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# STRONG COLLISION APPROACH TO CALCULATION OF DEPOLARIZATION FUNCTION FOR NEUTRON BEAM PASSING THROUGH FERROMAGNETIC BULK DOMAINS

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ABSTRACT

We propose the Markovian random walk approach for calculation of the depolarization function of the polarized neutron beam transmitted through a magnetic medium. This approach allows one to obtain exact analytical results for the depolarisation function $P(\lambda)$ which is valid for any wavelength $\lambda$. Two magnetic configurations were considered in the present work: random ferromagnetic domains, and staggered ferromagnetic domains.

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# 1 Introduction

The last 40-50 years in condensed matter physics are characterized by the more increased role of nuclear physics methods as an instrument for scientific investigations. Together with the nuclear magnetic resonance (NMR)[1] and the positive muon spin rotation ($\mu^+$SR)[2], the method of neutron depolarization stood as an attractive tool for exploring the internal structure of ferro- and antiferromagnetics as well as disordered spin systems. A base for interpretation of experimental data during long period was served by the theory of Halpern and Holstein [3] developed when there were no sources of polarized neutrons at all.

Nowadays in the world there are about a dozen of such sources, and the Time-Of-Flight spectrometers (e.g. in KEK (Japan) [4] and at JINR (Dubna, Russia)[5]) give the possibility to obtain the spectral dependence in the wavelength window. An actual task now is to find more refined approaches to calculate the neutron depolarization function in a magnetically disordered medium for understanding of the interconnection between the internal magnetic structures of such systems and the various kind of the experimental depolarization functions. The remarkable steps in this way were several papers using classical approach[6,7], quantum mechanical calculations of the neutron scattering process[8], and Gaussian two- momentum approximation[9].

Let us introduce briefly the neutron depolarization process in magnetic materials. The neutron is a particle possessing magnetic moment. When polarized neutron beam goes through magnetic material it changes its initial polarization due to magnetic interactions. This interaction can be treated in classical way for cold neutrons with typical wavelengths of the order $1-10$Å, passing through magnetic regions with typical sizes $> 10^4$Å. This is the case of polydomain ferromagnetics. To get an information about fields in the domains, their mutual orientation, sizes, etc. one has to analyze the wavelength dependence of the neutron polarization. Varying the wavelength actually corresponds to the change in dynamics of the magnetic fields seen by the neutron, leading to different regimes of the depolarization process. One can distinguish two important cases: (i) fast dynamics of the magnetic fields corresponding to the small wavelengths $\lambda \langle\delta\rangle H \ll C$, where $\langle\delta\rangle$ is the mean domain size and $H$ is the RMS value of the magnetic field on the neutron, $C$ – is a physical constant; and (ii) slow dynamics corresponding to the large wavelengths $\lambda \langle\delta\rangle H \gg C$. Another important parameter is the average number of domains $N = L/\langle\delta\rangle$ along the neutron beam. The form of the depolarization function strongly depends on the above mentioned conditions and, in addition, it is affected by the mutual domain orientation and distribution of the magnetization over the sample. The asymptotic values of the depolarization function were calculated only for a few magnetic configurations in these extreme cases – fast or slow dynamics, large or small $N$. The problem is how to conduct the correct time and configuration average of the neutron moment evolution. The situation becomes worse when there is some correlation in domain orientation.

We propose the "strong collision" or Markovian random-walk[10] approach for calculation of the neutron depolarization, which is widely used in various application of such experimental techniques as NMR and $\mu$SR. The probe particle's depolarization processes in all these methods have many similarities. Thus, the positive muon is localized in some site in the crystal lattice. The evolution of the muon spin in the sample is determined by the local internal magnetic fields. These fields can be either static or dynamic. The latter is realized for the muon diffusion or fluctuating magnetic fields on the muon. For these cases the analytical approaches to were developed to calculate the muon relaxation function. Notice, that the mechanism of the depolarization of the neutron beam passing through polydomain sample with static domain magnetic field distribution is very similar to muon spin depolarization by fluctuating fields. In the neutron frame its moment is affected by the abrupt change of the magnetic field when it goes from one to another domain. This analogy allows to apply the methods of the calculation of the muon depolarization functions to the process of neutron beam depolarization.

# 2 Neutron Depolarization Function in Strong Collision Model

When the neutron beam is passing through the single magnetic domain it is affected by the static magnetic field. The evolution of its magnetic moment in the field **H** is given by the Larmor equation

$$\frac{d\mathbf{m}}{dt} = \gamma_n \mathbf{m} \times \mathbf{H}, \tag{1}$$

where $\gamma_n$ is the gyromagnetic ratio of the neutron. It is convenient to write the solution of (1) in terms of evolution matrix $\hat{M}$:

$$\mathbf{m}(t) = \hat{M}(t)\mathbf{m}(0), \tag{2}$$

$$M_{\alpha\beta} = \frac{\omega_\alpha \omega_\beta}{\omega^2} + (\delta_{\alpha\beta} - \frac{\omega_\alpha \omega_\beta}{\omega^2})\cos(\omega t) + e_{\alpha\beta\gamma}\frac{\omega_\gamma}{\omega}\sin(\omega t), \tag{3}$$

where $\boldsymbol{\omega} = \gamma_n \mathbf{H}$. The polarization of the ensemble of neutrons in the magnetic fields with spectral distribution $W(\mathbf{H})$ is given by the averaged matrix:

$$g_{\alpha\beta}(t) = \langle M_{\alpha\beta} \rangle = \int M_{\alpha\beta}(\mathbf{H}, t) W(\mathbf{H}) d\mathbf{H}. \tag{4}$$

The neutron polarization given by the matrix $g_{\alpha\beta}(t)$ corresponds to the case of static fields on the neutron. In principle, one could imagine this situation for a thin sample which contains on an average one domain along the beam and many domains in the perpendicular plane. In reality there are many domains on the neutron path and to get the depolarization one should perform time averaging of the static depolarization matrix $g_{\alpha\beta}(t)$. When the neutron is passing from domain to domain the magnetic field on the neutron is changed. We will suppose that the field alternations are abrupt and that they occur like Markovian process. In the considered model the evolution of the magnetic moment in the domain is taken in the averaged form given by the matrix $\hat{g}(t)$. In general, one can suppose several types of domains configured in such way that the time averaging of polarization can not be performed independently. Let us assume that there are $M$ types of domains, and divide the neutron beam over the $M$ subbeams each of them is ended in the corresponding domains. The total polarization of the beam $\mathbf{P}(t)$ will be the sum of partial subbeam polarizations:

$$\mathbf{P}(t) = \sum_{i=1}^{M} \mathbf{P}_i(t), \tag{5}$$

In framework of Markovian random-walk model the partial polarizations $\mathbf{P}_i(t)$ are given by the set of integral equations/[10]/:

$$\mathbf{P}_i(t) = \mathrm{e}^{-\nu_i t}\hat{g}_i(t)A_i\mathbf{P}(0) + \sum_{k=1}^{M}\nu_{ik}\int_0^t \mathrm{e}^{-\nu_i(t-\tau)}\hat{g}_i(t-\tau)\mathbf{P}_k(\tau)d\tau, \qquad (6)$$

where $\hat{g}_i(t)$ – is the evolution matrix for $i$th-type domain, $\mathbf{P}(0)$ – is the initial polarization of the neutron beam, $A_i$ – is a weighted number of $i$th domain, $\nu_{ik}$ – is the rate of transitions from domain of $k$-type to $i$-type, $\nu_i = \sum_{k=1}^{M}\nu_{ki}$ – the full rate of leaving the $i$th domain. The matrix $\nu_{ik}$ is determined by the domains configuration along the neutron beam and by the average sizes of domains. With help of Laplace transformation the set of equations (6) is reduced to the algebraic set of linear equations:

$$\mathbf{P}_i(s) = \hat{g}_i(s+\nu_i)A_i\mathbf{P}(0) + \sum_{k=1}^{M}\nu_{ik}\hat{g}_i(s+\nu_i)\mathbf{P}_k(s), \qquad (7)$$

Solving (7) and performing the inverse Laplace transformation we will get the polarization at the time $t$. The final polarization is obtained for the time $t = L/v$ ($L$ – the sample length along the beam, $v$ – the neutron velocity). The dependence on the neutron wavelength comes to $\mathbf{P}(t)$ via $\nu_{ik}$ matrix. If we assume the domains to be of the same type and the absence of correlations between them, then the set of equations (7) is reduced to a single equation and the transition rate $\nu$ is given by the average domain size $\langle\delta\rangle$ and neutron wavelength $\lambda$ according to the relation $\nu = \frac{h}{m}\frac{1}{\lambda\langle\delta\rangle}$, where $m$ – is the mass of the neutron, $h$ – the Plank constant.

Further we will consider the examples of two different cases : (i) the magnetic field is changed to a new value which has no correlation with previous one; (ii) there is a strong correlation between the fields in neighbouring domains.

# 3 Depolarization Formulas for some Magnetic Configurations

## 3.1 Random Ferromagnetic Domains

The sample is considered as a set of uncorrelated ferromagnetic domains each of them has the same module of magnetization with random isotropic directions of magnetization. Let the initial polarization $\mathbf{P}(0)$ is directed along $z$-axis. The evolution of the $z$-component of polarization in the domain is given by $g_{zz}(t)$-component of the matrix (4).

$$g_{zz}(t) = \frac{1}{3} + \frac{2}{3}\cos(\omega t), \qquad (8)$$

where $\omega = \gamma_n H$, and $H$ is the module of the magnetic field in the domains. Since the magnetization of domains are not correlated, the transition matrix $\nu_{ik}$ is just the number $\nu = \frac{h}{m}\frac{1}{\lambda\langle\delta\rangle}$ and (7) is represented by one equation. Having performed the Laplace transform of (8) and substituting the result into the equation (7) we have the following $z$-component of Laplace form of the polarization:

Denominator

$$P_z(s) = \frac{s\,(s+2\,\nu) + \nu^2 + \frac{\omega^2}{3}}{s^2\,(s+2\,\nu) + (\nu^2+\omega^2)\,s + \frac{2\,\omega^2\nu}{3}}. \qquad (9)$$

Performing the inverse Laplace transformation and expressing the result in term of wavelengths, we obtain the depolarization formula:

$$P(\lambda) = (\frac{1}{3}+C_1)\exp(-\frac{N\,(v_1 - v_2 + 2)}{3})+\exp(\frac{N\,(v_1 - v_2 - 4)}{6})\left[(\frac{2}{3} - C_1)\cos a + C_2\sin a\right], \tag{10}$$

where the coefficients are:

$$C = 1 - 3\,l^2\omega^2 + 3\,l^4\omega^4,$$
$$v_1 = \sqrt[3]{3\sqrt{C}l\omega - 1},$$
$$v_2 = \sqrt[3]{1 + 3\sqrt{C}l\omega},$$

$$C_1 = \frac{1}{18\,l^2\omega^2 C}\Big( \left(1 - l^2\omega^2\right)\left({v_1}^2 + {v_2}^2\right) + +3\sqrt{C}l\omega\,(v_2 + v_1) - \left(1 - 2\,l^2\omega^2\left(2 - 3\,l^2\omega^2\right)\right)(v_2 - v_1)\Big),$$

$$C_2 = -\frac{\sqrt{3}}{18\,l^2\omega^2 C}\Big( \left(1 - l^2\omega^2\right)\left({v_1}^2 - {v_2}^2\right) + 3\sqrt{C}l\omega\,(v_2 - v_1) + \Big(\left(1 - 3\,l^2\omega^2\right)v_1\,v_2 - -l^2\omega^2\left(2 - 3\,l^2\omega^2\right)\Big)(v_2 + v_1)\Big),$$

$$a = \frac{N\sqrt{3}\,(v_2 + v_1)}{6},$$

with $l = \frac{\langle\delta\rangle\lambda}{(h/m)}$, and $N = \frac{L}{\langle\delta\rangle}$ – which is the average number of domains along the neutrons path. The plot of the depolarization formula (10) for several values of $N$ is presented in figure 1.

Usually the limits of a depolarization formula are used. They can be easily obtained for the polarization $P(\lambda)$ (10) for small wavelength $l\omega \to 0$ and it has the following form:

$$P(\lambda) = \exp\left(-\frac{2}{3}N\omega^2\lambda^2\delta^2/(h/m)^2\right).$$

In the limit of large wavelengths $l\omega \to \infty$ the polarization reads:

$$P(\lambda) = \exp(-\frac{2}{3}N)\Big(\frac{1}{3} + \frac{2}{3}\Big(\cos(L\omega\lambda/(h/m)) + \frac{(h/m)}{\omega\lambda\delta}\sin(L\omega\lambda/(h/m))\Big)\Big).$$

## 3.2 Opposite Orientations of the Magnetization in Neighbouring Ferromagnetic Domains

Now we consider the case of strong time correlation of the magnetic fields on the neutron. Let the sample consist of the domains with the magnetization directed along and against the $x$ axis in the neighbouring domains along the neutron beam. The initial neutron polarization $\mathbf{P}(0)$ is again along $z$-axis. The correlation between the domains is given by the transition matrix $\nu_{ik}$ which has the antisymmetric form:

$$\nu_{ik} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\nu.$$

The evolution matrices $\hat{g}_1(t)$ and $\hat{g}_2(t)$ are simply equal to (3) with substitutions $\boldsymbol{\omega}=(\pm\gamma_n H, 0, 0)$, where $H$ is the module of the magnetic field in the domains.

After substitution some transformations and substituting $\hat{g}_1(s)$, $\hat{g}_2(s)$ and $\nu_{ik}$ in (7), and some transformations we have the following set of linear equations:

$$\begin{cases} [\mathbf{I} - \nu^2 \hat{g}_1(s)\hat{g}_2(s)]\mathbf{P}_1(s) = \frac{1}{2}\hat{g}_1(s)(\mathbf{z} + \nu\hat{g}_2(s)\mathbf{z}), \\ [\mathbf{I} - \nu^2 \hat{g}_2(s)\hat{g}_1(s)]\mathbf{P}_2(s) = \frac{1}{2}\hat{g}_2(s)(\mathbf{z} + \nu\hat{g}_1(s)\mathbf{z}). \end{cases} \tag{11}$$

Note that the correlations between domains orientations are clearly seen in noncommutative multiplications of the evolution matrices. Solving the equation (11) we get the following formula for the Laplace transform of the depolarization function:

$$P_z(s) = P_{1z}(s) + P_{2z}(s) = \frac{2\nu + s}{s^2 + 2s\nu + \omega^2}. \tag{12}$$

And finally after performing the inverse Laplace transform of $P_z(s)$ we have the formula for the wavelength dependence of the neutron depolarization:

$$P(\lambda) = \frac{e^{-N}\left(\sin(N\sqrt{\omega^2 l^2 - 1}) + \cos(N\sqrt{\omega^2 l^2 - 1})\sqrt{\omega^2 l^2 - 1}\right)}{\sqrt{\omega^2 l^2 - 1}}, \tag{13}$$

where the meaning of the parameter $l$ is the same as in previous section. The limit cases of formula (13) are

$$P(\lambda) = \exp\Big(-\frac{1}{2}N\omega^2\lambda^2\delta^2/(h/m)^2\Big) \quad \text{for} \quad l\omega \to 0,$$

$$P(\lambda) = \exp(-N)\Big(\cos(L\omega\lambda/(h/m)) + \frac{(h/m)}{\omega\lambda\delta}\sin(L\omega\lambda/(h/m))\Big) \quad \text{for} \quad l\omega \to \infty.$$

# 4 Conclusion

The main advantage of this approach, in our opinion, is that in many interesting cases it gives exact analytical results for the neutron depolarization $P(\lambda)$ which is valid for any wavelength. Even when there is no analytical form of $P(\lambda)$, it can be obtained with the help of well developed numerical procedures for the Laplace transformation which are not CPU-time-consuming. A relative simplicity of getting the resulting formulas is due to the definite assumption about domain size distribution. Namely, if one supposes that the strong collisions take place as the Markovian process then the domain size distribution is actually chosen in the exponential form. However, taking into account that the domain size distribution is not usually known we tentatively suggest this method as a quite simple way to get at least qualitative picture of the internal magnetic field structures.

The calculations of the depolarization functions within the framework of present approach for more realistic models are in progress.

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## Figure Caption

**Figure 1.** The depolarization of the neutron beam as a function of $l = \frac{\langle\delta\rangle\lambda}{(\hbar/m)}$ for $\omega = 1$. $N$ – is the average number of domains along the neutrons path. Solid lines – random oriented ferromagnetic domains, dashed lines – opposite orientations of the magnetization in neighbouring ferromagnetic domains.

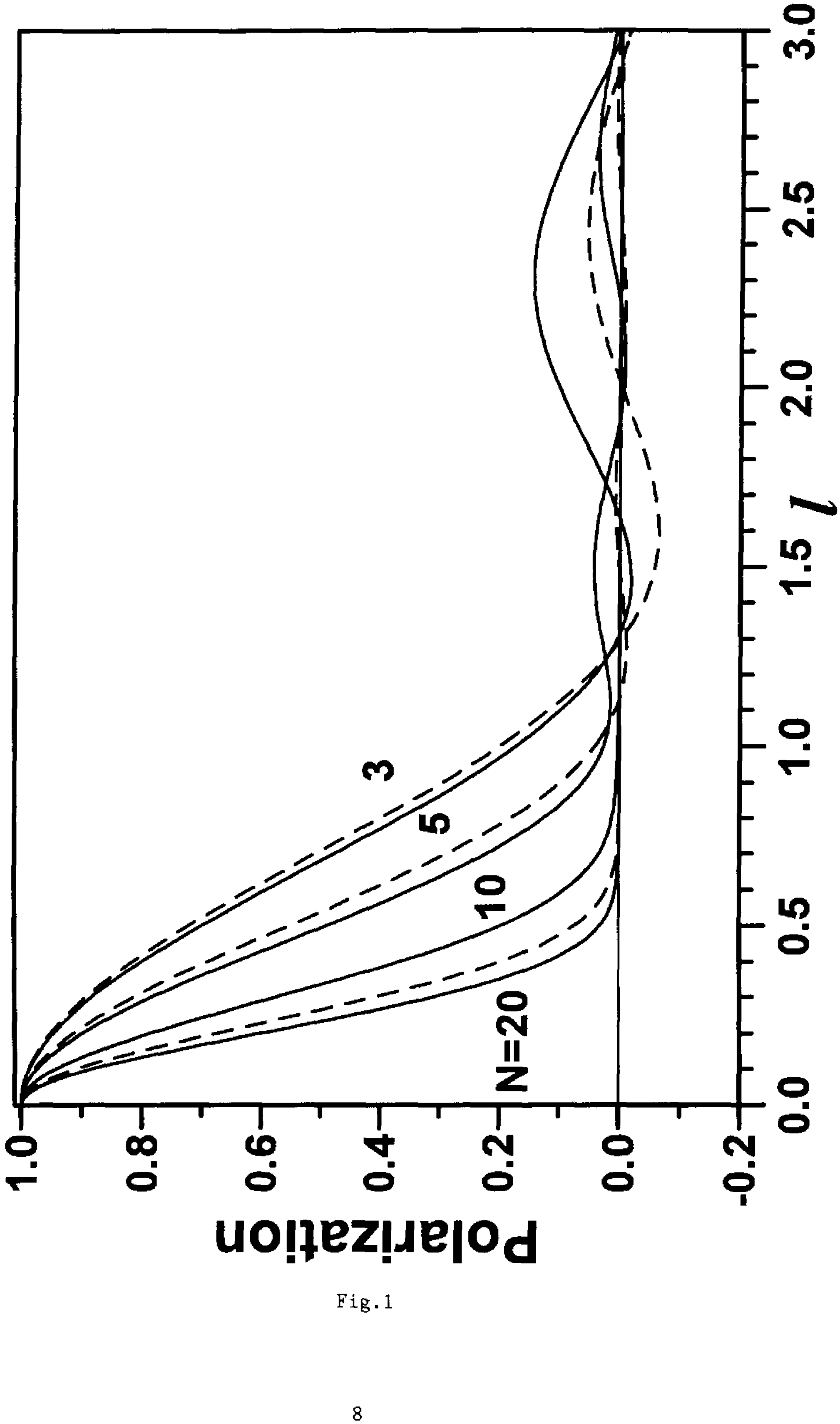


Fig.1