment $\mu \equiv \dfrac{q_\mathrm{m} l}{\mu_0}$

E-B formation

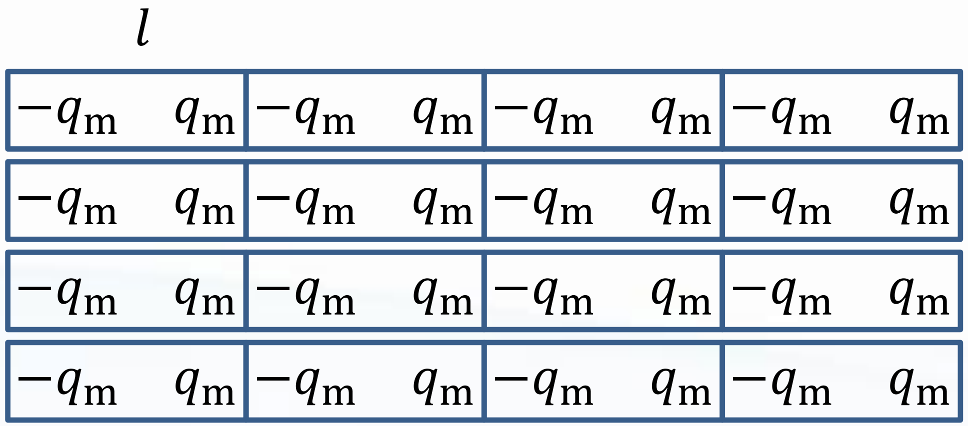


(a) Stable (b) Unstable

Dipole-dipole interaction: the dipoles feel each other's fields.

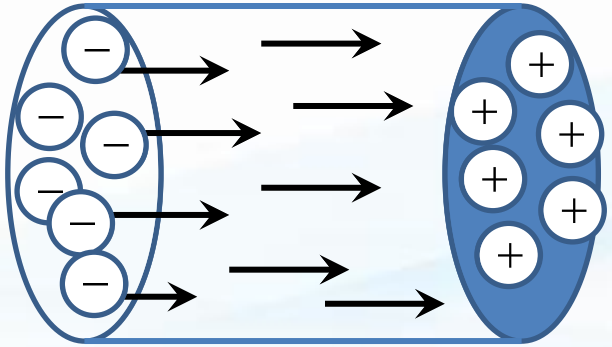
Potential: $U = \dfrac{1}{4\pi\mu_0 r^3}\left\{\boldsymbol{\mu}_1\cdot\boldsymbol{\mu}_2 - \dfrac{3}{r^2}(\boldsymbol{\mu}_1\cdot\boldsymbol{r})(\boldsymbol{\mu}_2\cdot\boldsymbol{r})\right\}$

A naïve dipole model of magnetization of materials



Set of small magnets

Density of magnets: N



Magnetic charges appear at the ends of the material

Magnetization: $\boldsymbol{M} = \sum_{\mathrm{unit\,vol.}} \boldsymbol{\mu} = N q_{\mathrm{m}} \boldsymbol{l} / \mu_0 \equiv \rho \boldsymbol{l} / \mu_0$

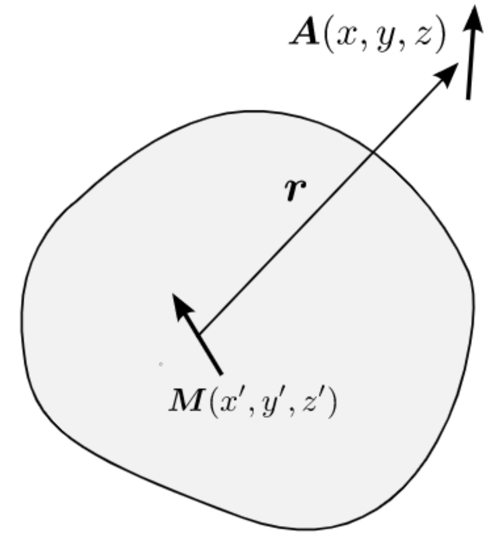
Surface density of magnetic charge $\sigma = q_{\mathrm{m}} s = q_{\mathrm{m}} N l = \mu_0 |\boldsymbol{M}|$

Expression with "equivalent current" in materials

Magnetic moments → vector potential

$$\boldsymbol{A} = \frac{\mu_0}{4\pi}\int_{\mathrm{mat}} dv' \frac{\boldsymbol{M}' \times \boldsymbol{r}}{r^3} = -\frac{\mu_0}{4\pi}\int_{\mathrm{mat}} dv' \left(\boldsymbol{M}' \times \nabla \frac{1}{r}\right)$$

$$= \frac{\mu_0}{4\pi}\int_{\mathrm{mat}} dv' \left(\boldsymbol{M}' \times \nabla' \frac{1}{r}\right)$$



Partial integration: $\boldsymbol{A} = \frac{\mu_0}{4\pi}\int_{\mathrm{mat}} dv' \frac{\nabla' \times \boldsymbol{M}'}{r}$

Equivalent current: $\boldsymbol{j}_M \equiv \nabla \times \boldsymbol{M} \longrightarrow \boldsymbol{A} = \frac{\mu_0}{4\pi}\int dv' \frac{\boldsymbol{j}' + \boldsymbol{j}'_M}{r}$

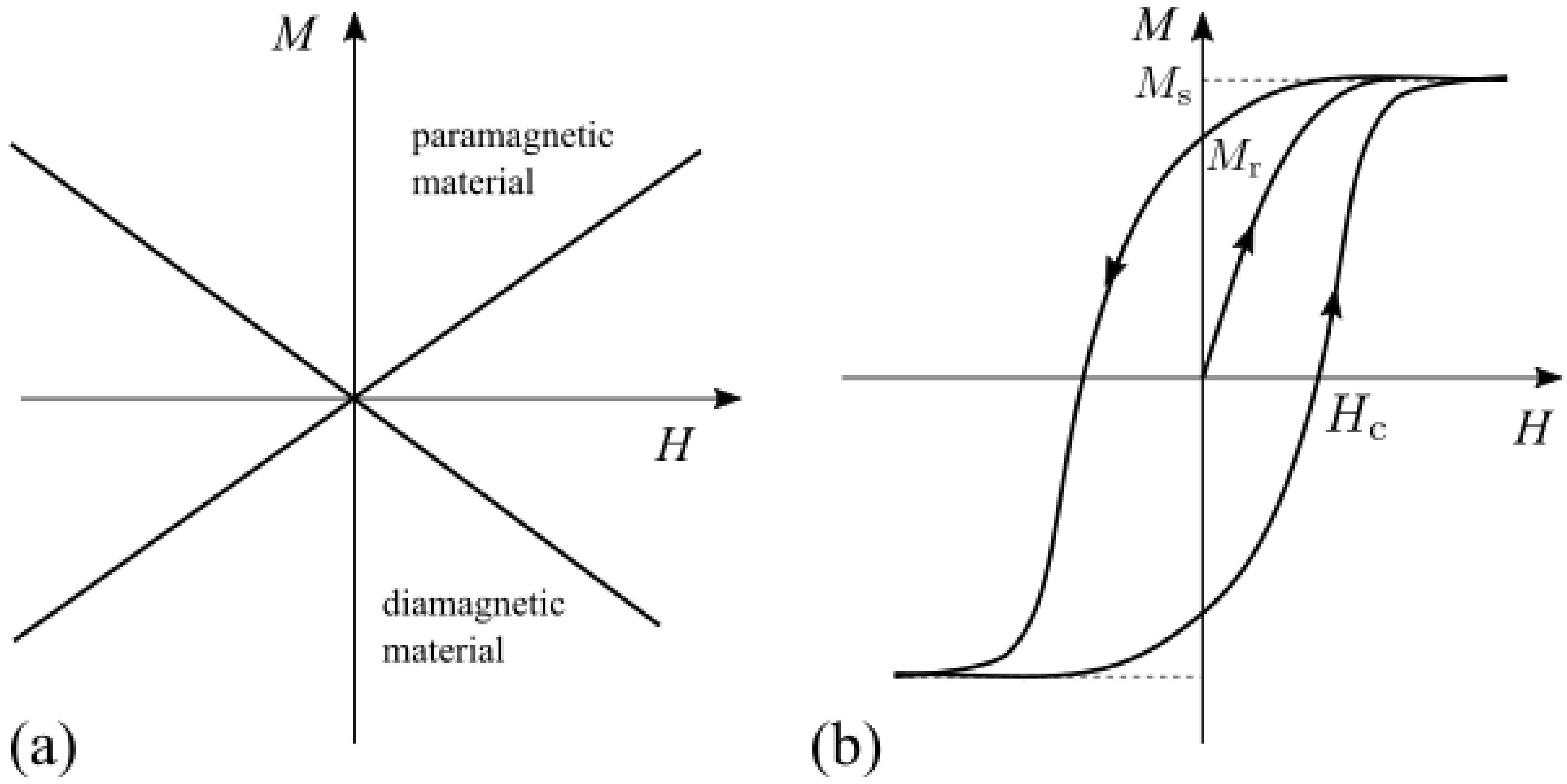
$$\nabla \times \boldsymbol{B} = \mu_0(\boldsymbol{j} + \boldsymbol{j}_M) = \mu_0 \boldsymbol{j} + \mu_0 \nabla \times \boldsymbol{M}$$

Introduction of magnetic field: $\boldsymbol{H} \equiv \boldsymbol{B}/\mu_0 - \boldsymbol{M}$

Maxwell equation with electric flux density $\nabla \times \boldsymbol{H} = \boldsymbol{j} + \frac{\partial \boldsymbol{D}}{\partial t}$

M-H curve

M-H relation



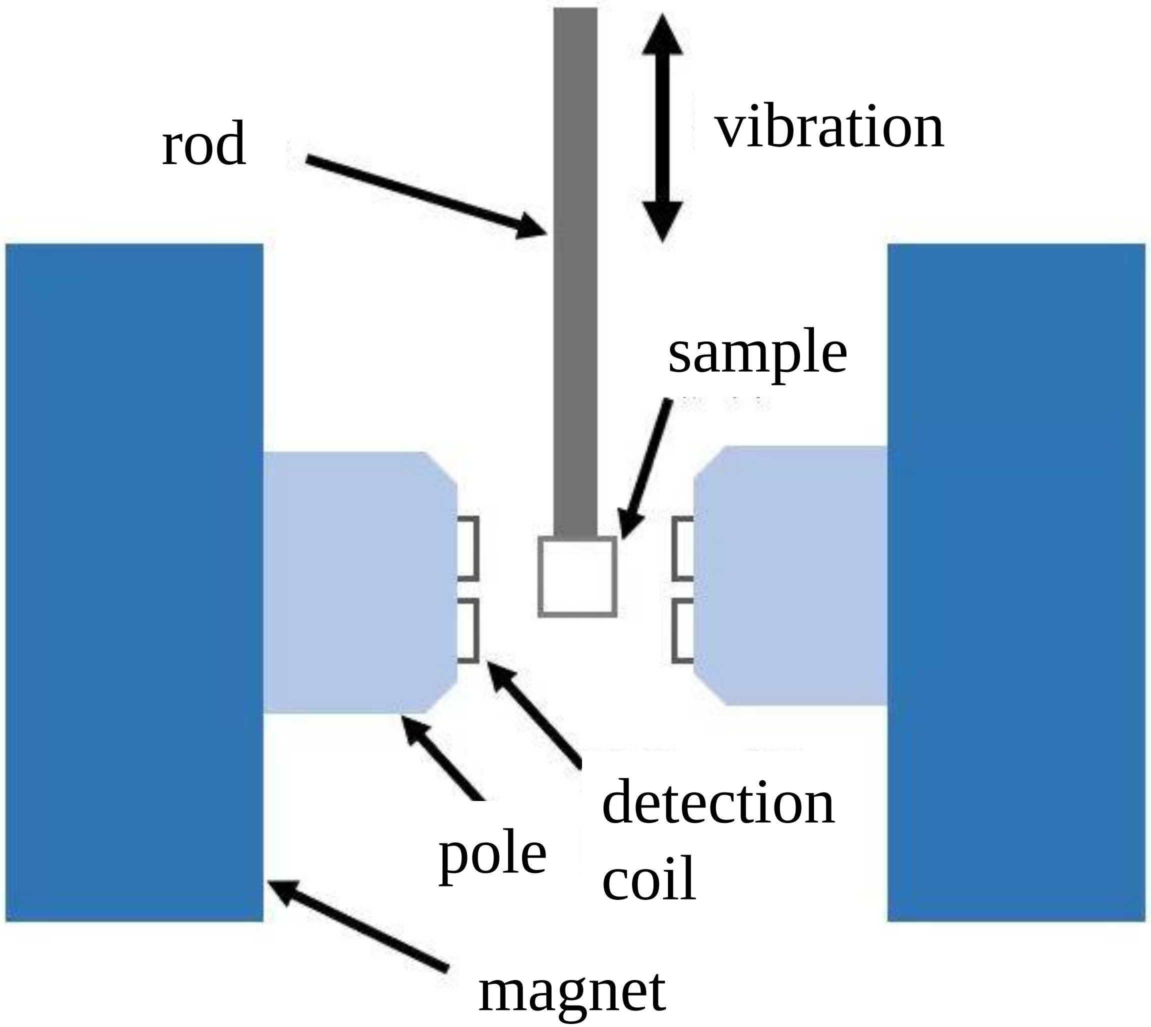
H_c: Coercive force,
M_r: Remanent magnetization,
M_s: Saturation magnetization

Linear: Paramagnetic materials, diamagnetic materials

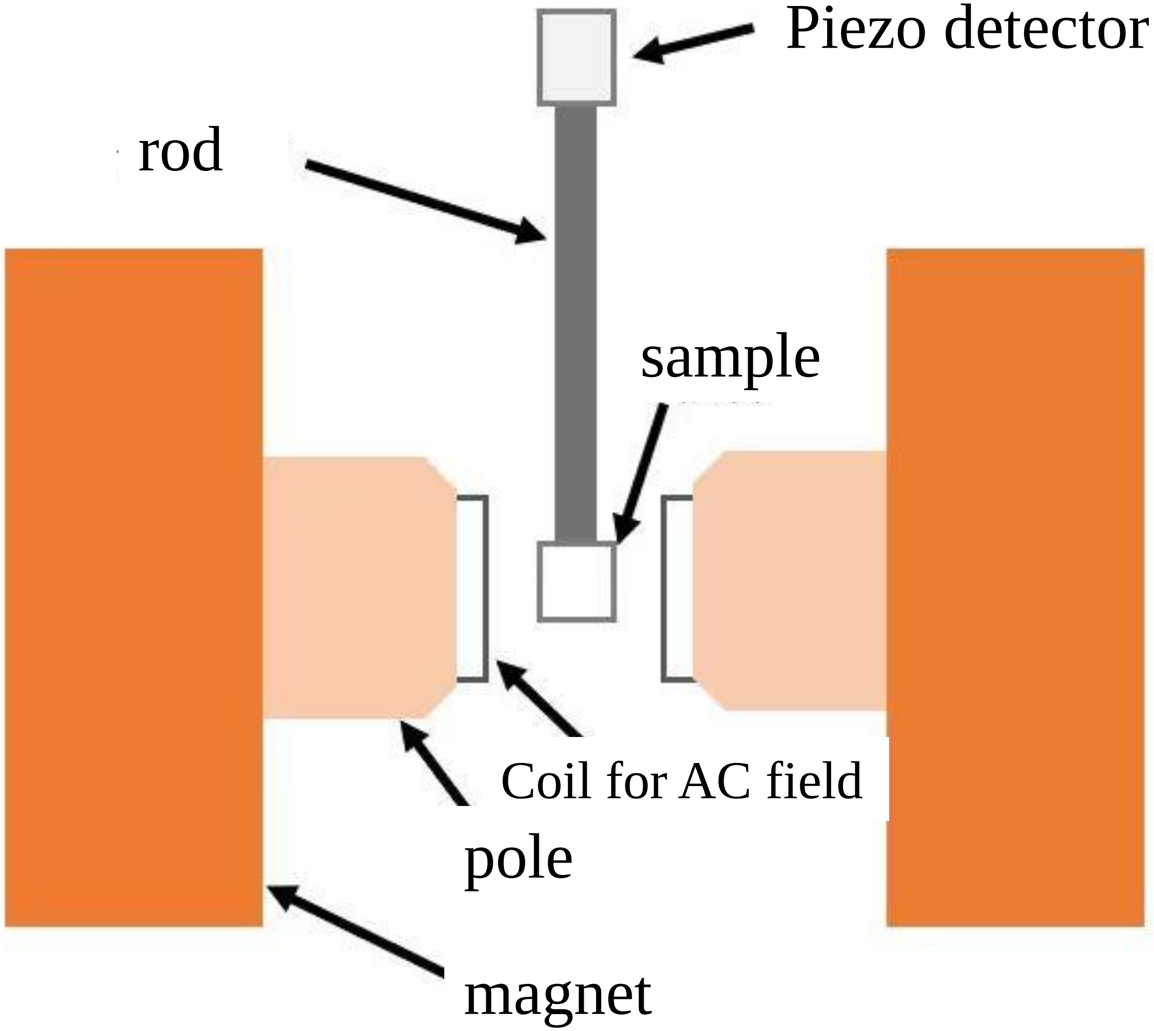
Strongly non-linear with hysteresis: Ferromagnetic materials, superconductors, …

Measurement of magnetization (1)

Vibrating sample magnetometer (VSM)

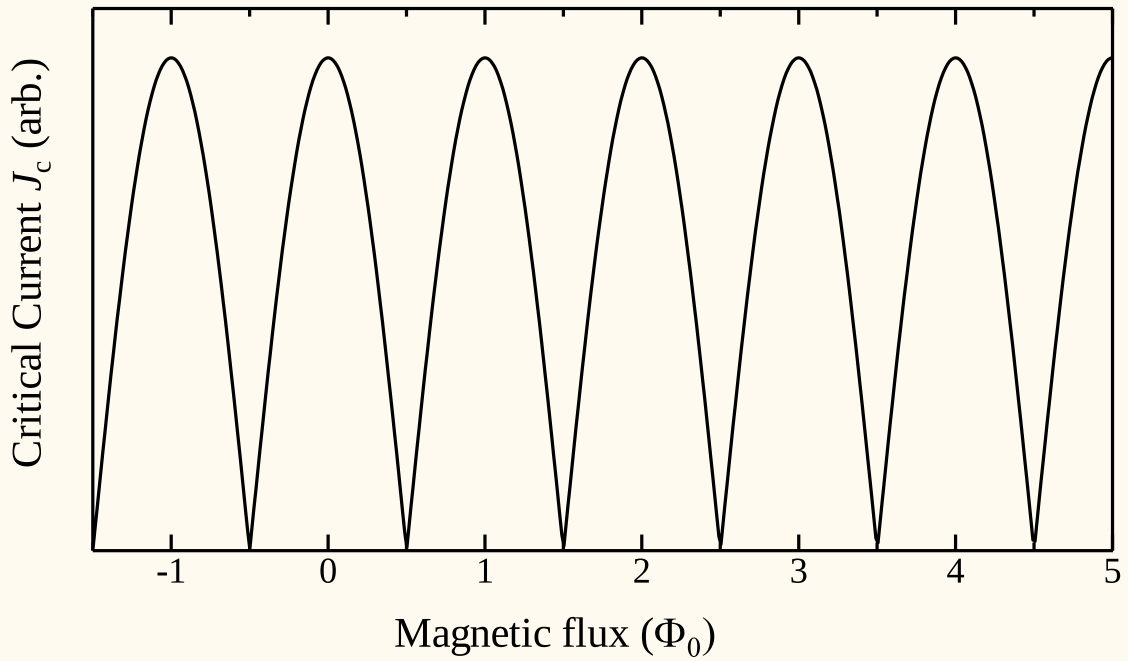


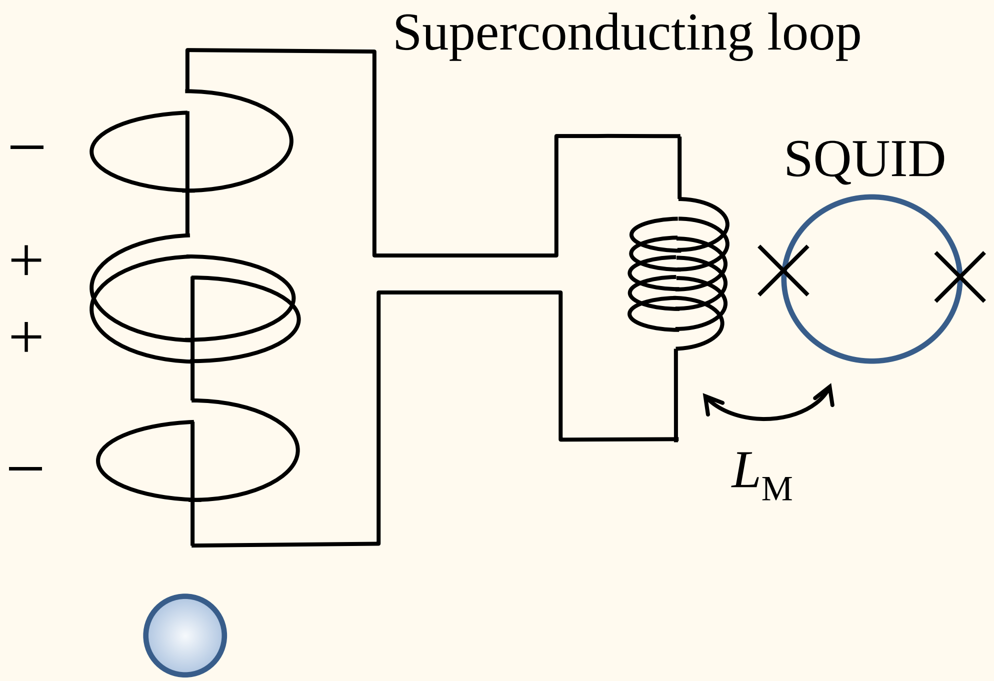
Alternating-gradient magnetometer (AGM)



Measurement of magnetization (2)

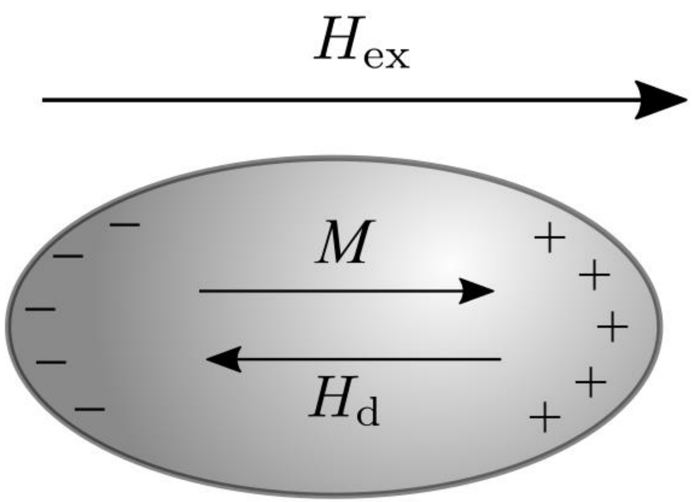
Superconducting quantum interference device (SQUID) magnetometer





$$\Phi_0 \equiv h/2e \approx 2.07 \times 10^{-15} \ \text{Wb}$$

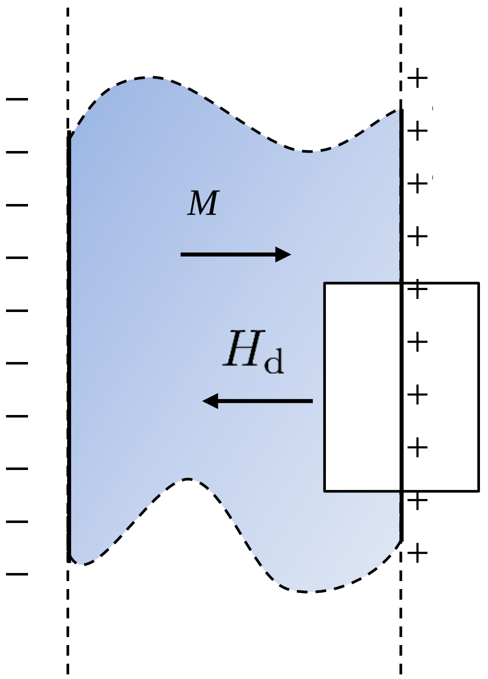
Effect of demagnetizing field



Magnetization causes creation of magnetic charges on the surface, which produces demagnetizing field inside.

$$H_{\mathrm{d}} = N \frac{M}{\mu_0}$$

N : demagnetizing factor
(depends only on shape)



In the case of infinite plate

$$\int_{\mathrm{surface}} H_{\mathrm{n}} ds = H_{\mathrm{d}} = \frac{M}{\mu_0}$$

$$\therefore N = 1$$

Example: Permalloy (Py)

Coercive force: 0.025 Oe
Saturation magnetization field: 3860 Oe

Classical treatment of magnetism

Paramagnetic moment

Model: set of molecules with independent magnetic moment μ in the magnetic field with flux density B along z-axis

Moment magnetic energy:

$$U = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\mu B \cos\theta$$

Average on classical distribution:

$$\begin{aligned}\langle \mu_z \rangle &= \int \exp\left(-\frac{U}{k_\mathrm{B}T}\right) \mu_z d\Omega \Big/ \int \exp\left(-\frac{U}{k_\mathrm{B}T}\right) d\Omega \\ &= \int \exp\left(\frac{\mu B\cos\theta}{k_\mathrm{B}T}\right) \mu\cos\theta d\Omega \Big/ \int \exp\left(\frac{\mu B\cos\theta}{k_\mathrm{B}T}\right) d\Omega \\ &= k_\mathrm{B}T \frac{\partial}{\partial B} \log\left[2\pi \int_0^\pi \exp\left(\frac{\mu B\cos\theta}{k_\mathrm{B}T}\right) \sin\theta d\theta\right] = \mu\left[\coth\left(\frac{\mu B}{k_\mathrm{B}T}\right) - \frac{k_\mathrm{B}T}{\mu B}\right]\end{aligned}$$

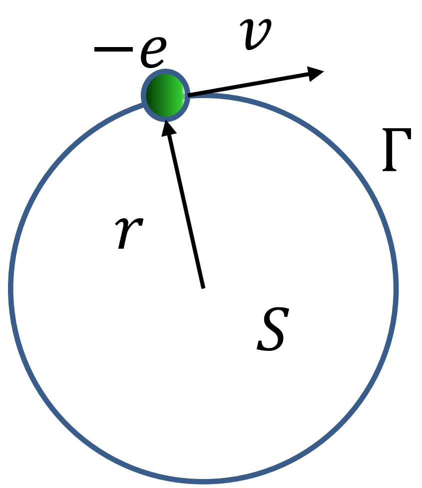
High temperature approximation:

$$\mu B \ll k_\mathrm{B}T$$

Curie law:

$$\frac{\langle \mu_z \rangle}{B} \sim \frac{\mu^2}{3k_\mathrm{B}} \frac{1}{T}$$

Classical paramagnetism



$$\oint_{\Gamma} \boldsymbol{E} \cdot d\boldsymbol{l} = -\frac{\partial}{\partial t} \int_{S} \boldsymbol{B} \cdot d\boldsymbol{\sigma}$$ Maxwell equation

$$2\pi r E = -\frac{\partial}{\partial t}\left(B\pi r^2\right) \qquad \therefore E = -\frac{r}{2}\frac{dB}{dt}$$

$$\frac{dL}{dt} = r \times (-eE) = e\frac{r^2}{2}\frac{dB}{dt}$$

Magnetic flux 0 $\rightarrow B$

$$\text{Angular momentum } 0 \rightarrow L = e\frac{r^2}{2}B$$

$$\mu = SJ = \pi r^2 \frac{ev}{2\pi r} = \pi r^2 \frac{L}{mr}\frac{e}{\pi r} = \frac{e}{2m} e\frac{r^2}{2} B$$

$$\mu = -\frac{e^2}{4m}\left\langle x^2 + y^2 \right\rangle_{\text{av}} B$$

Breakdown of classical magnetism

Hamiltonian $$\mathcal{H} = \frac{1}{2m}(\boldsymbol{p} + e\boldsymbol{A})^2 - e\phi$$

Symmetric gauge: $$\boldsymbol{A} = (\boldsymbol{B} \times \boldsymbol{r})/2$$

$$\mathcal{H} = \frac{\boldsymbol{p}^2}{2m} + \frac{e}{2m}(\boldsymbol{r} \times \boldsymbol{p}) \cdot \boldsymbol{B} + \frac{e^2}{8m}(\boldsymbol{B} \times \boldsymbol{r})^2$$

Dipole moment: $$\mu_{\mathrm{m}} = -\frac{\partial \mathcal{H}}{\partial B} = -\frac{e}{2m}(\boldsymbol{r} \times \boldsymbol{p}) - \frac{e^2}{4m}(\boldsymbol{r} \times (\boldsymbol{B} \times \boldsymbol{r}))$$

paramagnetic diamagnetic

N-electron system $$\mathcal{H}_N = \sum_{n=1}^{N} \left[\frac{1}{2m} (\boldsymbol{p}_n + e\boldsymbol{A}(\boldsymbol{r}_n))^2 - e\phi(\boldsymbol{r}_n) \right] + V(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_N)$$

Breakdown of classical magnetism (2)

Partition function: $Z = \prod_{n=1}^{N} \int \frac{d\boldsymbol{r}_n d\boldsymbol{p}_n}{h^3} e^{-\mathcal{H}/k_{\mathrm{B}}T}$

$$\boldsymbol{\pi}_n = \boldsymbol{p}_n + e\boldsymbol{A}(\boldsymbol{r})$$

$$Z = \prod_{n=1}^{N} \int \frac{d\boldsymbol{r}_n d\boldsymbol{\pi}_n}{h^3} e^{-\mathcal{H}'/k_{\mathrm{B}}T},$$

$$\mathcal{H}' = \sum_{n=1}^{N} \left[\frac{\boldsymbol{\pi}_n^2}{2m} - e\phi(\boldsymbol{r}_n) \right] + V(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_N)$$

Cancellation of paramagnetic and diamagnetic term $\langle \boldsymbol{\mu}_{\mathrm{m}} \rangle = -\frac{1}{N} \frac{\partial F}{\partial \boldsymbol{B}} = \frac{1}{N k_{\mathrm{B}} T} \frac{\partial \ln Z}{\partial \boldsymbol{B}} = \langle \boldsymbol{\mu}_{\mathrm{para}} \rangle + \langle \boldsymbol{\mu}_{\mathrm{dia}} \rangle = 0$

Bohr- van Leeuwen theorem

Electron spin from Dirac equation

Dirac equation and electron spin magnetic moment

Energy-momentum relation in Newtonian mechanics

$$E = \frac{p^2}{2m}$$

Quantum mechanical replacement to obtain Schroedinger equation:

$$E \to i\hbar\frac{\partial}{\partial t}, \quad p \to -i\hbar\frac{\partial}{\partial x}$$

Energy-momentum relation in relativity

$$E^2 = (pc)^2 + (mc^2)^2 \qquad (1)$$

However simple replacement is impossible: the wave equation must be the first-order in time

$$E = \sum_{k=1,2,3} \alpha_k p_k c + \beta mc^2 \qquad (2)$$

How to compromise (2) with (1) ?

These conditions require α_k and β to be 4×4 matrices.

$$\begin{cases} \alpha_k^2 = 1, \quad \beta^2 = 1, \\ \alpha_k\alpha_j + \alpha_j\alpha_k = 0 \ (k \neq j), \\ \alpha_k\beta + \beta\alpha_k = 0 \end{cases}$$

Pauli representation

Wave equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-i\hbar c\sum_{k=x,y,z}\alpha_k\frac{\partial}{\partial x_k} + \beta mc^2\right]\boldsymbol{\psi}$$

$$\equiv \mathcal{H}_{\mathrm{D}}\boldsymbol{\psi}, \quad \mathcal{H}_{\mathrm{D}} = c\boldsymbol{\alpha}\boldsymbol{p} + mc^2\beta$$

Dirac hamiltonian

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma_i\sigma_j = -\sigma_j\sigma_i = i\sigma_k, \quad \sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$$

Pauli representation

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

Spin angular momentum

$$\mathcal{H} = \mathcal{H}_{\mathrm{D}} + V(\boldsymbol{r})$$

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} \qquad [\boldsymbol{L}, \mathcal{H}] = i\boldsymbol{\alpha} \times \boldsymbol{p} \qquad \boldsymbol{\alpha} = \begin{pmatrix} \alpha_x \\ \alpha_y \\ \alpha_z \end{pmatrix}$$

L does not commute with Hamiltonian, is thus, not a constant of motion.

4×4 Pauli matrices: $\sigma_k^{(4)} = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}$ $\qquad [\boldsymbol{\sigma}, \mathcal{H}] = -2i\boldsymbol{\alpha} \times \boldsymbol{p}/\hbar$

Then $\boldsymbol{J} = \boldsymbol{L} + \dfrac{\hbar}{2}\boldsymbol{\sigma} \equiv \boldsymbol{L} + \boldsymbol{s}$ $\qquad [\boldsymbol{J}, \mathcal{H}] = 0$

Spin angular momentum: $\boldsymbol{s} \equiv (\hbar/2)\boldsymbol{\sigma}$

Magnetic moment of electron spin

Dirac eq. with electromagnetic field $i\hbar\frac{\partial\psi}{\partial t} = [c\boldsymbol{\alpha}(\boldsymbol{p}+e\boldsymbol{A}) + \beta m - e\phi]\,\psi$

$$\left[\left(i\hbar\frac{\partial}{\partial t}+e\phi\right) - c\sum_{j=x,y,z}\alpha_j\left(-i\hbar\frac{\partial}{\partial r_j}+eA_j\right) - \beta mc^2\right]\psi = 0$$

Operation from left: $i\hbar\frac{\partial}{\partial t}+e\phi + c\sum_{j=x,y,z}\alpha_j\left(-i\hbar\frac{\partial}{\partial r_j}+eA_j\right) + \beta mc^2$

We obtain

$$\left[\left(i\hbar\frac{\partial}{\partial t}+e\phi\right)^2 - c^2(\boldsymbol{p}+e\boldsymbol{A})^2 - m^2c^4 + ic\hbar e(\boldsymbol{\alpha}\cdot\boldsymbol{E}) + i\hbar c^2 e(\alpha_x\alpha_y B_z + \alpha_y\alpha_z B_x + \alpha_z\alpha_x B_y)\right]\psi = 0$$

Because $\alpha_x\alpha_y = i\sigma_z^{(4)},\quad \alpha_y\alpha_z = i\sigma_x^{(4)},\quad \alpha_z\alpha_x = i\sigma_y^{(4)}$

$$\left[\left(i\hbar\frac{\partial}{\partial t}+e\phi\right)^2 - c^2(\boldsymbol{p}+e\boldsymbol{A})^2 - m^2c^4 + ic\hbar e(\boldsymbol{\alpha}\cdot\boldsymbol{E}) - \hbar c^2 e\boldsymbol{\sigma}\cdot\boldsymbol{B}\right]\psi = 0$$

Magnetic moment of electron spin (2)

Stationary solution: $\psi(\boldsymbol{r},t) = \exp(-i\epsilon t/\hbar)\varphi(\boldsymbol{r})$

$$\left[(\epsilon + e\phi)^2 - c^2(\boldsymbol{p} + e\boldsymbol{A})^2 - m^2c^4 + ic\hbar e(\boldsymbol{\alpha}\cdot\boldsymbol{E}) - \hbar c^2 e\boldsymbol{\sigma}\cdot\boldsymbol{B}\right]\varphi = 0$$

$$\phi = 0,\ \boldsymbol{E} = 0$$

Low energy expansion

$$\epsilon = mc^2 + \delta$$

We take first order in $\dfrac{\delta}{mc^2}$

$$\left[\frac{1}{2m}(\boldsymbol{p} + e\boldsymbol{A})^2 + \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B}\right]\varphi = \delta\varphi$$

Bohr magneton $\mu_{\mathrm{B}} \equiv \dfrac{e\hbar}{2m} \approx 9.274\times 10^{-24}\ \mathrm{JT^{-1}}$

$$\frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B} = \mu_{\mathrm{B}}\boldsymbol{\sigma}\cdot\boldsymbol{B} = \frac{2}{\hbar}\mu_{\mathrm{B}}\boldsymbol{s}\cdot\boldsymbol{B}$$

Therefore the magnetic moment is $-2\mu_{\mathrm{B}}\boldsymbol{s}/\hbar$

Summary

1. Introduction of magnetic moment
2. Measurement of magnetization
3. Magnetism in classical interpretation and its breakdown
4. Introduction of electron spin along Dirac equation