Polarized neutron reflectometry plus (PNR+)

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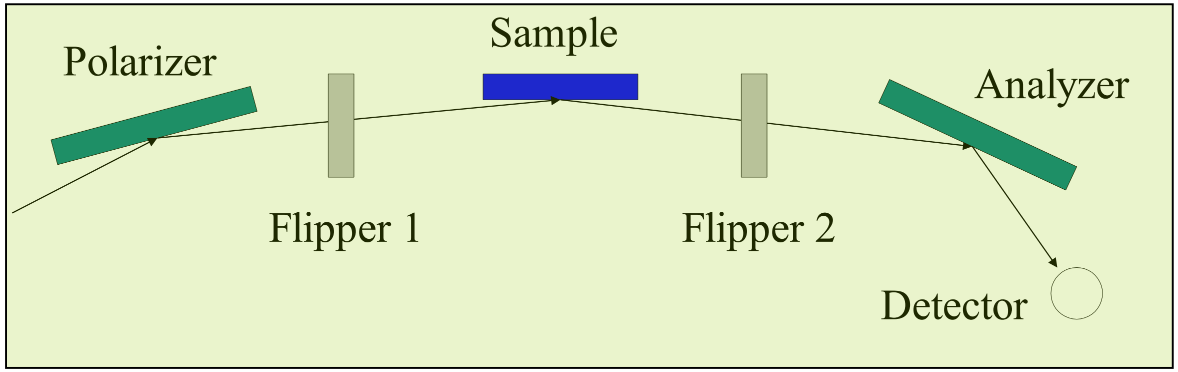
Polarized neutron reflectometry (PNR)

Standard scheme

$\pm\mathbf{P}_0 \| \mathbf{B}_0$



REFLECTION OF POLARIZED NEUTRONS

the reflection operator couples the spinors of the incident and reflected neutrons through their values at the sample surface

$$\left|\psi_r(0)\right\rangle = \hat{r}\left|\psi_i(0)\right\rangle$$

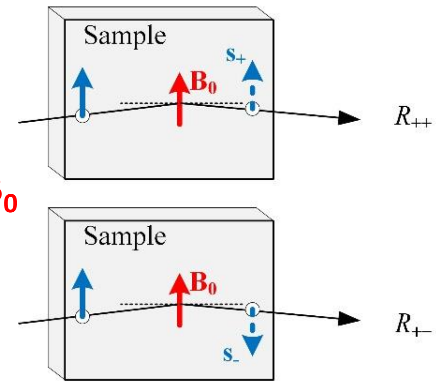
the reflection operator in the basis of the eigenvectors of the operator of the spin projection on the quantization axis Z||B$_0$ is represented by the reflection matrix

$$\hat{r} = \begin{pmatrix} r_{++} & r_{-+} \\ r_{+-} & r_{--} \end{pmatrix}_{\mathbf{B}_0}$$

reflection matrix elements

$$r_{++} \equiv |r_{++}|\exp(i\varphi_{++}),\ r_{-+} \equiv |r_{-+}|\exp(i\varphi_{-+}),$$
$$r_{+-} \equiv |r_{+-}|\exp(i\varphi_{+-}),\ r_{--} \equiv |r_{--}|\exp(i\varphi_{--})$$

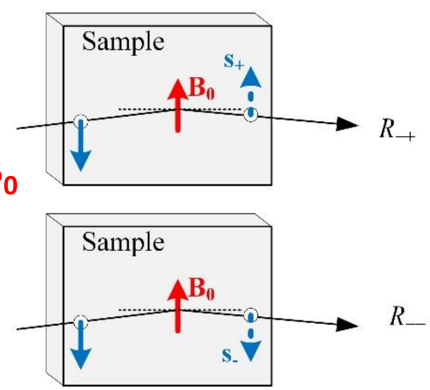
$\mathbf{P}_0 \| \mathbf{B}_0$



$$R_{++} = |r_{++}|^2$$

$$R_{+-} = \frac{k_0^-}{k_0^+}|r_{+-}|^2$$

$-\mathbf{P}_0 \| \mathbf{B}_0$



$$R_{-+} = \frac{k_0^+}{k_0^-}|r_{-+}|^2$$

$$R_{--} = |r_{--}|^2$$

Polarized neutron reflectometry plus (PNR+)

$$\mathrm{r} = \begin{pmatrix} |r_{++}|\exp(i\varphi_{++}) & |r_{-+}|\exp(i\varphi_{-+}) \\ |r_{+-}|\exp(i\varphi_{+-}) & |r_{--}|\exp(i\varphi_{--}) \end{pmatrix}_{\mathbf{B}_0}$$

DEFINITIONS

Difference phasometry is an experimental method of extracting the phase differences of the elements of the reflection matrix in any representation.

PNR+ is polarized neutron reflectometry (PNR) supplemented with the difference phasometry.

BASED ON THE PROVEN STATEMENTS

1. Only the differences of the phases of the reflection matrix elements can be directly measured by polarized neutron reflectometry. Of the six possible phase differences, only three may be independent, e.g., $\Delta_d = \varphi_{++} - \varphi_{--},\ \Delta_+ = \varphi_{++} - \varphi_{-+},\ \Delta_- = \varphi_{+-} - \varphi_{--}.$

2. The reflection matrix represents the reflection operator in the basis of the eigenvectors of the operator of the spin projection onto a certain axis Z. Choosing the quantization axis Z (Cartesian frame XYZ), one specifies the reflection matrix, e.g. $\hat{\mathrm{r}} = \begin{pmatrix} r_{++} & r_{-+} \\ r_{+-} & r_{--} \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} r_{\uparrow\uparrow} & r_{\downarrow\uparrow} \\ r_{\uparrow\downarrow} & r_{\downarrow\downarrow} \end{pmatrix}_{Z'}$

3. The moduli and phase differences of the elements of the reflection matrix in one representation determine the moduli and phase differences of the elements of the reflection matrix in another representation.

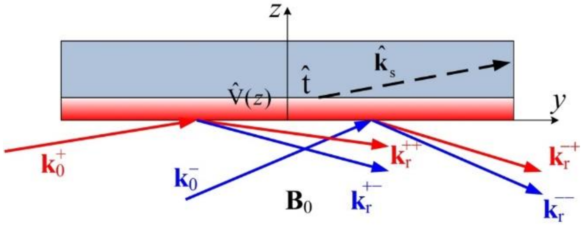
Polarized neutron reflectometry plus (PNR+)

Tasks of development of PNR+:

- to substantiate the method theoretically;
- to introduce methods of obtaining the phase information;
- to suggest measurement schemes.

Some aspects of polarized neutron reflection come to foreground, which had not been discussed in the literature at all or in sufficient detail.

Schrödinger equation: transition from 3D to 1D



$$\left(-\frac{\hbar^2}{2m}\Delta + V(z) - \mu_n \hat{\boldsymbol{\sigma}} \mathbf{B}(z)\right)|\Psi(\mathbf{r})\rangle = E|\Psi(\mathbf{r})\rangle$$

3D-equation with 1D-potential for a neutron

$$|\Psi(\mathbf{r})\rangle = \exp(i\hat{k}_{0,x}x)\exp(i\hat{k}_{0,y}y)|\psi(z)\rangle$$

incident-plane-wave solution

$$\mathbf{k}_0^\pm = (k_{0,x}^\pm, k_{0,y}^\pm, k_{0,z}^\pm) \qquad \mathbf{b}_0 = \mathbf{B}_0 / B_0$$

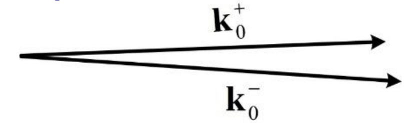
$$k_0^\pm = \hbar^{-1}\sqrt{2m_n[E - (V_0 \pm |\mu_n| B_0)]}$$

$$\hat{k}_{0,x} = (k_{0,x}^+ + k_{0,x}^-)/2 + \hat{\boldsymbol{\sigma}}\mathbf{b}_0 \cdot (k_{0,x}^+ - k_{0,x}^-)/2$$

$$\hat{k}_{0,y} = (k_{0,y}^+ + k_{0,y}^-)/2 + \hat{\boldsymbol{\sigma}}\mathbf{b}_0 \cdot (k_{0,y}^+ - k_{0,y}^-)/2$$

$$\exp(i\hat{k}_{0,x}x) = \begin{pmatrix} \exp(ik_{0,x}^+ x) & 0 \\ 0 & \exp(ik_{0,x}^- x) \end{pmatrix}_{\mathbf{B}_0}$$

$$\exp(i\hat{k}_{0,y}y) = \begin{pmatrix} \exp(ik_{0,y}^+ y) & 0 \\ 0 & \exp(ik_{0,y}^- y) \end{pmatrix}_{\mathbf{B}_0}$$



$$\hat{E}_\perp = E - \hbar^2(\hat{k}_{0,x}^2 + \hat{k}_{0,y}^2)/2m$$

normal motion energy operator

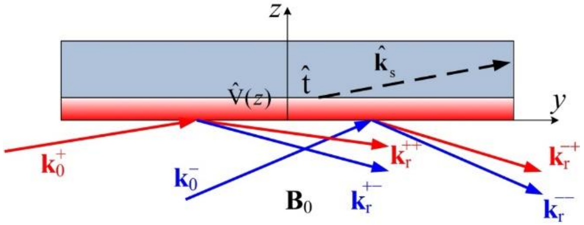
$$E_\perp^\pm = E - \hbar^2[(k_{0,x}^\pm)^2 + (k_{0,y}^\pm)^2)]/2m$$

$$\hat{E}_\perp = \begin{pmatrix} E_\perp^+ & 0 \\ 0 & E_\perp^- \end{pmatrix}_{\mathbf{B}_0}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right) e^{i\hat{k}_{0,x}x} e^{i\hat{k}_{0,y}y}|\psi(z)\rangle = \hat{E}_\perp e^{i\hat{k}_{0,x}x} e^{i\hat{k}_{0,y}y}|\psi(z)\rangle$$

The Schrödinger 3D-equation for a neutron in a 1D-potential is not reduced to 1D-equation in the general case (the phase factors are operators, which cannot be reduced).

Schrödinger equation: transition from 3D to 1D

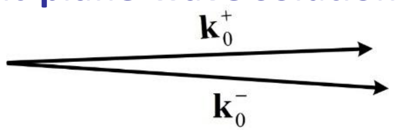


$$\left(-\frac{\hbar^2}{2m}\Delta + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)|\Psi(\mathbf{r})\rangle = E|\Psi(\mathbf{r})\rangle$$

3D-equation with 1D-potential for a neutron

$$|\Psi(\mathbf{r})\rangle = \exp(i\hat{k}_{0,x}x)\exp(i\hat{k}_{0,y}y)|\psi(z)\rangle$$

incident-plane-wave solution



$$\mathbf{k}_0^\pm = (k_{0,x}^\pm, k_{0,y}^\pm, k_{0,z}^\pm)$$

$$\mathbf{b}_0 = \mathbf{B}_0 / B_0$$

$$k_0^\pm = \hbar^{-1}\sqrt{2m_n[E - (V_0 \pm |\mu_n| B_0)]}$$

$$\hat{k}_{0,x} = (k_{0,x}^+ + k_{0,x}^-)/2 + \hat{\boldsymbol{\sigma}}\mathbf{b}_0 \cdot (k_{0,x}^+ - k_{0,x}^-)/2$$

$$\hat{k}_{0,y} = (k_{0,y}^+ + k_{0,y}^-)/2 + \hat{\boldsymbol{\sigma}}\mathbf{b}_0 \cdot (k_{0,y}^+ - k_{0,y}^-)/2$$

$$\exp(i\hat{k}_{0,x}x) = \begin{pmatrix} \exp(ik_{0,x}^+ x) & 0 \\ 0 & \exp(ik_{0,x}^- x) \end{pmatrix}_{\mathbf{B}_0}$$

$$\exp(i\hat{k}_{0,y}y) = \begin{pmatrix} \exp(ik_{0,y}^+ y) & 0 \\ 0 & \exp(ik_{0,y}^- y) \end{pmatrix}_{\mathbf{B}_0}$$

$$\hat{E}_\perp = E - \hbar^2(\hat{k}_{0,x}^2 + \hat{k}_{0,y}^2)/2m$$

normal motion energy operator

$$E_\perp^\pm = E - \hbar^2[(k_{0,x}^\pm)^2 + (k_{0,y}^\pm)^2)]/2m$$

$$\hat{E}_\perp = \begin{pmatrix} E_\perp^+ & 0 \\ 0 & E_\perp^- \end{pmatrix}_{\mathbf{B}_0}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)e^{i\hat{k}_{0,x}x}e^{i\hat{k}_{0,y}y}|\psi(z)\rangle = \hat{E}_\perp e^{i\hat{k}_{0,x}x}e^{i\hat{k}_{0,y}y}|\psi(z)\rangle$$

When the incident beam is polarized either up or down the guide field (like in the Standard scheme of PNR), then the 3D-equation splits into two 1D-equations with different normal-motion energies (different for spin-up and spin-down neutrons).

Standard scheme :

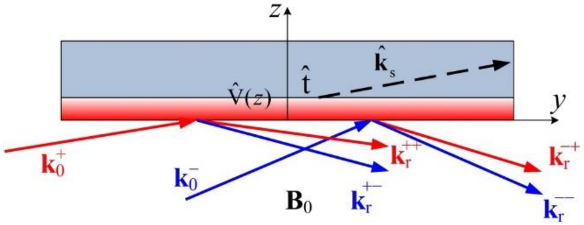
$\pm\mathbf{P}_0 || \mathbf{B}_0$

$$|\Psi(\mathbf{r})\rangle = \exp(ik_{0,x}^\pm x)\exp(ik_{0,y}^\pm y)|\psi(z)\rangle$$

Two 1D-equations $E_\perp^+ \neq E_\perp^-$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)|\psi(z)\rangle = E_\perp^\pm|\psi(z)\rangle$$

Schrödinger equation: transition from 3D to 1D



$$\left(-\frac{\hbar^2}{2m}\Delta + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)|\Psi(\mathbf{r})\rangle = E|\Psi(\mathbf{r})\rangle$$

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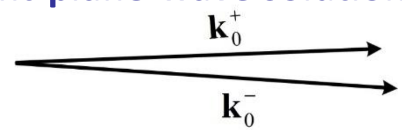
incident-plane-wave solution



$$\mathbf{k}_0^\pm = (k_{0,x}^\pm, k_{0,y}^\pm, k_{0,z}^\pm) \qquad \mathbf{b}_0 = \mathbf{B}_0 / B_0$$

$$k_0^\pm = \hbar^{-1}\sqrt{2m_n[E - (V_0 \pm |\mu_n| B_0)]}$$

$$\hat{k}_{0,x} = (k_{0,x}^+ + k_{0,x}^-)/2 + \hat{\boldsymbol{\sigma}}\mathbf{b}_0 \cdot (k_{0,x}^+ - k_{0,x}^-)/2$$

$$\hat{k}_{0,y} = (k_{0,y}^+ + k_{0,y}^-)/2 + \hat{\boldsymbol{\sigma}}\mathbf{b}_0 \cdot (k_{0,y}^+ - k_{0,y}^-)/2$$

$$\exp(i\hat{k}_{0,x}x) = \begin{pmatrix} \exp(ik_{0,x}^+x) & 0 \\ 0 & \exp(ik_{0,x}^-x) \end{pmatrix}_{\mathbf{B}_0}$$

$$\exp(i\hat{k}_{0,y}y) = \begin{pmatrix} \exp(ik_{0,y}^+y) & 0 \\ 0 & \exp(ik_{0,y}^-y) \end{pmatrix}_{\mathbf{B}_0}$$

$$\hat{E}_\perp = E - \hbar^2(\hat{k}_{0,x}^2 + \hat{k}_{0,y}^2)/2m$$

normal motion energy operator

$$E_\perp^\pm = E - \hbar^2[(k_{0,x}^\pm)^2 + (k_{0,y}^\pm)^2]/2m$$

$$\hat{E}_\perp = \begin{pmatrix} E_\perp^+ & 0 \\ 0 & E_\perp^- \end{pmatrix}_{\mathbf{B}_0}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)e^{i\hat{k}_{0,x}x}e^{i\hat{k}_{0,y}y}|\psi(z)\rangle = \hat{E}_\perp e^{i\hat{k}_{0,x}x}e^{i\hat{k}_{0,y}y}|\psi(z)\rangle$$

When the lateral components of the wavevectors for the incident neutron in the states with the opposite spins, (+) and (-), are equal, then $E_\perp^+ = E_\perp^-$, the 3D-equation reduces to 1D...

$$k_{0,x}^+ = k_{0,x}^- = k_{0,x} \qquad k_{0,y}^+ = k_{0,y}^- = k_{0,y}$$

$\mathbf{P}_0 \# \mathbf{B}_0$

$$\exp(i\hat{k}_{0,x}x) = \exp(ik_{0,x}x) \qquad \exp(i\hat{k}_{0,y}y) = \exp(ik_{0,y}y)$$

$$E_\perp^+ = E_\perp^- = E_\perp$$

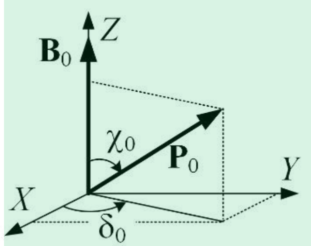
1D-equation:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)|\psi(z)\rangle = E_\perp|\psi(z)\rangle$$

Non-frontal precession

$k^{+}_{0,x} = k^{-}_{0,x} = k_{0,x}$ $\quad k^{+}_{0,y} = k^{-}_{0,y} = k_{0,y}$

$E^{+}_{\perp} = E^{-}_{\perp} = E_{\perp}$



$a^{+}_{0} = \cos(\chi_0 / 2)$

$a^{-}_{0} = \sin(\chi_0 / 2)$

$\delta_0 = \alpha^{-}_{0} - \alpha^{+}_{0}$

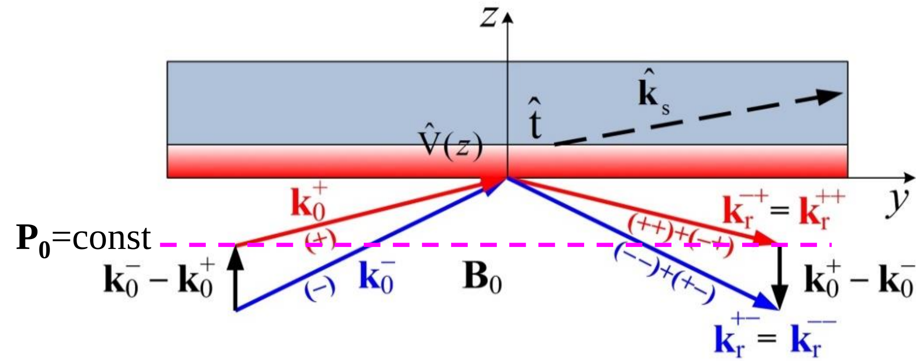
$$|\Psi_0(\mathbf{r})\rangle = \begin{pmatrix} a^{+}_{0} \exp[i(\mathbf{k}^{+}_{0}\mathbf{r} + \alpha^{+}_{0})] \\ a^{-}_{0} \exp[i(\mathbf{k}^{-}_{0}\mathbf{r} + \alpha^{-}_{0})] \end{pmatrix}_{\mathbf{B}_0}$$

incident neutron wave function

1D-equation:

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V(z) - \mu_n \hat{\boldsymbol{\sigma}}\mathbf{B}(z) \right) |\psi(z)\rangle = E_{\perp} |\psi(z)\rangle$$

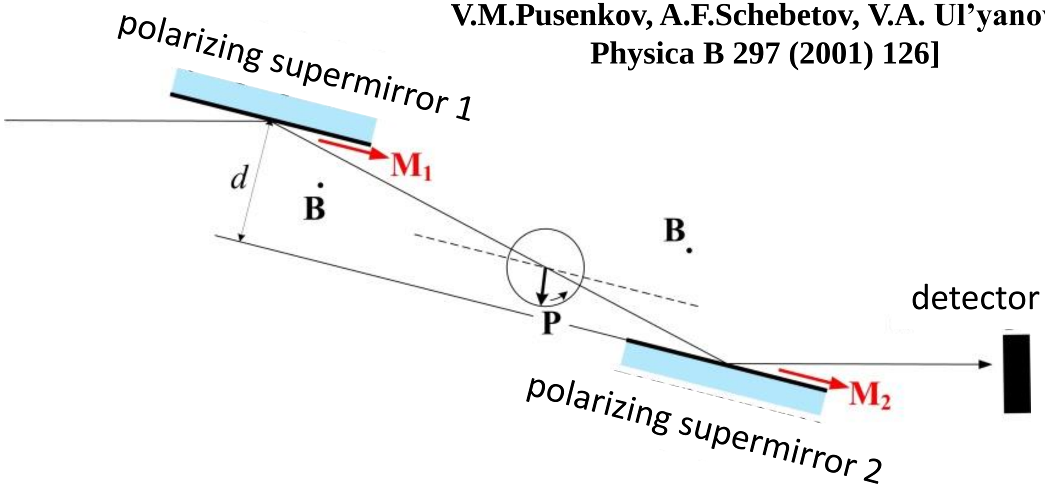
$(k^{-}_{0,z} - k^{+}_{0,z})z = \mathrm{const}$ $\longleftrightarrow$ $\mathbf{P_0}$=const

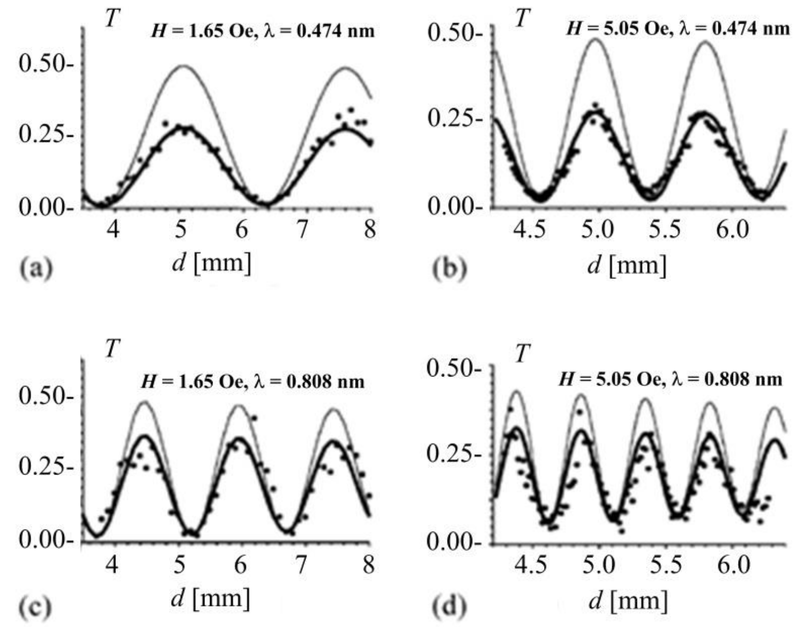


1. The precession front in the incident beam is parallel to the sample surface (!). The same orientation of the neutron spin at the sample surface is <u>needed for phasometry (PNR+)</u>.
2. Such a spin precession should be assigned to <u>each neutron</u>.
3. <u>Neutron spin optics</u> would provide solutions for preparing <u>such beams</u> of neutrons with the precession front parallel to the sample surface at small angles with the beam direction. **[N.K. Pleshanov, Neutron spin optics: Fundamentals and verification. – NIM A 853 (2017) 61]**

Precession: observation with remanent supermirrors

[N.K. Pleshanov, V. Bodnarchuk, R.Gähler, D.A. Korneev, A. Menelle, S.V.Metelev, V.M.Pusenkov, A.F.Schebetov, V.A. Ul'yanov, Physica B 297 (2001) 126]





Schrödinger 1D-equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V(z)-\mu_n\hat{\boldsymbol{\sigma}}\mathbf{B}(z)\right)\left|\psi(z)\right\rangle = E_\perp\left|\psi(z)\right\rangle$$ **1D-equation**

!!! Only z-components of the wavevectors remain, so the lower index z will be omitted, e.g.

$$\hat{k}_0 \equiv \hat{k}_{0,z} \qquad k_0^\pm \equiv k_{0,z}^\pm$$

$$\left|\psi_r(0)\right\rangle = \hat{r}\left|\psi_0(0)\right\rangle \qquad \hat{r} = \begin{pmatrix} r_{++} & r_{-+} \\ r_{+-} & r_{--} \end{pmatrix}_{\mathbf{B}_0}$$ **reflection matrix**

(1D) $$\left|\psi_0(z)\right\rangle = \exp(i\hat{k}_0 z)\left|\psi_0(0)\right\rangle = \begin{pmatrix} a_0^+\exp(ik_0^+ z) \\ a_0^-\exp(i\delta_0)\exp(ik_0^- z) \end{pmatrix}_{\mathbf{B}_0}$$ **incident neutron state "as-prepared"**

$$\left|\psi_r(z)\right\rangle = \exp(-i\hat{k}_0 z)\hat{r}\left|\psi_0(0)\right\rangle = \begin{pmatrix} [r_{++}a_0^+ + r_{-+}a_0^-\exp(i\delta_0)]\exp(-ik_0^+ z) \\ [r_{+-}a_0^+ + r_{--}a_0^-\exp(i\delta_0)]\exp(-ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} A_+e^{-ik_0^+ z} \\ A_-e^{-ik_0^- z} \end{pmatrix}_{\mathbf{B}_0}$$ **reflected neutron wavefunction**

$$A_+ \equiv r_{++}a_0^+ + r_{-+}a_0^- e^{i\delta_0},\ A_- \equiv r_{+-}a_0^+ + r_{--}a_0^- e^{i\delta_0}$$

Reflectivities of polarized neutrons

$$\mathbf{j}(\mathbf{r}) = <\hat{\mathbf{j}}(\mathbf{r})> = \mathrm{Re}\left(\frac{\hbar}{m_\mathrm{n} i}\langle\Psi(\mathbf{r})|\delta(\mathbf{r}'-\mathbf{r})\nabla|\Psi(\mathbf{r})\rangle\right)$$

(3D) **probability current**

$$j(z) = <\hat{\mathrm{j}}(z)> = \mathrm{Re}\left(\hbar/im_\mathrm{n}\,\langle\psi(z)|\delta(z'-z)\,\partial/\partial z\,|\psi(z)\rangle\right)$$

(1D) **flux density (~ j_z)**

The reflectivity is the ratio of the reflected and incident neutron flux densities.

(1D)

$$|\psi(z)\rangle \to |\psi_0(z)\rangle: \quad j_0 \equiv \langle\hat{\mathrm{j}}_0(0)\rangle$$

$$|\psi(z)\rangle \to |\psi_\mathrm{r}(z)\rangle: \quad j_\mathrm{r} \equiv \langle\hat{\mathrm{j}}_\mathrm{r}(0)\rangle$$

$$R = \frac{j_\mathrm{r}}{j_0} = \frac{|A_+|^2 k_0^+ + |A_-|^2 k_0^-}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-}$$

$$A_+ \equiv r_{++} a_0^+ + r_{-+} a_0^- e^{i\delta_0}, \; A_- \equiv r_{+-} a_0^+ + r_{--} a_0^- e^{i\delta_0}$$

Reflectivities of polarized neutrons

$$|\psi_0(z)\rangle = \begin{pmatrix} a_0^+ \exp(ik_0^+ z) \\ a_0^- \exp(i\delta_0)\exp(ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^+(z) \\ \psi_0^-(z) \end{pmatrix}_{\mathbf{B}_0}$$

incident neutron wavefunction

$$|\psi_r(z)\rangle = \begin{pmatrix} [r_{++}a_0^+ + r_{-+}a_0^- \exp(i\delta_0)]\exp(-ik_0^+ z) \\ [r_{+-}a_0^+ + r_{--}a_0^- \exp(i\delta_0)]\exp(-ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} A_+ e^{-ik_0^+ z} \\ A_- e^{-ik_0^- z} \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_r^+(z) \\ \psi_r^-(z) \end{pmatrix}_{\mathbf{B}_0}$$

reflected neutron wavefunction

<u>With the analyzer</u> the reflectivities R± for neutrons with the spin up and down the external field are obtained by using the upper and lower spin components of the reflected neutron wavefunction

(1D)

$$|\psi(z)\rangle \to |\psi_0(z)\rangle: \quad j_0 \equiv \langle \hat{j}_0(0)\rangle$$

$$|\psi(z)\rangle \to \psi_r^+(z): \quad j_r^+ \equiv \langle \hat{j}_r^+(0)\rangle$$

$$|\psi(z)\rangle \to \psi_r^-(z): \quad j_r^- \equiv \langle \hat{j}_r^-(0)\rangle$$

$$R^+ = \frac{j_r^+}{j_0} = \frac{|A_+|^2 k_0^+}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-} \qquad R^- = \frac{j_r^-}{j_0} = \frac{|A_-|^2 k_0^-}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-}$$

in the standard scheme of PNR

$a_0^+ = 1,\ a_0^- = 0 \Rightarrow R_{++} = |r_{++}|^2 \quad R_{+-} = (k_0^- / k_0^+)|r_{+-}|^2$

$a_0^+ = 0,\ a_0^- = 1 \Rightarrow R_{-+} = (k_0^+ / k_0^-)|r_{-+}|^2 \quad R_{--} = |r_{--}|^2$

Z-components of

(Z||B$_0$) **neutron flux polarization** **neutron polarization**

incident beam

$$\tilde{P}_{0,z} = \frac{j_0^+ - j_0^-}{j_0^+ + j_0^-} = \frac{(a_0^+)^2 k_0^+ - (a_0^-)^2 k_0^-}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-} = \cos\tilde{\chi}_0 \neq P_{0,z} = \frac{(a_0^+)^2 - (a_0^-)^2}{(a_0^+)^2 + (a_0^-)^2} = \cos\chi_0$$

reflected beam

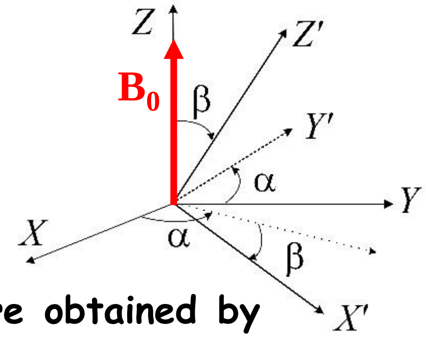
$$\tilde{P}_{r,z} = \frac{j_r^+ - j_r^-}{j_r^+ + j_r^-} = \frac{|A_+|^2 k_0^+ - |A_-|^2 k_0^-}{|A_+|^2 k_0^+ + |A_-|^2 k_0^-} \neq P_{r,z} = \frac{|A_+|^2 - |A_-|^2}{|A_+|^2 + |A_-|^2}$$

Conclusion: <u>neutron flux polarization</u> and <u>neutron polarization</u> differ (neutron flux polarization is defined with the flux densities and neutron polarization - with the probability densities of neutrons with the opposite spins).

Reflectivities of polarized neutrons

$$|\psi_0(z)\rangle = \begin{pmatrix} a_0^+ \exp(ik_0^+ z) \\ a_0^- \exp(i\delta_0)\exp(ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^+(z) \\ \psi_0^-(z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^\uparrow(z) \\ \psi_0^\downarrow(z) \end{pmatrix}_{Z'}$$

$$|\psi_r(z)\rangle = \begin{pmatrix} [r_{++}a_0^+ + r_{-+}a_0^- \exp(i\delta_0)]\exp(-ik_0^+ z) \\ [r_{+-}a_0^+ + r_{--}a_0^- \exp(i\delta_0)]\exp(-ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} A_+ e^{-ik_0^+ z} \\ A_- e^{-ik_0^- z} \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_r^+(z) \\ \psi_r^-(z) \end{pmatrix}_{\mathbf{B}_0} \equiv \begin{pmatrix} \psi_0^\uparrow(z) \\ \psi_0^\downarrow(z) \end{pmatrix}_{Z'}$$



The reflectivities for neutrons with the spin inclined to the external field are obtained by using the spin components of the reflected neutron wavefunction in respective representation

(1D)

$$|\psi(z)\rangle \to \psi_0^\uparrow(z): \quad j_0^\uparrow \equiv \langle \hat{j}_0^\uparrow(0) \rangle \qquad |\psi(z)\rangle \to \psi_r^\uparrow(z): \quad j_r^\uparrow \equiv \langle \hat{j}_r^\uparrow(0) \rangle$$

$$|\psi(z)\rangle \to \psi_0^\downarrow(z): \quad j_0^\downarrow \equiv \langle \hat{j}_0^\downarrow(0) \rangle \qquad |\psi(z)\rangle \to \psi_r^\downarrow(z): \quad j_r^\downarrow \equiv \langle \hat{j}_r^\downarrow(0) \rangle$$

$(Z' \parallel X)$

$Z'(\alpha=0,\ \beta=\pi/2) \parallel X \qquad \tilde{\mathbf{P}}_r \parallel X: \qquad j_r^\uparrow > 0,\ \ j_r^\downarrow < 0 \ \Rightarrow\ \tilde{P}_{r,X} = \dfrac{j_r^\uparrow - j_r^\downarrow}{j_r^\uparrow + j_r^\downarrow} > 1$ **(???)**

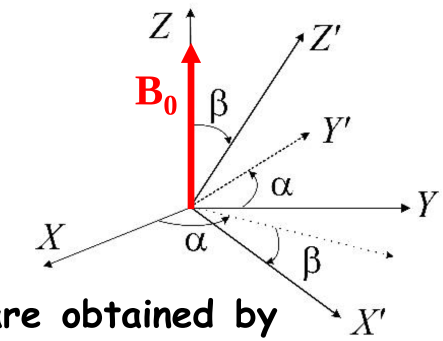
$R^\uparrow > 0,\ \ R^\downarrow < 0$ **(???)**

When the neutron flux polarization is along the X-axis, the reflectivity of neutrons with the spin opposite to the X-axis is negative.

Neutron flux polarization and neutron polarization

$$|\psi_0(z)\rangle = \begin{pmatrix} a_0^+ \exp(ik_0^+ z) \\ a_0^- \exp(i\delta_0)\exp(ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^+(z) \\ \psi_0^-(z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^\uparrow(z) \\ \psi_0^\downarrow(z) \end{pmatrix}_{Z'}$$

$$|\psi_r(z)\rangle = \begin{pmatrix} [r_{++}a_0^+ + r_{-+}a_0^- \exp(i\delta_0)]\exp(-ik_0^+ z) \\ [r_{+-}a_0^+ + r_{--}a_0^- \exp(i\delta_0)]\exp(-ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} A_+ e^{-ik_0^+ z} \\ A_- e^{-ik_0^- z} \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_r^+(z) \\ \psi_r^-(z) \end{pmatrix}_{\mathbf{B}_0} \equiv \begin{pmatrix} \psi_0^\uparrow(z) \\ \psi_0^\downarrow(z) \end{pmatrix}_{Z'}$$



The reflectivities for neutrons with the spin inclined to the external field are obtained by using the spin components of the reflected neutron wavefunction in respective representation

($Z'\#\mathbf{B}_0$) **(1D)**

$$|\psi(z)\rangle \to \psi_0^\uparrow(z): \quad j_0^\uparrow \equiv \langle \hat{j}_0^\uparrow(0)\rangle \qquad |\psi(z)\rangle \to \psi_r^\uparrow(z): \quad j_r^\uparrow \equiv \langle \hat{j}_r^\uparrow(0)\rangle$$

$$|\psi(z)\rangle \to \psi_0^\downarrow(z): \quad j_0^\downarrow \equiv \langle \hat{j}_0^\downarrow(0)\rangle \qquad |\psi(z)\rangle \to \psi_r^\downarrow(z): \quad j_r^\downarrow \equiv \langle \hat{j}_r^\downarrow(0)\rangle$$

		neutron flux polarization		neutron polarization
precessing components	**($Z'\perp\mathbf{B}_0$)**	$\tilde{P}_{0,XY} = \dfrac{j_0^\uparrow - j_0^\downarrow}{j_0^\uparrow + j_0^\downarrow} = \dfrac{a_0^+ a_0^- (k_0^+ + k_0^-)}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-}$	$>$	$P_{0,XY} = 2a_0^+ a_0^- = \sin\chi_0$
***Z*-components**	**($Z\Vert\mathbf{B}_0$)**	$\tilde{P}_{0,Z} = \dfrac{j_0^+ - j_0^-}{j_0^+ + j_0^-} = \dfrac{(a_0^+)^2 k_0^+ - (a_0^-)^2 k_0^-}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-} = \cos\tilde{\chi}_0$	$<$	$P_{r,Z} = \dfrac{(a_0^+)^2 - (a_0^-)^2}{(a_0^+)^2 + (a_0^-)^2} = \cos\chi_0$
$\tilde{P}_0 = \sqrt{(\tilde{P}_{0,XY})^2 + (\tilde{P}_{0,Z})^2}$		$\tilde{P}_0 = \dfrac{\sqrt{(a_0^+ k_0^+)^2 + (a_0^- k_0^-)^2}}{(a_0^+)^2 k_0^+ + (a_0^-)^2 k_0^-} > 1$ **(???)**		$P_0 = 1$

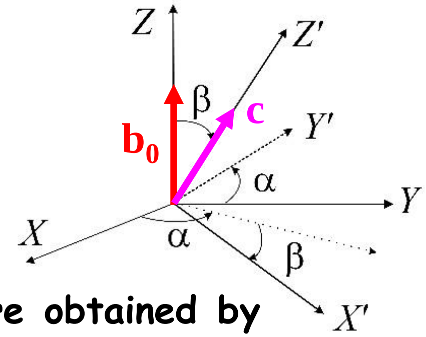
$$P_0 = \sqrt{(P_{0,XY})^2 + (P_{0,Z})^2}$$

More generally, whenever the quantization axis Z' # $\mathbf{B}_0$, the length of the neutron flux polarization exceeds 1.

Reflectivities of polarized neutrons

$$|\psi_0(z)\rangle = \begin{pmatrix} a_0^+ \exp(ik_0^+ z) \\ a_0^- \exp(i\delta_0)\exp(ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^+(z) \\ \psi_0^-(z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_0^\uparrow(z) \\ \psi_0^\downarrow(z) \end{pmatrix}_{Z'}$$

$$|\psi_r(z)\rangle = \begin{pmatrix} [r_{++}a_0^+ + r_{-+}a_0^- \exp(i\delta_0)]\exp(-ik_0^+ z) \\ [r_{+-}a_0^+ + r_{--}a_0^- \exp(i\delta_0)]\exp(-ik_0^- z) \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} A_+ e^{-ik_0^+ z} \\ A_- e^{-ik_0^- z} \end{pmatrix}_{\mathbf{B}_0} = \begin{pmatrix} \psi_r^+(z) \\ \psi_r^-(z) \end{pmatrix}_{\mathbf{B}_0} \equiv \begin{pmatrix} \psi_0^\uparrow(z) \\ \psi_0^\downarrow(z) \end{pmatrix}_{Z'}$$



The reflectivities for neutrons with the spin inclined to the external field are obtained by using the spin components of the reflected neutron wavefunction in respective representation

($Z' \# \mathbf{B}_0$) **(1D)**

$$|\psi(z)\rangle \to \psi_0^\uparrow(z): \quad j_0^\uparrow \equiv \langle \hat{\mathrm{j}}_0^\uparrow(0)\rangle \qquad |\psi(z)\rangle \to \psi_r^\uparrow(z): \quad j_r^\uparrow \equiv \langle \hat{\mathrm{j}}_r^\uparrow(0)\rangle$$

$$|\psi(z)\rangle \to \psi_0^\downarrow(z): \quad j_0^\downarrow \equiv \langle \hat{\mathrm{j}}_0^\downarrow(0)\rangle \qquad |\psi(z)\rangle \to \psi_r^\downarrow(z): \quad j_r^\downarrow \equiv \langle \hat{\mathrm{j}}_r^\downarrow(0)\rangle$$

The strange results may be explained by noticing that

c is the unit vector along *Z′*, $\mathbf{b}_0 = \mathbf{B}_0 / B_0$

$$[\hat{\mathrm{j}}_0(z), \hat{\boldsymbol{\sigma}}\mathbf{c}] = i(\hbar/m_n)\delta(z'-z)(k_0^+ - k_0^-)[\hat{\boldsymbol{\sigma}}\mathbf{b}_0, \hat{\boldsymbol{\sigma}}\mathbf{c}] = i(\hbar/m_n)\delta(z'-z)(k_0^+ - k_0^-)\cdot(\mathbf{b}_0 \times \mathbf{c})\hat{\boldsymbol{\sigma}}$$

The probability current operator does not commute with the operator of the spin projection onto any axis **c**, inclined to the field direction. That means that the respective flux density and the reflectivity are not defined unambiguously. No analyzer could be imagined that would <u>perfectly</u> separate neutrons with the opposite spins inclined to the field.

Weak external field approximation

$|\mu_n| B_0 | / E_\perp \ll 1$ **criterion for the weak field**

$E_\perp = E \sin^2 \theta$

$|\mu_n| B_0 | = 60\,[\mathrm{neV}]$ for 1 [T]

$|\mu_n| B_0 | = 0.06\,[\mathrm{neV}]$ for 1 [mT]

E.g., $E_\perp = 56\,[\mathrm{neV}]$ at the total reflection edge of Si

$|\mu_n| B_0 | / E_\perp = 0.001$

$$\frac{k_0^- - k_0^+}{(k_0^+ + k_0^-)/2} = |\mu_n| B_0 / E_\perp \quad \Rightarrow \quad k_0^- = k_0^+ = k$$

(except for the phase terms of type $(k_0^- - k_0^+) z = k\, z |\mu_n| B_0 / E_\perp$

which describe the precession at macroscopic distances *z*)

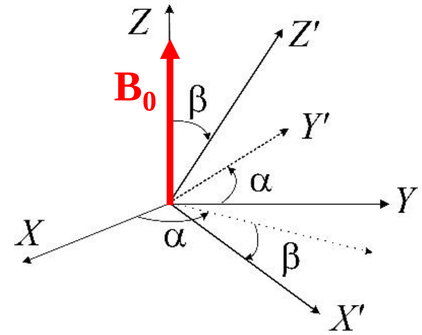
$$[\hat{\mathrm{j}}_0(z), \hat{\boldsymbol{\sigma}}\mathbf{c}] = i(\hbar / m_n)\delta(z' - z)(k_0^+ - k_0^-)[\hat{\boldsymbol{\sigma}}\mathbf{b}_0, \hat{\boldsymbol{\sigma}}\mathbf{c}] = i(\hbar / m_n)\delta(z' - z)(k_0^+ - k_0^-) \cdot (\mathbf{b}_0 \times \mathbf{c})\hat{\boldsymbol{\sigma}} \simeq 0$$

Due to restrictions on the magnitude of external fields in phasometry, the commutator tends to 0, and the reflectivity of neutrons with any spin orientation is well defined.

Relationship between two representations

$$R_{++} = |r_{++}|^2 \qquad R_{+-} = |r_{+-}|^2 \qquad R_{-+} = |r_{-+}|^2 \qquad R_{--} = |r_{--}|^2$$

$$R_{\uparrow\uparrow} = |r_{\uparrow\uparrow}|^2 \qquad R_{+-} = |r_{\uparrow\downarrow}|^2 \qquad R_{\downarrow\uparrow} = |r_{\downarrow\uparrow}|^2 \qquad R_{\downarrow\downarrow} = |r_{\downarrow\downarrow}|^2$$



The relations between the elements of the reflection matrices in representations with the quantization axes $Z||B_0$ and Z' :

$$\begin{pmatrix} r_{\uparrow\uparrow} & r_{\downarrow\uparrow} \\ r_{\uparrow\downarrow} & r_{\downarrow\downarrow} \end{pmatrix}_{Z'} = \mathrm{U}(\alpha,\beta) \begin{pmatrix} r_{++} & r_{-+} \\ r_{+-} & r_{--} \end{pmatrix}_{\mathbf{B}_0} \mathrm{U}^{-1}(\alpha,\beta) \Rightarrow$$

$$r_{\uparrow\uparrow} = r_{++}\cos^2(\beta/2) + r_{--}\sin^2(\beta/2) + \sin\beta[r_{-+}\exp(i\alpha) + r_{+-}\exp(-i\alpha)]/2,$$

$$r_{\downarrow\uparrow} = \sin\beta(r_{--} - r_{++})/2 + r_{-+}\cos^2(\beta/2)\exp(i\alpha) - r_{+-}\sin^2(\beta/2)\exp(-i\alpha),$$

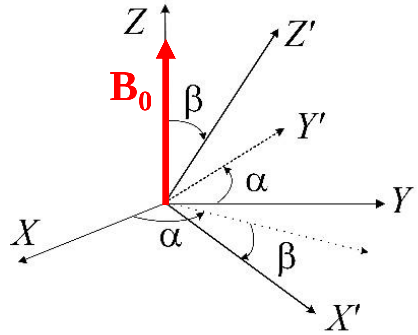
$$r_{\uparrow\downarrow} = \sin\beta(r_{--} - r_{++})/2 - r_{-+}\sin^2(\beta/2)\exp(i\alpha) + r_{+-}\cos^2(\beta/2)\exp(-i\alpha),$$

$$r_{\downarrow\downarrow} = r_{++}\sin^2(\beta/2) + r_{--}\cos^2(\beta/2) - \sin\beta[r_{-+}\exp(i\alpha) + r_{+-}\exp(-i\alpha)]/2.$$

Two sets of the reflectivities, corresponding to the reflection matrices in two representations, can be measured. They define the phase differences.

Relationship between two representations

The relations between squares of the moduli of the elements of the reflection matrices in representations with the quantization axes $Z||B_0$ and Z' :



$$|r'_{\uparrow\uparrow}|^2 = F_1 + \sin\beta\left(G_1\cos^2(\beta/2) + G_2\sin^2(\beta/2)\right) + (H_1/4)\sin^2\beta,$$

$$|r'_{\downarrow\uparrow}|^2 = F_2 + \sin\beta\left(G_3\cos^2(\beta/2) - G_4\sin^2(\beta/2)\right) + (H_2/4)\sin^2\beta,$$

$$|r'_{\uparrow\downarrow}|^2 = F_3 - \sin\beta\left(G_3\cos^2(\beta/2) - G_4\sin^2(\beta/2)\right) + (H_2/4)\sin^2\beta,$$

$$|r'_{\downarrow\downarrow}|^2 = F_4 - \sin\beta\left(G_1\sin^2(\beta/2) + G_2\cos^2(\beta/2)\right) + (H_1/4)\sin^2\beta,$$

$$F_1 = |r_{++}|^2\cos^4(\beta/2) + |r_{--}|^2\sin^4(\beta/2),\ \ F_2 = |r_{-+}|^2\cos^4(\beta/2) + |r_{+-}|^2\sin^4(\beta/2),$$

$$F_3 = |r_{-+}|^2\sin^4(\beta/2) + |r_{+-}|^2\cos^4(\beta/2),\ \ F_4 = |r_{++}|^2\sin^4(\beta/2) + |r_{--}|^2\cos^4(\beta/2),$$

$$G_1 = |r_{++}||r_{-+}|\cos(\varphi_{++} - \varphi_{-+} - \alpha) + |r_{++}||r_{+-}|\cos(\varphi_{++} - \varphi_{+-} + \alpha),$$

$$G_2 = |r_{--}||r_{-+}|\cos(\varphi_{-+} - \varphi_{--} + \alpha) + |r_{--}||r_{+-}|\cos(\varphi_{+-} - \varphi_{--} - \alpha),$$

$$G_3 = |r_{--}||r_{-+}|\cos(\varphi_{-+} - \varphi_{--} + \alpha) - |r_{++}||r_{-+}|\cos(\varphi_{++} - \varphi_{-+} - \alpha),$$

$$G_4 = |r_{--}||r_{+-}|\cos(\varphi_{+-} - \varphi_{--} - \alpha) - |r_{++}||r_{+-}|\cos(\varphi_{++} - \varphi_{+-} + \alpha),$$

$$H_1 = |r_{+-}|^2 + |r_{-+}|^2 + 2|r_{++}||r_{--}|\cos(\varphi_{++} - \varphi_{--}) + 2|r_{+-}||r_{-+}|\cos(\varphi_{-+} - \varphi_{+-} + 2\alpha),$$

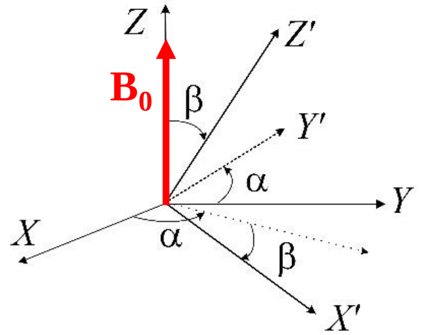
$$H_2 = |r_{++}|^2 + |r_{--}|^2 - 2|r_{++}||r_{--}|\cos(\varphi_{++} - \varphi_{--}) - 2|r_{+-}||r_{-+}|\cos(\varphi_{-+} - \varphi_{+-} + 2\alpha).$$

$$\Delta_d = \varphi_{++} - \varphi_{--},\ \ \Delta_+ = \varphi_{++} - \varphi_{-+},\ \ \Delta_- = \varphi_{+-} - \varphi_{--}$$

$$\varphi_{-+} - \varphi_{--} = \Delta_d - \Delta_+,\ \ \varphi_{++} - \varphi_{+-} = \Delta_d - \Delta_-,\ \ \varphi_{-+} - \varphi_{+-} = \Delta_d - \Delta_+ - \Delta_-$$

Relationship between two representations

The relations between squares of the moduli of the elements of the reflection matrices in representations with the quantization axes $Z\|B_0$ and Z' :



$$|r'_{\uparrow\uparrow}|^2-|r'_{\downarrow\downarrow}|^2+|r'_{\downarrow\uparrow}|^2-|r'_{\uparrow\downarrow}|^2=(|r_{++}|^2-|r_{--}|^2+|r_{-+}|^2-|r_{+-}|^2)\cos\beta+$$
$$+2[|r_{++}||r_{+-}|\cos(\Delta_d-\Delta_-+\alpha)+|r_{--}||r_{-+}|\cos(\Delta_d-\Delta_++\alpha)]\sin\beta,$$

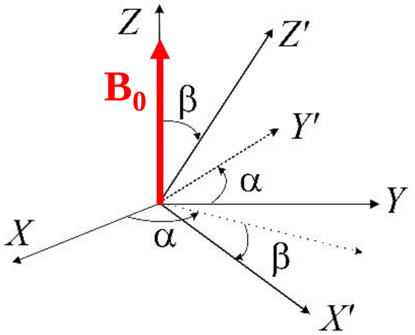
$$|r'_{\uparrow\uparrow}|^2-|r'_{\downarrow\downarrow}|^2-|r'_{\downarrow\uparrow}|^2+|r'_{\uparrow\downarrow}|^2=(|r_{++}|^2-|r_{--}|^2-|r_{-+}|^2+|r_{+-}|^2)\cos\beta+$$
$$+2[|r_{++}||r_{-+}|\cos(\Delta_+-\alpha)+|r_{--}||r_{+-}|\cos(\Delta_--\alpha)]\sin\beta,$$

$$|r'_{\uparrow\uparrow}|^2+|r'_{\downarrow\downarrow}|^2-|r'_{\downarrow\uparrow}|^2-|r'_{\uparrow\downarrow}|^2=(|r_{++}|^2+|r_{--}|^2-|r_{-+}|^2-|r_{+-}|^2)\cos^2\beta+$$
$$+2[|r_{++}||r_{--}|\cos\Delta_d+|r_{-+}||r_{+-}|\cos(\Delta_d-\Delta_+-\Delta_-+2\alpha)]\sin^2\beta+$$
$$+2[|r_{++}||r_{-+}|\cos(\Delta_+-\alpha)-|r_{--}||r_{+-}|\cos(\Delta_--\alpha)+|r_{++}||r_{+-}|\cos(\Delta_d-\Delta_-+\alpha)-$$
$$-|r_{--}||r_{-+}|\cos(\Delta_d-\Delta_++\alpha)]\sin\beta\cos\beta,$$

$$|r'_{\uparrow\uparrow}|^2+|r'_{\downarrow\downarrow}|^2+|r'_{\downarrow\uparrow}|^2+|r'_{\uparrow\downarrow}|^2=|r_{++}|^2+|r_{--}|^2+|r_{-+}|^2+|r_{+-}|^2.$$ **(!!!)**

$$\Delta_d=\varphi_{++}-\varphi_{--},\ \ \Delta_+=\varphi_{++}-\varphi_{-+},\ \ \Delta_-=\varphi_{+-}-\varphi_{--}$$

The relations between squares of the moduli of the elements of the reflection matrices in representations with the quantization axes *Z*||B_0 and *Z′* :



$\beta = \pi/2$:

$$|r'_{\uparrow\uparrow}|^2 - |r'_{\downarrow\downarrow}|^2 + |r'_{\downarrow\uparrow}|^2 - |r'_{\uparrow\downarrow}|^2 = 2[|r_{++}||r_{+-}|\cos(\Delta_d - \Delta_- + \alpha) + |r_{--}||r_{-+}|\cos(\Delta_d - \Delta_+ + \alpha)],$$

$$|r'_{\uparrow\uparrow}|^2 - |r'_{\downarrow\downarrow}|^2 - |r'_{\downarrow\uparrow}|^2 + |r'_{\uparrow\downarrow}|^2 = 2[|r_{++}||r_{-+}|\cos(\Delta_+ - \alpha) + |r_{--}||r_{+-}|\cos(\Delta_- - \alpha)],$$

$$|r'_{\uparrow\uparrow}|^2 + |r'_{\downarrow\downarrow}|^2 - |r'_{\downarrow\uparrow}|^2 - |r'_{\uparrow\downarrow}|^2 = 2[|r_{++}||r_{--}|\cos\Delta_d + |r_{-+}||r_{+-}|\cos(\Delta_d - \Delta_+ - \Delta_- + 2\alpha)].$$

$$\Delta_d = \varphi_{++} - \varphi_{--},\ \Delta_+ = \varphi_{++} - \varphi_{-+},\ \Delta_- = \varphi_{+-} - \varphi_{--}$$

Conclusion

Tasks on development of PNR+:

√ - to substantiate the method theoretically;

- to introduce methods of obtaining the phase information;
- to suggest measurement schemes.

The methods of difference phasometry :

- guide field tilt method;
- sample rotation method;
- spin tilt method;
- cross-interference method;
- 3D-polarization analysis.

In the first three methods the manipulations with the field, sample, or neutron spins provide two sets of moduli of the reflection matrix elements. More exquisite methods use cross-interference and 3D-polarization analysis.

Final remark

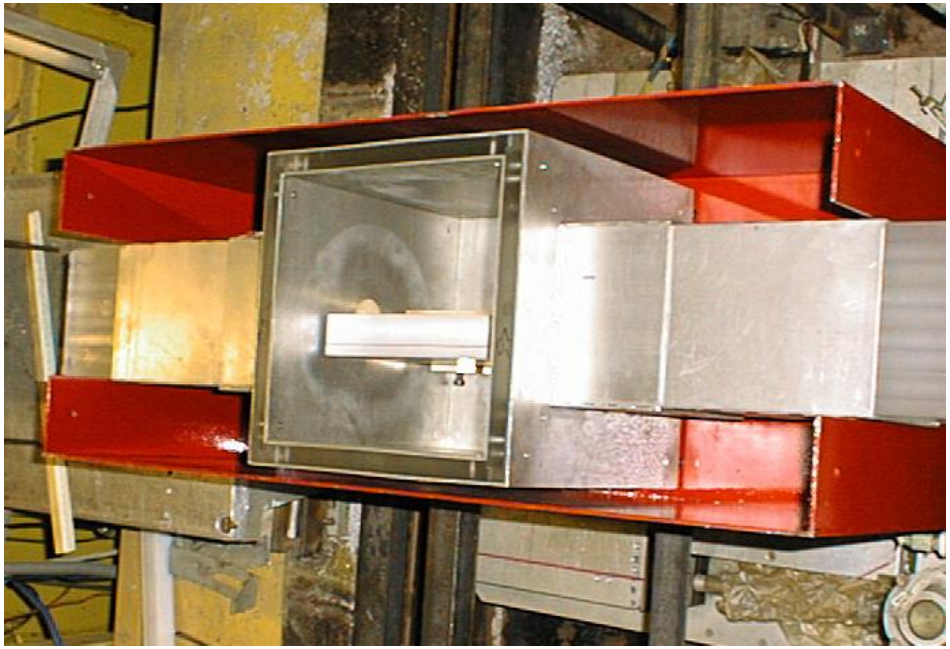


Photo: The spin manipulator with a sample holder in the process of its assembly at the neutron reflectometer NR-4M (beam 13, WWR-M reactor, Gatchina) for measurements with 3D-polarization analysis with the sample in zero field, in the absence of spin precession.

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Thanks for
your attention!