EUROPEAN
SPALLATION
SOURCE

Precessions in neutron scattering experiments

Erice

July 2, 2017

F. Mezei
Technical coordinator

Eugene P. Wigner:

”If my work seemed trivial to some people, I did not care. Throughout my life, I have found it best to seek physics problems whose solutions seem initially simple. In complete form, their details revealed, such problems become barely manageable. Solving physics problems that are exacting from the first often becomes hopeless undertakings.”

Eugene P. Wigner:

”If my work seemed trivial to some people, I did not care. Throughout my life, I have found it best to seek physics problems whose solutions seem initially simple. In complete form, their details revealed, such problems become barely manageable. Solving physics problems that are exacting from the first often becomes hopeless undertakings.”

Solving the Schrödinger equation for a neutron scattering experiment (instrument + sample + multiple scattering + polarization +….) does not simple from the outset. **What makes it still simple** – most of the time?

Otto R. Frisch, H. von Halban Jr, J. Koch, 1937, Copenhagen

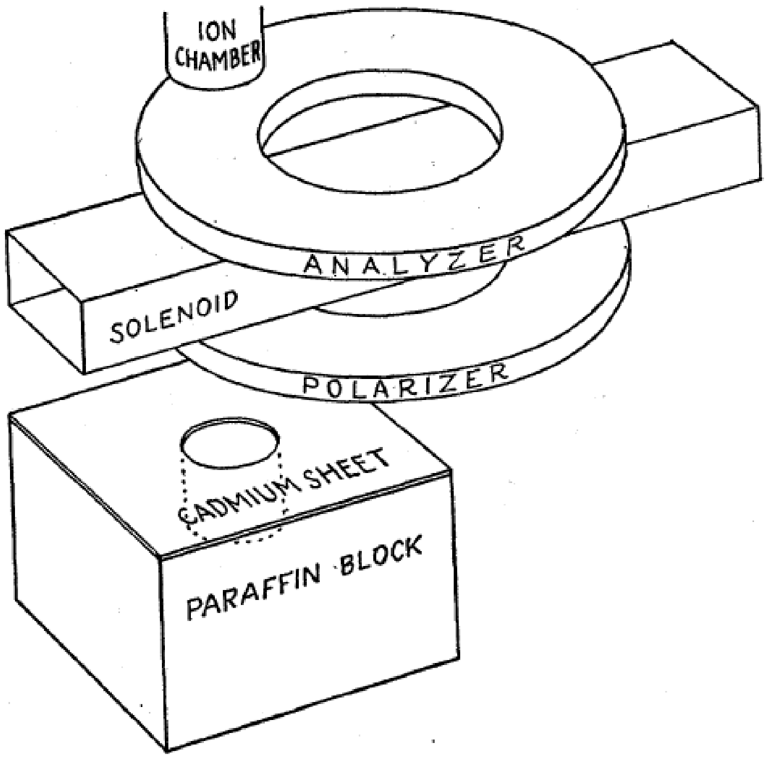


FIG. 1. Experimental arrangement for the demonstration of the precession of neutrons. The path of the neutrons from the hole in the paraffin block to the ionization chamber was almost entirely surrounded by boron and cadmium sheets (not shown in the figure) to suppress scattered neutrons.

Larmor precessions
(next: 1969 Drabkin et al)

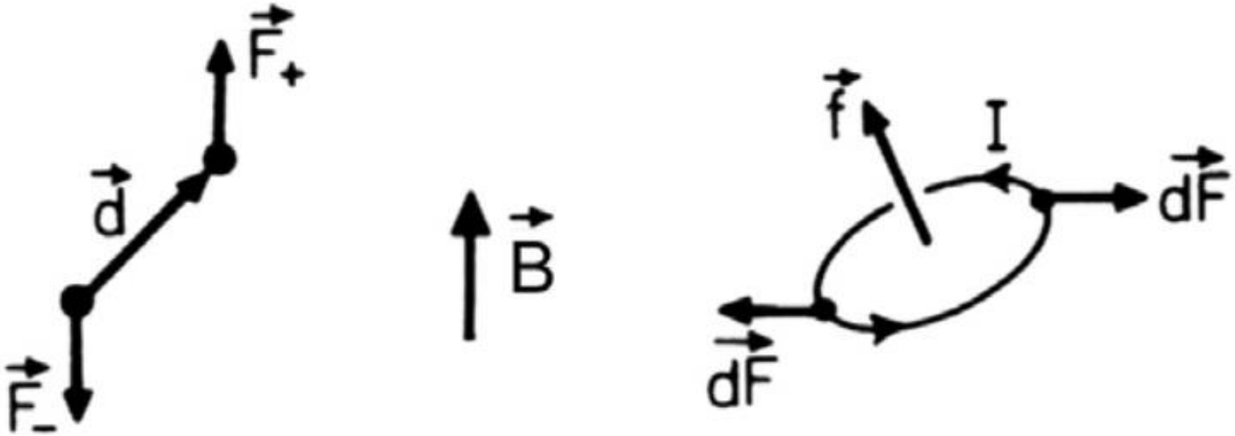
Larmor frequency → $\mu_n \sim 2\ \mu_B/1840$

Larmor precession in Fe:
scales with **B** (not **H**)
(debated until 1951)

"15 years law" ?

What is a magnetic moment?

Forces on model magnetic moments: (outside magnetic media **B** = **H**)



$$\mathbf{F_d} = \mathbf{F}^+ + \mathbf{F}^- = (\boldsymbol{\mu}\cdot grad)\mathbf{B} = grad(\boldsymbol{\mu}\cdot\mathbf{B}) - \boldsymbol{\mu}\times curl\ \mathbf{B}$$

$$\mathbf{F_c} = \oint \mathrm{d}\mathbf{F} = \frac{I}{c}\oint \mathrm{d}\mathbf{l}\times\mathbf{B} = \frac{I}{c}\int grad(\mathbf{B}\cdot\mathrm{d}\mathbf{f}) - \frac{I}{c}\int (div\,\mathbf{B})\mathrm{d}\mathbf{f} =$$
$$= grad(\boldsymbol{\mu}\cdot\mathbf{B})$$

↑

Bona fide potential

Ambiguous if j≠ 0: $curl\ \mathbf{B} = 4\pi\mathbf{j}/c$

What does the neutron see?

Bloch (July 9, 1936)

A neutron inside condensed matter is influenced by

"(1)…interaction of the neutron with atomic nucleus….
(2)…inhomogeneous ***magnetic field*** *in its surrounding acting on the magnetic moment of the neutron."*

(2) is much weaker but *"acts on distances so much larger"*

$\rightarrow$ The neutron sees nuclear spins, but does not directly see magnetic moments!

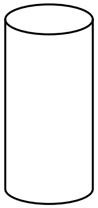
What is Bloch's "magnetic field"? Bloch 1936: dipolar fields

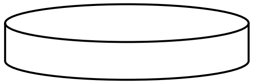
Electromagnetism theory had no answer to the new problem posed by the neutron and quantum mechanics: it can **overlap with the sources of magnetic** fields (electrons or current in wires).

What does the neutron see?

Schwinger (January 11, 1937): gets a different expression by using quantum mechanical formalism (Dirac operator)

Bloch (April 28, 1937): the two results rather depend on the shape of the “hole” the neutron sits in: avoid overlap of electrons and neutrons



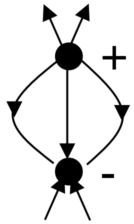
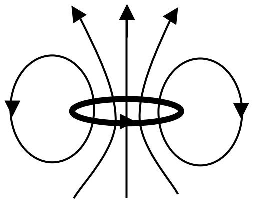


Field in the hole: **= H** (Bloch) **= B** (Schwinger)

Reality: in quantum mechanics **electrons and neutrons overlap** and the field inside a source of magnetic field depends on the model of magnetism:

Dipoles or current loops?

What is the source of field seen by neutron ?

H:  or **B:** 

(**B** = **H** + 4π**M**)

Migdal (1938): it is **B,** if done right (i.e. take the formulae from Landau's textbook)

O. Haplern and M. H. Johnson (1939): theory of neutron polarization by allowing the scattering system to change spin, otherwise agrees with Schwinger & Migdal: *"…the neutron…produces in its neighborhood a field analogous to classical magnetic dipole which owes its existence to a stationary current distribution ….div H = 0."*

Eckstein (1949): theory cannot decide, experiments needed (with 3+ Nobel laurates involved: Fermi,…)

Shull, Wollan and Strauser (December 8, 1950, appeared February 1951)
Hughes & Burgy (September 25, 1950, appeared March 1951)

All magnetic moments are current loops

Shull, Wollan and Strauser (1951)

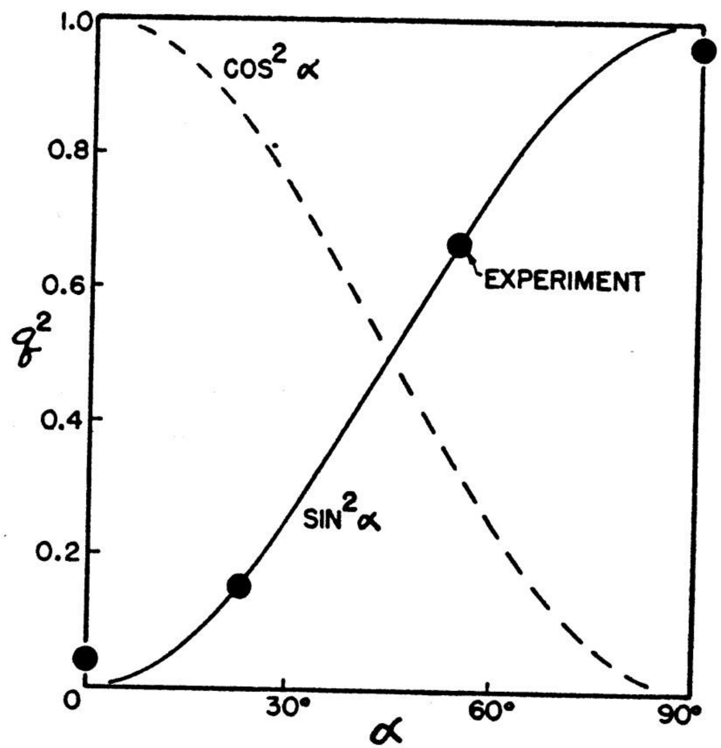


FIG. 2. Variation of q^2 with the angle α between the scattering and magnetization vectors. The experimental points have been normalized to the unmagnetized value of $q^2 = 2/3$.

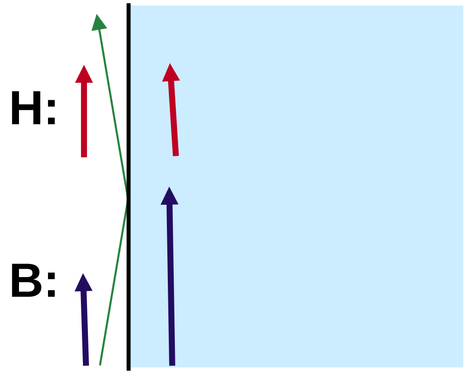
Magnetic Bragg peak intensity in magnetite observed as a function of the angle between $\mathbf{H}_{ext}$ and $\mathbf{Q}_{111}$

De Gennes: the $\sin^2\alpha$ factor can be taken into account by considering $\mathbf{M}_\perp$ and $\mathbf{j}$ = c curl $\mathbf{M}$

All magnetic moments are current loops

Hughes & Burgy (1951):

neutron total reflection on optically flat iron surface (critical angle < 1°)



Since the component of **H** parallel to the surface between two materials must be continuous across the surface, there **should be no magnetic contribution** in neutron reflection for layers polarized in the plane of the mirror.

Hamiltonian for (slow) neutron propagation including Larmor precessions

$$H(\mathbf{r},t) = \frac{1}{2}mv^2 - \boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{r},t) + mgh + \frac{2\pi\hbar^2}{m}\sum_i b_i(1 + c_i\mathbf{I}_i\cdot\boldsymbol{\sigma})\delta(\mathbf{r}-\mathbf{r}_i(t))$$

Note: wavelength is relative, only difference in wavenumber/momentum **k** is absolute!

Space + spin quantum states

General free particle wave function:

$$\Phi = \int \left(a_\uparrow(\mathbf{k}) e^{i(\boldsymbol{kr} - \omega t)} \left| \uparrow \right\rangle + a_\downarrow(\mathbf{k}) e^{i(\boldsymbol{kr} - \omega t)} \left| \downarrow \right\rangle \right) \mathrm{d}\mathbf{k} = \int \left| \chi(\mathbf{k}) \right\rangle a(\mathbf{k}) e^{i(\boldsymbol{kr} - \omega t)} \mathrm{d}\mathbf{k} \neq$$

$$\neq \left| \chi \right\rangle \int a(\mathbf{k}) e^{i(\boldsymbol{kr} - \omega t)} \mathrm{d}\mathbf{k}$$

1)

Not: $|\chi\rangle\phi(\boldsymbol{r})$. Instead:

- **For each value of *k*** the spin wave function $|(\boldsymbol{k})\rangle$ is a simple superposition of $|\uparrow\rangle$ and $|\downarrow\rangle$ spin eigenstates.
- $S_\alpha = \langle(\boldsymbol{k})|\sigma_\alpha|(\boldsymbol{k})\rangle$ for $\alpha = x,y,z$ form a classical spin direction vector $\boldsymbol{S}(\mathbf{k})$ of unit length (full polarization).
- The spin direction vector evolves according to the classical Larmor precessions:

$$\frac{d\boldsymbol{S}}{dt} = \gamma \, [\boldsymbol{S}(\mathbf{k}) \times \boldsymbol{B}]$$

Space + spin quantum states

EUROPEAN SPALLATION SOURCE

2)
- Wave packet expands according to classical velocity difference in $|a(\mathbf{k})|^2$ distribution
- **The expansion by uncertainty principle is small for a minimum size wave packet** (e.g. ~30 % for 0.1 mm rms size over 100 m for v = 1000 m/s)

3)
- The **deviation from geometrical optics is negligible** in waves for which the path differences in collimated beams $\Delta \approx d^2/2l \gg \lambda$ (true for neutrons beams, not for synchrotron radiation or light)

4)
- Due to random phase statistics in an ensemble of particles : $\langle a^*(\boldsymbol{k}) a(\boldsymbol{k'}) \rangle = 0$ if $\boldsymbol{k} \neq \boldsymbol{k'}$, i.e. **there is no intrinsic coherence** except for stimulated and externally modulated emission of Bosons or if $\Delta \approx d^2/2l < \lambda$ or similar. No experimental evidence found yet for the crossover between $\boldsymbol{k} \neq \boldsymbol{k'}$ to $\boldsymbol{k} = \boldsymbol{k'}$,

“Exact” solution of neutron propagation

Within at all observable precision, the “exact” solution of the neutron propagation Schrödinger equation can be obtained by the following rules for common neutron scattering experimental conditions, in particularly including Larmor precessions:

1) Between probabilistic scattering and absorption events within small correlated volumes inside matter the neutrons propagate deterministically as point like classical particles with “infinitely” well-defined trajectories ***r***(*t*), each carrying a classical magnetic moment with perfectly well-defined direction at any instance of time. (This is no contradiction to the uncertainty principle: a) classical distribution of particle parameters also provide measurement uncertainties masking smaller effects, b) for a large number *N* of detected particles the principal uncertainty limit is divided by $\sqrt{N}$ and c) the volume is small where quantum transition to the new happens

“Exact” solution of neutron propagation

EUROPEAN SPALLATION SOURCE

2) The magnetic moment direction vector follows the classical Larmor precession motion governed by the Zeeman energy: $-\mu\,\boldsymbol{B}(\boldsymbol{r}(t), t)$, where the magnetic induction field ***B*** shows time dependence as seen by the point-like neutron along its infinitely well-defined classical trajectory across the magnetic fields both inside and out-side materials. This energy represents a conservative potential if the ***B*** field is in itself time independent ***B*** = ***B***(***r***), and the sum of the kinetic and all potential energies of the remains a constant over the classical trajectory of the point-like neutron.

3) The neutrons also follow classical mechanical trajectories between quantum probabilistic scattering processes inside matter (as determined including the volume average nuclear potential $\boldsymbol{V}_{\mathrm{n}}$). The probabilistic beam attenuation due to scattering and absorption by nuclear reactions needs to factored into the effective description of the classical trajectories ***r***(*t*). Note: Van Hove scattering formalism translates plane wave states $\approx$ point-like classical particles with well defined velocity.

“Exact” solution of neutron propagation

4) Neutrons do not interact with magnetic moments in any other way than via the Zeeman interaction with the ***B*** field, that can equally well be created by macroscopic currents and microscopic ones related to magnetism in matters via the relation *curl* ***M*** *=* ***j****/c.*

5) The neutron scattering processes inside matter are of wave mechanical nature, in contrast to the classical point-like particle propagation 1-3) between probabilistic scattering events. They need to be determined using adequate quantum mechanical approaches for both the Zeeman term in the Hamiltonian if the ***B*** field shows short range variations and the term with the sum of the nuclear interaction potentials of individual nuclei.

“Exact” solution of neutron propagation

EUROPEAN SPALLATION SOURCE

6) Scattering events that can be handled by approximate theories such as first Born approximation involve **correlated / coherence volumes of the scattering matter, which are most often point-like small** ($\ll$ 1 mm) on the scale of neutron scattering sample volumes. Exceptions are large perfect crystals (including neutron interferometers made from such crystals), for which the Schrödinger equation must be essentially solved exactly without much approximation.

7) In contrast to the finite structurally correlated volumes that can coherently contribute to the neutron scattering processes inside materials, the neutron radiation by itself has no inherent limit of coherence lengths. Observations of apparently limited coherence are due to classical averaging of the results over the classical (velocity) distribution of the effectively detected particles: beam shaping is the only source of coherence length. In neutron beam interference only involvement a single well defined wavenumber **k** component of the initial particle state could be observed by now, classically averaged over the classical distribution of particle states **k**.

Apparent paradoxes

EUROPEAN SPALLATION SOURCE

Wave packets can quantum mechanically best described in most cases in neutron research by an ensemble of classical, point-like particles with perfectly well defined velocities and classical spin vectors

Wave packets cannot be assumed to have a well defined spin, factorized spatial and spin wave functions do not reflect general quantum behavior, while ensemble of classical particles can do

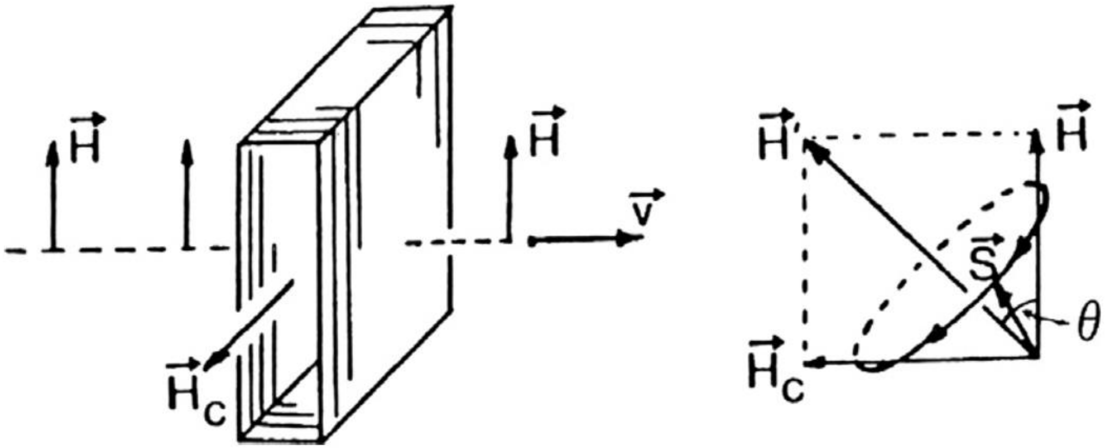
Neutron scattering theory: transition probabilities from a plane wave state to another, but it can happen in a very small correlated sample volume (natural limit of intrinsic Q resolution).

Classical behavior can be the result of precise quantum treatment (Landau's ideal solution)

Elementary examples

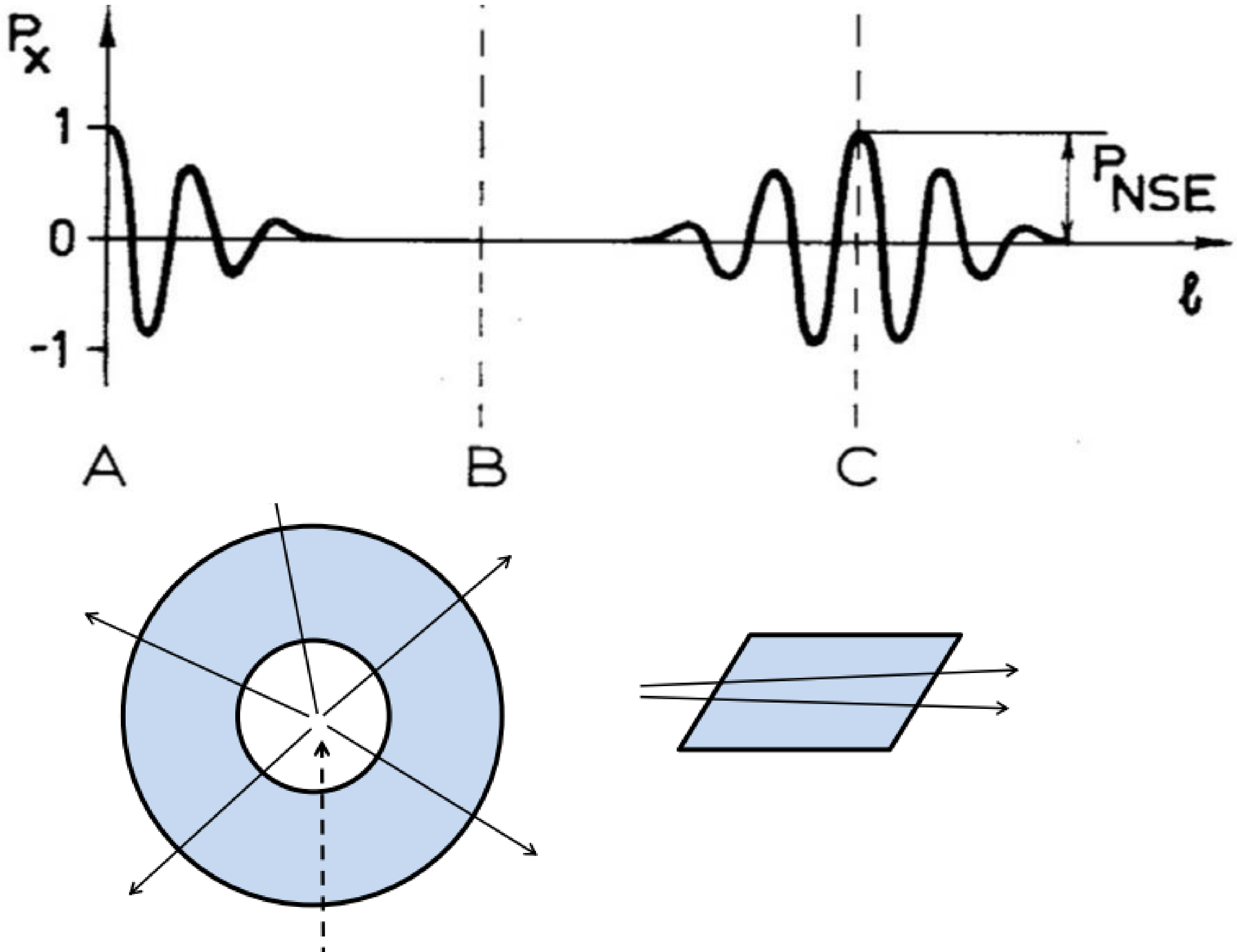
$\boldsymbol{B}(\boldsymbol{t}) = \boldsymbol{B}(\boldsymbol{r}(\boldsymbol{t}))$ **as seen by the neutron** advancing along the trajectory $\boldsymbol{r}(t)$.

Adiabatic limit: If the change of the direction of field $\boldsymbol{B}(t)$ is slow compared to the angular velocity of the Larmor precession $\omega_L(t) = 2\gamma_L B(t)$, the angle between $\boldsymbol{B}(t)$ and $\boldsymbol{S}(t)$ remains a constant.
Majorana limit: If the change of the direction of field $\boldsymbol{B}(t)$ is fast compared to the angular velocity of the Larmor precession $\omega_L(t)$ the direction of ***S*** remains unchanged during the time of the rapid jump of the direction of $\boldsymbol{B}(t)$.



Elementary examples

Precession field geometries and particle trajectories: time-of-flight is exact measure of velocity (in NSE to 1 ppm!)



Thanks for your attentions…

and examples for deviations from “exact” approximation most welcome!

ELSEVIER

Experimental Methods in the Physical Sciences

Volume 48, 2015, Pages 1-42

Chapter 1 - Neutron Optics and Spin Labeling Methods

Janos Major[1], Bela Farago[2], Ferenc Mezei[3, 4]