EPR imaging characterization of natural and synthetic materials

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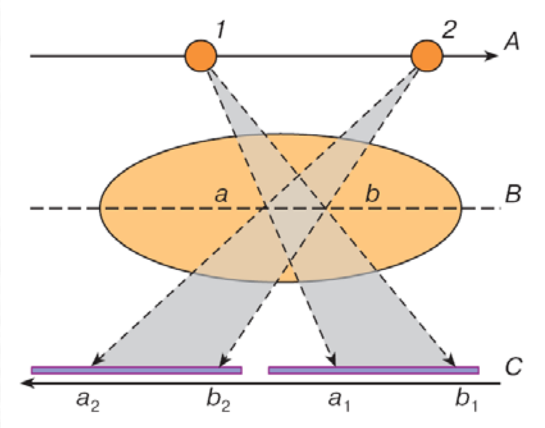
Contents:

- Introduction
- MR theory
- Mathematical problems of computer-aided tomography
- EPR imaging
- Conclusion

Tomography (gr. tomos - layer, grapho - write)

Simple methods:

- anatomic
- linear X-ray



Computer methods:

- computed (CT, SCT)
- magnetic-resonance (MRT)
- positron-emission (PET)
- ultrasonic (US)
- laser
- electron-impedance

Introduction

Questions to be answered during report:

- What a magnetic-resonance phenomenon is?
- How can we obtain useful information from spectra?
- Which

Intro – subject review

- What is the aim of tomography actually for living science?
- T is an individual frame of knowledge with application in medicine, nanotechnology, chemistry and so on
- EPR imaging is the only method of inspection electron density distribution in a sample

Magnetic properties of atom

$$\vec{\mu} = \gamma \cdot \hbar\vec{I} = g_N \vec{I}$$

$$\vec{p} = \hbar\vec{I}$$

Nucleus:

– has a spin momentum **I**

I = 0; 1/2; 1; 3/2...

Electron:

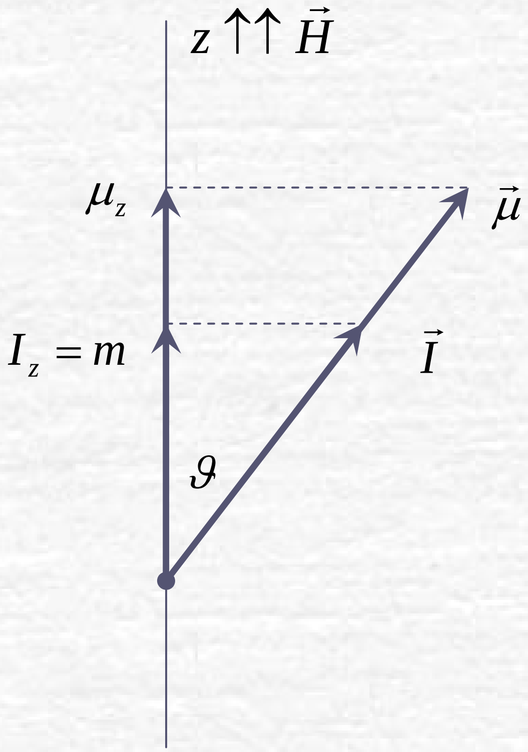
– has a orbital momentum **L**

L = 0; 1; 2; 3...

– has a spin momentum **S**

S = 1/2

Magnetic properties of atom



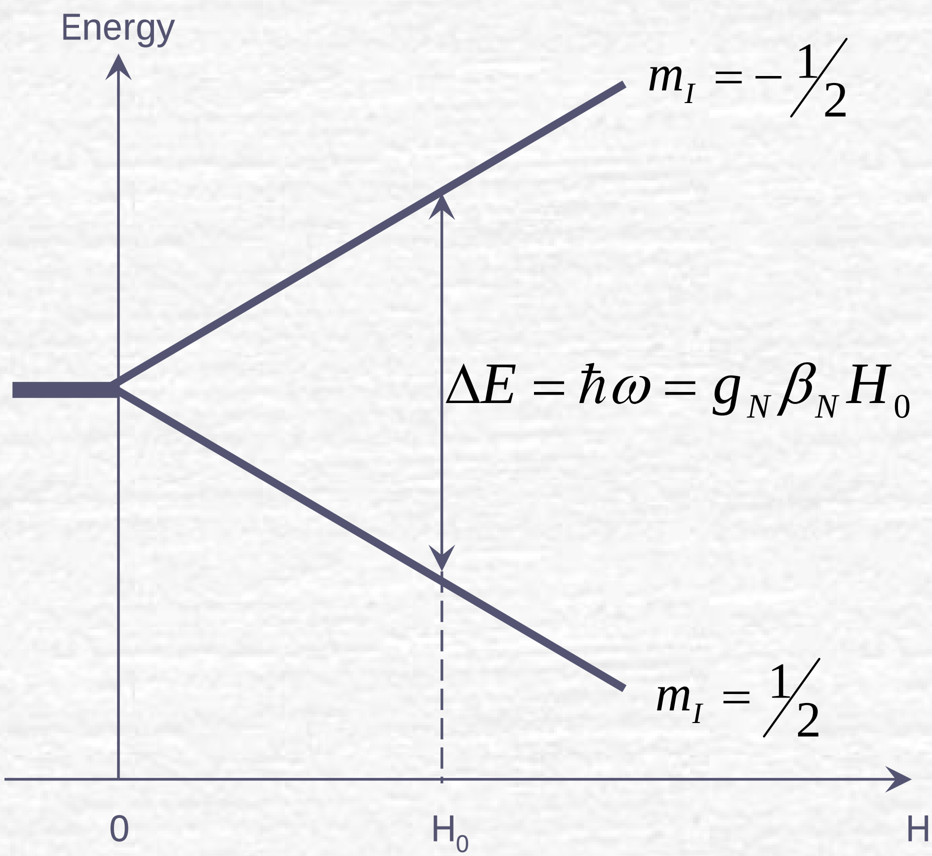
Interaction with external field:

$$E = -(\vec{\mu}, \vec{H}) = -\mu H \cos\vartheta = -\mu_z H$$

Fixed momentum orientations

Discreet energy levels

Energy levels of nucleus



Interaction energy:

$$E = -\gamma \cdot \hbar H I_z = -g_N \beta_N H I_z$$

$$\beta_N = \frac{eh}{2Mc}$$ nuclear magneton

Energy levels of electron

MR theory – classification

- NMR
- Nuclei with non-zero nuclear spin (H)
- Ask help

- EPR
- Substance with odd number of e (^{1}H)
- Substance with unpaired es on valence shell without chem link (VO)
- Free radicals (mithil-r)

MR theory – absorption line

- Which information can we obtain from EPR spectra?
- FS & HFS & SHFS
- g-factor
- Line width & line shape
- Integral intensity

MR theory – CW-method

- Block-scheme of spectrometer
- Sweeping magnetic field and synchronous detecting of signal
- First derivative form of absorption line
- Aims of sweeping field

MR theory – my examples

- Ask S.M. about good examples...
- in progress

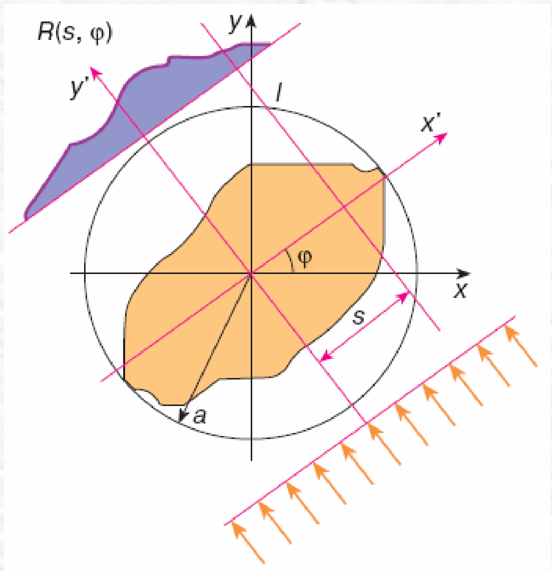
Radon transformation

1. The methods of projection data acquisition;

2. Means of tomographic images reconstruction:
   - Back-projection algorithm;
   - De-convolution algorithm;

3. Examples

Radon transformation



Equation of line l in x-y-frame:

$$x\cos\varphi + y\sin\varphi - s = 0$$

Rotation of axes:
$$\begin{cases} x = x'\cos\varphi - y'\sin\varphi \\ y = y'\sin\varphi + y'\cos\varphi \end{cases}$$

Equation of line l in new coordinates: $x' - s = 0$

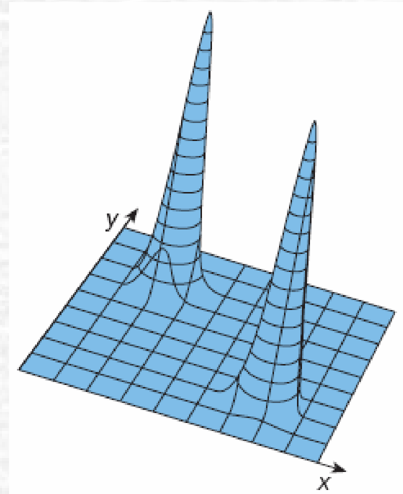
Radon image:

$$R(s,\varphi) = \int_{-\infty}^{\infty} f(s\cos\varphi - y'\sin\varphi, s\sin\varphi + y'\cos\varphi)\,dy'$$

$$R(s,\varphi) = \int_{-\sqrt{a^2-s^2}}^{\sqrt{a^2-s^2}} f(s\cos\varphi - y'\sin\varphi, s\sin\varphi + y'\cos\varphi)\,dy'$$

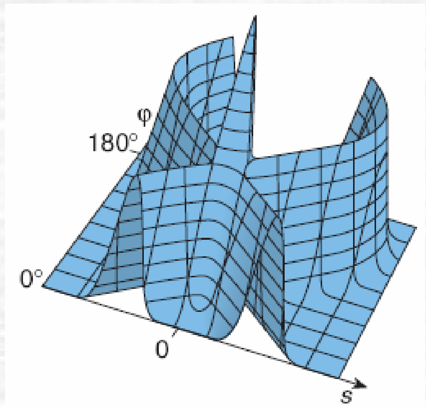
Radon transformation

2 Gauss impulses:



$$f(x,y)=\sum_{i=1}^{2}\exp\left\{-\frac{(x-x_i)^2+(y-y_i)^2}{2b^2}\right\}$$

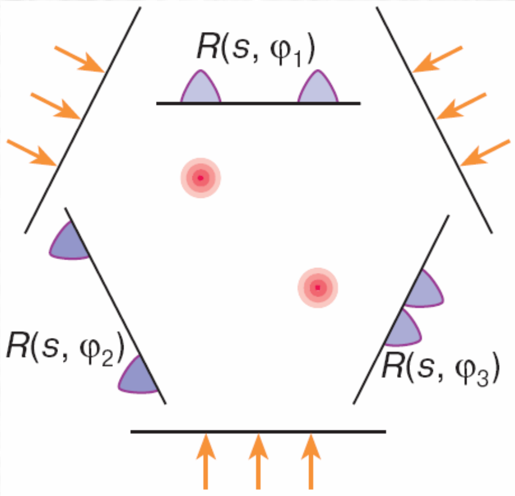
Radon image of *f(x,y)*:



$$R(s,\varphi)=\sum_{i=1}^{2}b\sqrt{2\pi}\exp\left\{-\frac{(x_i\cos\varphi+y_i\sin\varphi-s)^2}{2b^2}\right\}$$

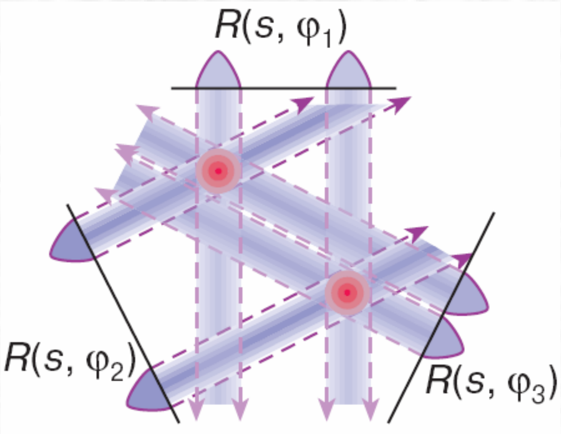
Back projection algorithm

1. Fixing the angel φ in R(s, φ)
2. Stretch 1D function R(s, φ) in *x*-*y*-plane



Back-projected image:

$$R_\varphi(x,y) = R(x\cos\varphi + y\sin\varphi, \varphi)$$



Summary image:

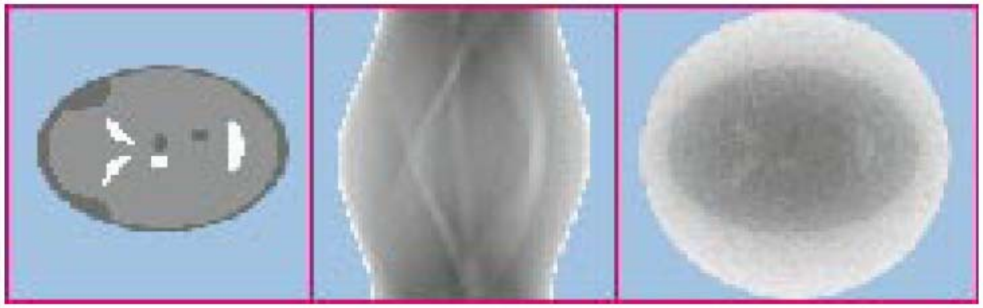
$$\hat{f}_{on}(x,y) = \int_0^\pi R(x\cos\varphi + y\sin\varphi, \varphi)\,d\varphi$$

Back projection algorithm

Main disadvantage:

Image contrast is too low :(

1. Original phantom
2. Radon image (180 projection)
3. Back-projected phantom



1 2 3

Deconvolution algorithm

$$f(x,y)=\int_0^{\pi}\tilde{R}(x\cos\varphi+y\sin\varphi,\varphi)d\varphi$$

- original function

$$\tilde{R}(x\cos\varphi+y\sin\varphi,\varphi)=\tilde{R}(s,\varphi)=\int_{-a}^{a}h(s_1)R(s-s_1,\varphi)ds_1$$

- convolution product

$$h(s_1)=\frac{1}{2\pi}\int_{-\infty}^{\infty}|\omega|\cos(\omega s_1)d\omega$$

- Fourier image of |ω|

1 2 3 4 5

EPR Imaging – experiment

- Summing up 2 theories
- Adding MF gradient
- Spectral line broadening, frequency coding
- Radon transform application

EPR Imaging - properties

- EPR imaging resolution (compare with MRI)
- Practical limitations

EPR Imaging – examples

- Radicals
- Applications to mineral samples (radiation defects)
- Skin experiments

Conclusion

- Development difficulty
- Limitations of using *in vivo*
- Further perspectives and so on