Solid-state NMR methods

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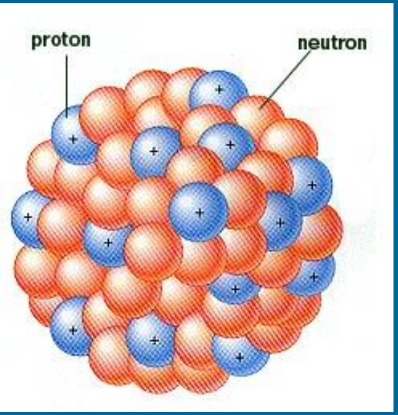
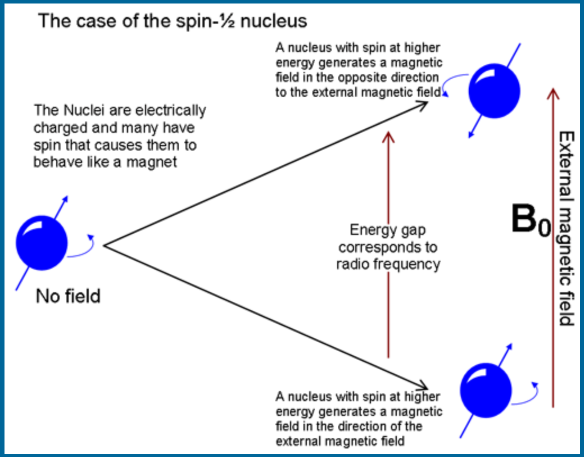
Outline

- Introduction to NMR:
  - Interaction of nuclei magnetic fields.
  - Spin precession.
    - Larmor frequency.
  - Nuclear paramagnetistm.
  - Nuclear spin transitions.

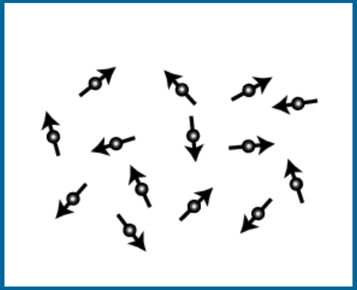
Interaction energies – order of magnitude



Nuclear interaction: $E_n \sim$ keV = 10^3 eV



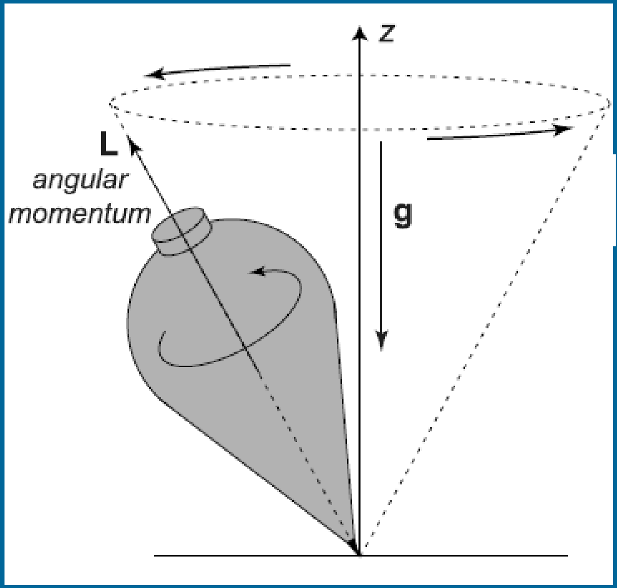
Magnetic interaction between a nucleus and an external magnetic field: $E_m \sim \mu$eV = 10^{-6} eV

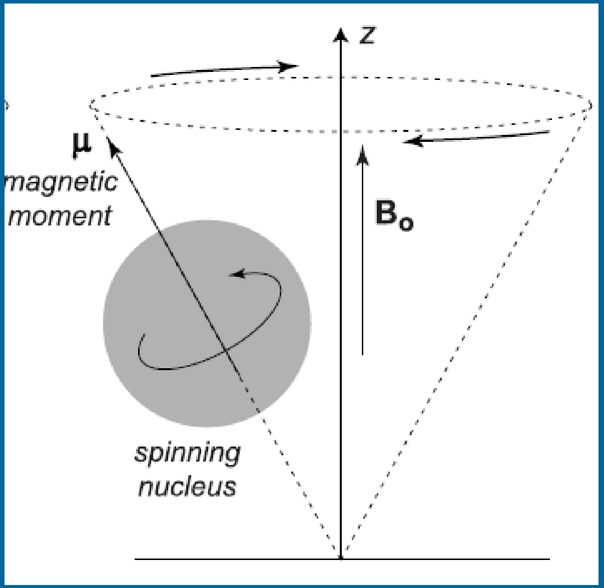


Thermal energy: $E_T \sim k_B T \sim 10^{-2}$ eV

Spin precession

Atomic nucleus in the presence of a static magnetic field:





$$\vec{\tau} = \vec{r} \times m\vec{g}$$

$$\omega = \frac{mgr}{L}$$

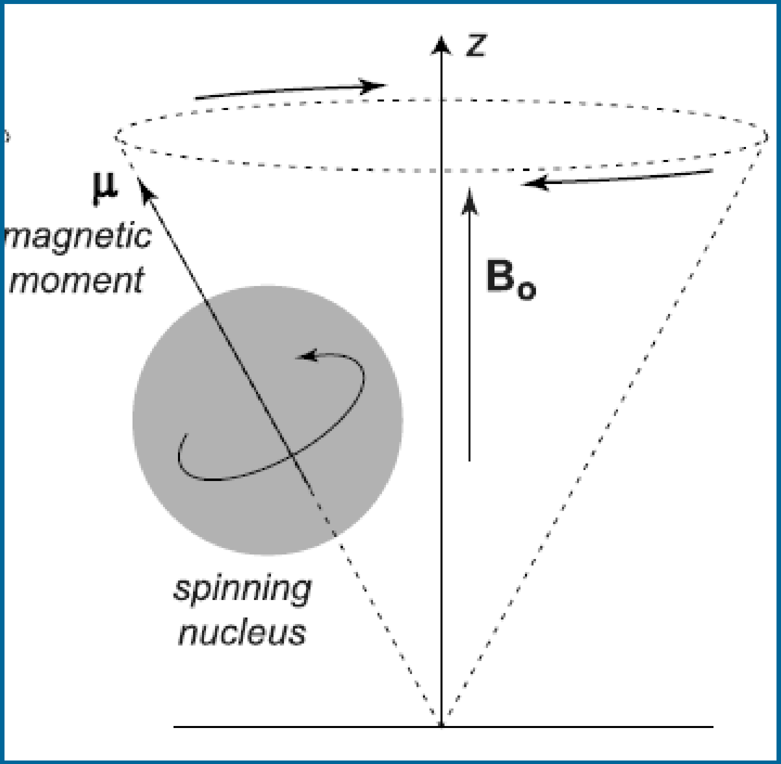
$$\vec{\mu} = \gamma \vec{I}$$

$$\vec{\tau} = \vec{\mu} \times \vec{B}_0$$

$$\omega_L = \gamma B_0$$

Spin precession

Atomic nucleus in the presence of a static magnetic field:



Larmor frequency:

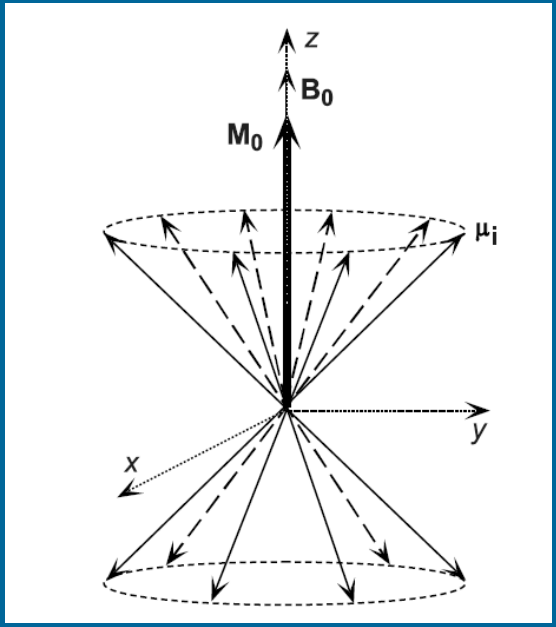
$$\omega_L = \gamma B_0$$ (~10^7 rad/s)

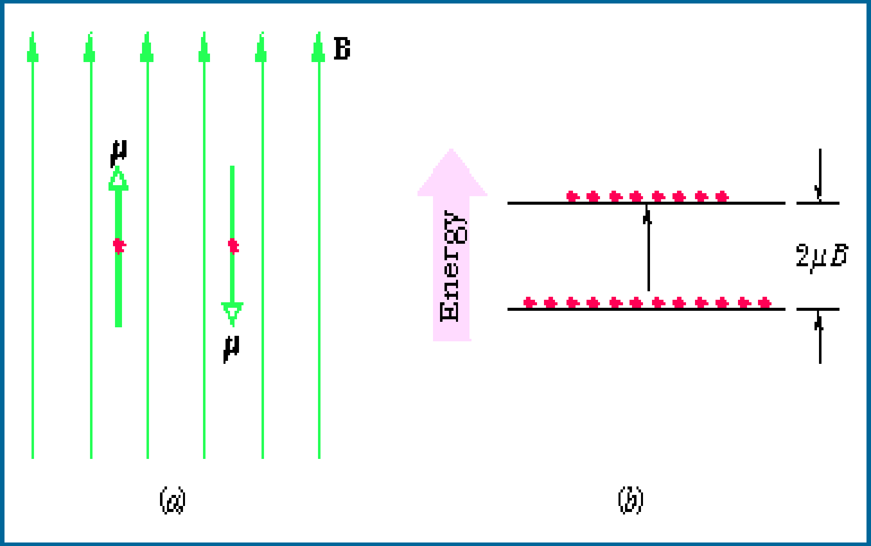
$$f_L = \gamma B_0 / 2\pi$$ (~MHz)

↓

radiofrequency (RF)

Nuclear paramagnetism



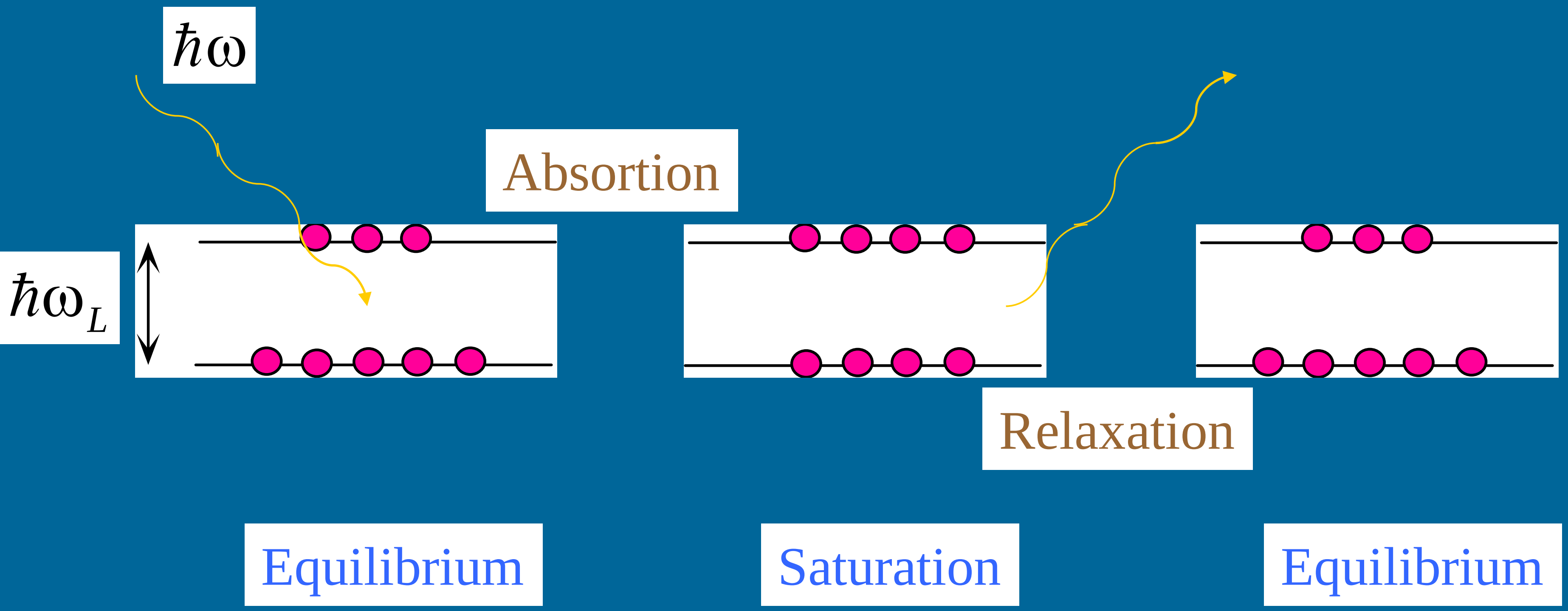


$$M_0 = \frac{N\mu^2 B_0}{3kT}$$

$$E = -\vec{\mu}\cdot\vec{B}_0 = -\gamma m\hbar B_0 = -m\hbar\omega_L$$

$$\frac{n_-}{n_+} = e^{(-\hbar\omega_L / kT)}$$

Nuclear spin transitions



Transition probability: $P_{m\rightarrow n} = P_{n\rightarrow m} \propto \gamma^2 B_1^2 \left| \langle m | \mathbf{I}_x | n \rangle \right|^2 \delta(\omega - \omega_L)$

Recommended bibliography

- Principles of NMR:

  - “Spin dynamics”, M. H. Levitt. John Wiley & Sons, 2002.
  - “Principles of magnetic resonance”, C. P. Slichter. Springer, 1996.
  - “Ressonância magnética nuclear: fundamentos, métodos e aplicações”, V. M. S. Gil, C. F. G. C. Geraldes. Fundação Calouste Gulbekian, 1987.
  - “NMR nomenclature. Nuclear spin properties and conventions for chemical shifts (IUPAC recommendations 2001)”, R. K. Harris, E. D. Becker, S. M. Cabral de Menezes, R. Goodfelow, P. Granger. *Pure Appl. Chem.* 2001;73:1795-1818.
  - http://www.magritek.com/support/videos (Lectures presented by Prof. Paul Callagham on the principles of NMR and MRI.)