Reflection of neutrons from fan-like magnetic systems

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Abstract
An analytical solution is found for neutron reflectivity from so called fan-like magnetic mirrors with perpendicular exchange-spring multilayered magnetic structure. The main feature of the reflection curves related to this type of magnetization is pointed out. The results of numerical calculations for some parameters of the system are presented. The problems of time parity and detailed balance violation in the model are discussed.

Keywords
Multilayers, Neutron Scattering, Diffraction, Polarization, Magnetism

1. Introduction
Investigation of neutron reflection from multilayered systems belongs to the field of nanostructure research. Magnetic multilayered systems with magnetization vector varying in space can be grown artificially by consecutive evaporation or sputtering techniques of magnetic layers with different coercivity, or they can appear naturally under the action of anisotropic exchange forces [1-4]. A representative example is a soft-magnetic layer (SL), which is magnetically coupled to a hard-magnetic layer (HL) [5-8], when the last one is magnetized non-parallel with respect to the external field orientation. As a result, the SL becomes virtually separated into magnetic sub layers (domains) with different orientations of the magnetization vector, which turns from a direction almost parallel to the external field to a direction defined by the HL magnetization vector. This turn can go along a spiral, giving rise to a helicoidal structure, often referred to as spring magnet, or this turn can be confined in the plane perpendicular to the sample interface. In the last case, the magnetization in the SL is fan-like and is referred to as perpendicular exchange-spring multilayer [9,10]. Neutron scattering on helicoidal structures was investigated in [11]. Here we consider the neutron scattering on a fan-like system. Such a magnetic state in fact consists of a large number of magnetic layers with magnetization slightly turned with respect to each other, and the neutron scattering on them can be calculated numerically by making use of generalized matrix methods [12-15]. However it is possible to model the system by a magnet with continuous rotation of the magnetization vector, and to calculate neutron scattering on it analytically. We show here that neutron scattering on such a system is similar to scattering on helicoidal magnets. For instance, reflection curves for both configurations exhibit a resonance in some range of values of the normal wave vector component of the incident neutrons.

In the next section we find an analytical solution of the Schrödinger equation in an infinite medium with fan-like magnetization. In section III reflectivity of polarized neutrons from a semi infinite magnetic medium is analytically calculated in the absence of an external field. In this case, the quantization axis for the neutron spin s is chosen along the axis q of the magnetization rotation, and the neutron scattering becomes dependent on correlation s·q , which violates time parity and detailed balance theorem. In section IV analytical expressions for reflectivity from a magnetic slab of finite thickness in zero external field is given. The results are further generalized in section V for nonzero external field. In section VI we consider a SL/HL magnetic
heterostructure and calculate the neutron reflectivity curves from the front and back sides of the sample similar to that used in the experiment [6]. The results are summarized in section VII.

2. Neutron Propagation in a Homogeneous Medium with Fan-Like Magnetization

Let’s consider a semi-infinite \((z>0)\) mirror and an arbitrary external field. Magnetic induction in the medium consists of two parts: one part is constant, \(\mathbf{B}=B(1,0,0)\) and directed along \(x\)-axis. The other one, \(b(z)=b(0,\cos(2qz), \sin(2qz))\), rotates around \(x\)-axis (the factor 2 is selected for convenience). Our task is to find the neutron reflection from such a system. For that we need to know the neutron wave function inside the mirror, i.e. to find a solution of the Schrödinger:

\[
\left( \frac{d^2}{dz^2} + u_0 - 2b [\sigma_y \cos(2qz) + \sigma_z \sin(2qz)] - 2B \sigma_x + k^2 \right) \psi(z) = 0 \tag{1}
\]

where \(\sigma_{x,y,z}\) are the Pauli matrices, \(u_0\) is the medium optical potential multiplied by the factor \(2m/\hbar^2\) (\(m\) is the neutron mass), and magnetic fields include the factor \(\mu m/\hbar^2\) (\(\mu\) is the neutron magnetic moment).

In the real class of perpendicular exchange-spring magnetic multilayers [9,10] the magnetization changes stepwise in neighboring magnetic domains, but for analytical calculations we can approximate such a change by a model of a continuous rotation of the magnetization.

For solution of (1) we use the relation:

\[
\sigma_y \cos(2qz) + \sigma_z \sin(2qz) = \exp(-i\sigma \cdot \mathbf{q} \cdot z) \sigma_y \exp(i\sigma \cdot \mathbf{q} \cdot z) \tag{2}
\]

and represent the wave function \(|\psi(z)\rangle\) in the form:

\[
|\psi(z)\rangle = \exp(-i\sigma \cdot \mathbf{q} \cdot z) |\phi(z)\rangle \tag{3}
\]

where

\[
|\phi(0)\rangle = |\psi(0)\rangle \tag{4}
\]

and \(|\psi(0)\rangle\) corresponds to an arbitrary spin state. Substitution of (2) and (3) into Eq.(1) gives:

\[
\left( \frac{d^2}{dz^2} - 2q \sigma_x \frac{d}{dz} - u_0 - 2b \sigma_y - 2B \sigma_x + k^2 - q^2 \right) |\phi(z)\rangle = 0 \tag{5}
\]

2.1. A solution by Calvo [4]

Such a type of equation was solved in [4] by substitution

\[
|\phi(z)\rangle = \exp(ipz) |\phi(0)\rangle \tag{6}
\]

with constant parameter \(p\) and some spinor state \(|\phi(0)\rangle\). After substitution one reduces (5) to

\[
\left( -p^2 + 2q \sigma_x p - u_0 - 2b \sigma_y - 2B \sigma_x + k^2 - q^2 \right) |\psi(0)\rangle = 0 \tag{7}
\]

which is of the type

\[
\hat{M}|\phi(0)\rangle = 0 \tag{8}
\]

with constant matrix \(\hat{M}\).

There are three types of solutions for such an equation:

1. The trivial one \(|\phi(0)\rangle = 0\) is not interesting and rejected.
2. A solution \(\hat{M} = 0\). Since every matrix can be represented as a linear combination of 4 independent matrices (unit one and 3 Pauli matrices), the Eq. \(\hat{M} = 0\) means that all the coefficients in this linear combination are zero. It means that in (7) \(b=0\) and \((B/q)^2 = k^2 - q^2 - u_0\), which for considered system in general can not be satisfied.
3. The standard solution: some eiven vector \(|\phi(0)\rangle\) of \(\hat{M}\) with zero eigen value. This solution exists only, if \(\det \hat{M} = 0\).

Only the last solution is possible, if the wave function is represented by (6). The condition \(\det \hat{M} = 0\) gives an algebraic equation of 4-th order for \(p\)

\[
\left( p^2 - k^2 + q^2 + u_0 \right) - 4(pq - B)^2 - 4b^2 = 0 \tag{9}
\]

which at \(B=0\) is reduced to a biquadratic equation. For every root \(p_i\) of (9) there is a spinor state \(|\phi_i\rangle\). Two positive roots give two spinor eigen states propagating along \(z\)-axis, and two negative roots give the eigen states propagating in opposite directions.

The obtained solutions can be then used to find reflection and transmission of a magnetic mirror with the considered magnetization. However matching of the wave function even at a single interface leads in general to 4 linear equations with 4 unknowns, and, if we have two interfaces, the number of equations doubles. All they can be solved but only numerically. Below we show how to avoid this huge number of equations and find an analytical solution for a general problem of the neutron reflection and transmission of a magnetic mirror with a finite thickness.

2.2. Our solution

Our solution will proceed along the lines of the work [11]. We substitute in Eq. (5) a solution for a wave, going to the right, in the form

\[
|\psi(z)\rangle = \exp(i(a \mathbf{l} + \mathbf{p} \cdot \sigma)z) |\chi\rangle \tag{10}
\]

where \(|\chi\rangle\) is an arbitrary spinor, the parameter \(a\) is positive, \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) is the vector of the Pauli matrices and \(\mathbf{l}\) denotes the unit 2x2 matrix, which will be usually omitted below.
The distinguishing feature of our approach is that $|\chi\rangle$ is an arbitrary spin state, which is very important for simplification of analytical calculations. With account of (3) the total solution of Eq.(1) looks

$$\psi(z) = \exp(-i\sigma_z q z) \exp\left[i(\alpha l + \tilde{p} \cdot \sigma) z\right] |\chi\rangle \quad (11)$$

Now we can demonstrate advantage of our solution comparing to the Calvo’s one. In order to calculate reflection from a semi-infinite fan-like medium at $z>0$ we need to match the inside and outside wave functions at the interface $z=0$. Suppose that outside field is $B_0$. It can have an arbitrary value and direction. The total wave function for reflection of the incident wave going from the left (in vacuum) toward the interface is equal to:

$$\psi(z) = \left\{ \Theta(z < 0) \left[ \exp(i k z) + \exp(-i k z) \tilde{t} \right] \right\} |\chi\rangle + \Theta(z > 0) \exp(-i \sigma_z z) \exp\left[ i(\alpha l + \tilde{p} \cdot \sigma) z \right] |\tilde{\chi}\rangle \quad (12)$$

where $\Theta$ is a step function equal to unity, when inequality in its argument is satisfied, and to zero in the opposite case. The function (12) at $z<0$ contains an incident wave with an reflection matrix amplitude $r$ and the reflected one with the refraction matrix amplitude $\tilde{t}$. The wave vector in the external field $B_0$ is the matrix $\hat{k} = \sqrt{k^2 I - 2B_0 \cdot \sigma}$. The internal function is represented by (11) and contains refraction matrix amplitude $\tilde{t}$. Requirement of continuity for the function (12) and its derivative at the point $z=0$ leads to the equations [11,12]:

$$\left( I + \tilde{t} \right) |\chi\rangle, \left( \hat{k} [1 - \tilde{t}] \right) = \left[ -q \sigma_x + a l + \tilde{p} \cdot \sigma \right] |\tilde{\chi}\rangle \quad (13)$$

Since these equations should be satisfied for any spinor $|\tilde{\chi}\rangle$, they are equivalent to

$$I + \tilde{t} = \tilde{t}, \quad \hat{k} [1 - \tilde{t}] = \left[ -q \sigma_x + a l + \tilde{p} \cdot \sigma \right] \tilde{t} \quad (14)$$

The solution of these equations is:

$$\tilde{t} = \left( \hat{k} - q \sigma_x + a l + \tilde{p} \cdot \sigma \right)^{-1} \left( \hat{k} + q \sigma_x - a l + \tilde{p} \cdot \sigma \right), \quad \tilde{t} = 2 \left( \hat{k} - q \sigma_x + a l + \tilde{p} \cdot \sigma \right)^{-1} \hat{k} \quad (15)$$

In the absence of magnetic fields it is immediately reduced to the well-known scalar case

$$\tilde{t} = \frac{k - k'}{k + k'}, \quad \tilde{t} = \frac{2k}{k + k'}, \quad k^2 - u_0 \quad (16)$$

The function (10) has four unknown parameters $a$ and $\tilde{p}$. A solution for a wave going to the left can be written as:

$$\psi(z) = \exp\left(-i(\alpha l + \tilde{p} \cdot \sigma) z\right) |\chi\rangle \quad (17)$$

again with four unknown parameters $a$ and $\tilde{p}$.

To find the parameters of the wave (10) we substitute (10) into (5) and get:

$$\begin{align*}
-a^2 - \tilde{p}^2 + 2q \tilde{p}^2 - u_0 + k^2 - q^2 &= 0, \\
ap x - qa + B &= 0, ap y + iq \tilde{p} z + b &= 0, ap z - iq \tilde{p} y &= 0 \quad (19)
\end{align*}$$

From the last three equations it follows that:

$$\tilde{p}_x = q \frac{B}{a}, \quad \tilde{p}_y = \frac{ab}{q^2 - a^2}, \quad \tilde{p}_z = \frac{qb}{q^2 - a^2}, \quad \tilde{p}^2 = \left( q - \frac{B^2}{a} \right) + \frac{b^2}{a^2 - q^2} \quad (22)$$

and substitution of (22) into (20) leads to:

$$a^2 + \frac{B^2}{a^2} + \frac{b^2}{a^2 - q^2} = k^2 - u_0 \quad (23)$$

which is a cubic equation for $a^2$.

### 2.3. Solution of the Cubic Equation

We denote $x = a^2$ and $K^2 = k^2 - u_0$, and transform (23) to

$$x^3 - x \left( K^2 + q^2 \right) + x(a^2 - q^2) - B^2 q^2 = 0 \quad (24)$$

A further change of variables $x = y + (K^2 + q^2)/3$ transforms it to:

$$y^3 - \alpha y - \beta = 0 \quad (25)$$

where

$$\alpha = \frac{(K^2 + q^2)^2}{3} - B^2 - b^2 - K^2 q^2, \quad \beta = \frac{K^2 + q^2}{3} \left( \alpha - \frac{(K^2 + q^2)^2}{9} \right) + B^2 q^2 \quad (26)$$
Substitution of \( y = z + \alpha/3z \), reduces Eq. (25) to
\[
z^3 + \alpha^3/27z^3 - \beta = 0,
\]
and solutions of it can be written as:
\[
z_n = \exp(2\pi i n/3) \sqrt{\beta \pm \sqrt{\beta^2 - 4\alpha^3/27}}/2
\]
with \( n=0,1,2 \). The parameter \( a(k) \) can be represented as:
\[
a = \sqrt{(K^2 + q^2)/3 + z_n + \alpha/3z_n},
\]
and it is a challenge now how to choose a single correct physical root. We can look for the correct one between the roots of the form:
\[
\left\{-a^2 - \frac{p^2 - 2a(\tilde{p} \cdot \sigma)}{a} - 2q(\tilde{\sigma})_p, a + (\tilde{p} \cdot \sigma)\right\}
\]
\[
-\frac{u_0 - 2b\sigma_j - 2B\sigma_q + k^2 - q^2}{|\phi(z)|} = 0
\]
which differs from (18) only by the sign of \( q \). The relation (32) is equivalent to 4 equations similar to (21-22) with negative \( q \). Their solutions read:
\[
\hat{p}_x = -\frac{q - q}{a}, \hat{p}_y = \frac{ab}{q^2 - a^2},
\]
\[
\hat{p}_z = \frac{-q - b}{q^2 - a^2}, \hat{p}^2 = \left(\frac{q + B}{a}\right)^2 + \frac{b^2}{a^2 - q^2}
\]
and eq. for \( a \) is identical to (23).

### 3. Reflection from the Interface of a Semi Infinite Fan-Like Mirror

Above in (15) we have already found the reflection and refraction matrix amplitudes at a single interface. In the absence of fields they are reduced to (16), and in the limit \( q=0 \) we obtain the formulas for refraction at the interface of a medium with a uniform magnetization \( b+B \).

With the analytical expression (15) we can easily calculate reflection coefficients from a semi infinite mirror with and without spin flip. Their dependence on the wave number \( k \) of the incident neutrons are shown in Fig. 1 for the simplest case of zero external field, when quantization axis is chosen along the rotation vector \( q \), i.e. along the \( x \)-axis. In calculations, the value of \( k \) is defined in units \( \sqrt{u_0} \).

![Fig. 1. Dependence on wave number k of reflectivities: a) without and b) with spin flip. The solid curves are for initial polarization along x-axis, and the dashed curves are for the initial polarization along -x. Calculations were made for parameters \( B=0, u_0=4-0.01i, b=0.5, B=0.1, q=2 \).](image)
The most striking feature of the Fig.1b), is the presence of 
a resonant peak with the center at the point \( k = \sqrt{q^2 + u_0} \) and 
the width determined by the field \( \Delta k = \sqrt{b^2 + B^2} \). The peak 
corresponds to almost total reflection with spin-flip, and it 
exists only for polarization of the incident neutron against the 
vector \( q \), which characterizes the rotation of the field in the 
mirror.

It is interesting to compare the obtained results to the case 
\( B=0 \), when we can use the quadratic equation (30) in stead of 
the cubic one (23). The results for the same parameters 
except \( B=0 \) are shown in Fig.2.

At the point \( z=1 \) near the entrance surface the reflected 
wave of (37) is equal to

\[
\exp(-i\sigma_x q l) \exp(i (a + \tilde{p} \cdot \sigma) l) \hat{r}' \hat{X} \hat{\chi}.
\]

Now we are well equipped to calculate reflection from a 
slab of thickness \( l \). Let’s denote the wave incident from inside 
the matter upon the exit interface at \( z=l \) as \( \hat{X} \hat{\chi} \). For \( \hat{X} \) we 
can construct a self consistent equation:

\[
\hat{X} = \exp(-i\sigma_x q l) \exp(i (a + \tilde{p} \cdot \sigma) l) \hat{\chi}
\]

which has the following solution:

\[
\hat{X} = (1 + \exp(-i\sigma_x q l) \exp(i (a + \tilde{p} \cdot \sigma) l) \hat{r}')^{-1} \exp(-i\sigma_x q l) \exp(i (a + \tilde{p} \cdot \sigma) l) \hat{r} \hat{\chi}.
\]
With the help of \( \hat{X} \) we can easily find the reflection, \( \hat{R} \), and the transmission, \( \hat{T} \), matrix amplitudes, which read:

\[
\hat{R} = i \hat{r} \exp(\im \sigma_l q l) \exp(i(a - \hat{p} \cdot \sigma)l) \hat{r} \hat{X}, \quad \hat{T} = i \hat{t} \hat{X}.
\]  

(43)

Using the analytical expressions (43) we can directly calculate matrix elements and find reflection and transmission probabilities with and without spin-flip as a function of \( k \).

The results of the calculations for \( l=8 \) and for the simplest case \( B_0 = 0 \) are shown in Fig.3. Again, we clearly see the occurrence of the resonant peak. Its height decreases with decrease of \( l \).

5. Reflectivities for \( B_0 \neq 0 \)

When external magnetic induction \( B_0 \neq 0 \), the quantization axis is to be chosen along \( B_0 \). If \( B_0 \) is parallel oriented with respect to the \( y \)-axis, then the incident neutron has a polarization \( \ket{\chi_{\pm}} \), which is a superposition of two opposite polarizations \( \ket{\chi_{\pm}} \):

\[
\ket{\chi_{\pm}} = \frac{1+i}{2} \ket{\chi_{+}} + \frac{1-i}{2} \ket{\chi_{-}}.
\]  

(44)

Therefore, the reflection amplitudes with spin flip, \( \hat{R}_{\pm, \mp} \), and without spin-flip \( \hat{R}_{\pm, \mp} \), contain contributions of the resonant amplitude \( \hat{R}_{\pm, \mp} \). This is clearly seen in Fig.4. The results of the calculations show that the amplitudes with spin-flip are equal for both initial polarizations, and that the reflection amplitudes without spin-flip also contain a resonant peak at \( \sqrt{q^2 + u_0 - 2b} < k < \sqrt{q^2 + u_0 + 2b} \).

6. Reflection from Composition of Soft and Hard Magnetics

Above we have considered the reflection from an abstract fan-like magnetic system. In reality, a fan-like magnetization state can appear in a SL which is magnetically coupled to a HL. In the following we assume that the HL of thickness \( l_h \) with optical potential \( u_h \) has a uniform magnetization \( b \), which coincides with the magnetization of the SL at the exit interface \( z=l \). The total reflection matrix amplitude from the two magnetic layers at the side of the soft and hard ones
are\[5,6\]:

\[ R_{sh} = \bar{R} + T \bar{R} \left( I - \bar{R} \bar{R} \right)^{-1} T , \]

where \( R_{sh} \) and \( T_{sh} \) are the reflection and transmission matrices of the separate HL in vacuum and for the same external field on both sides of it:

\[ R_{sh} = r_{h} - (1-r_{h}) \exp(i k_{s_{h}} / h) [1 - \exp(-i k_{s_{h}} / h)]^{-1} \exp(-i k_{s_{h}} / h) (I + r_{h}) , \]

\[ T_{sh} = (1-r_{h}) \exp(i k_{s_{h}} / h) [1 - \exp(-i k_{s_{h}} / h)]^{-1} \exp(-i k_{s_{h}} / h) (I + r_{h}) . \]

The results of the calculations for \( u_{0} = 3.5 - 0.01i \) and \( l_{0} = 1.1 \) are shown in Fig.6. The top panels show reflectivities from the SL side a) without and b) with spin-flip, and the bottom panels show the analogous reflectivities from the HL side. The top and bottom figures are different. The resonance peak seen on the top figures, is replaced with the second total reflection edge when reflection is from the HL side. This is in good agreement with measured reflectivity curves of [6]. When the external field changes, the shapes of the top and bottom curves also change.

The results obtained by analytical methods were checked by numerical simulations with the generalized matrix method [12,13]. Both types of calculations are in good agreement. For the numerical calculation, the SL was subdivided into 50 sub-layers with different directions of magnetization. The angular increment between two neighboring sub-layers was constant.

By making use of the numerical method, it is also possible to calculate reflectivities when rotation of the field is not uniform, and we can expect that nonuniform rotation will lead to broadening of the resonant peak and to a lowering of its height.

\[ \text{Fig. 6. Dependence on } k \text{ of the reflectivities from (top) the SL side (bottom) from HL side. On the left panels the reflectivities without spin flip when initial polarization is against field } B_{0} \text{ (solid curve) and along it (dashed curve) are shown. On the right panels the spin-flip reflectivities are shown. They are the same for both polarizations, therefore only one curve is plotted. For the calculations the following parameters have been used: } B_{0} = 0.2, u_{0} = 4 - 0.0001i, b = 1, q = 1, l = 3, u_{h} = 3.5 - 0.001i \text{ and } l_{h} = 1.1. \text{ In these calculations an additional phase } \phi = 0.1 \text{ in expression for } b(z) \text{ in (1) was taken into account.} \]

7. Violation of Some Fundamental Principles in the Considered Model

The resonant spin flip reflection from samples with rotating field (see also [11]) shows some features, which are very important with respect to fundamental principles. Reflectivity and transmissivity of samples with a field rotating around a \( q \) vector contain a \( T \)-odd correlation \( q \cdot s \), where \( R_{sh} \) and \( T_{sh} \) are the reflection and transmission matrices of the separate HL in vacuum and for the same external field on both sides of it:
example, however is very useful. It shows that observation in an experiment of T-odd or P-odd correlations should not be accepted as a proof of violation of P- or T-invariance.

In our problem we meet also violation of the detailed balance principle, related to the principle of maximal entropy. According to this principle the flux reflected with spin flip from the initial state \( |\xi_{-x}\rangle \) is to be equal to the flux reflected with spin flip from the initial state \( |\xi_{+x}\rangle \). Such equality is necessary because, if the mirror would be immersed in an isotropic distribution of unpolarized neutrons, the reflectivity would neither change the isotropy nor create polarization. In the case of the mirror with a rotating field it is not so. The neutrons in the state \( |\xi_{-x}\rangle \) are reflected almost totally with spin flip, while the oppositely polarized neutrons are not totally reflected. It seems that, if we take a vessel with isotropic unpolarized neutron gas and partition it off by a magnetized foil with a rotating magnetization (helicoidal, fan-like or some other) then the neutrons from, say, the left part of the vessel will spill completely polarized through the foil into the right part of the vessel. Indeed the neutrons in the left part, which are polarized along \(-x\), after reflection become polarized along \(+x\) and these neutrons are easily transmitted without depolarization into the right side. So all the neutrons will go to the right side and they will be polarized along \(+x\).

However such a terrible violation of the maximal entropy principle does not happen, because for neutrons on the right side of the foil the field in the foil looks rotating in the opposite direction, therefore the states \( |\xi_{+x}\rangle \) are reflected almost totally with spin flip, and the states \( |\xi_{-x}\rangle \) are easily transmitted to the left side. Nevertheless there appears a cycle in the phase space, which violates principle of the detailed balance. This violation is attributed to presence of rotation in space. If there were two opposite rotations the space could be considered having an equilibrium state, and the detailed balance would be not violated. With a single hand rotation the space is not in the equilibrium, and because of that the detailed balance is violated.

8. Conclusion

We have obtained analytical expressions for calculation of reflectivities and transmissivity of neutrons through magnetic media with fan-like and helicoidal magnetization. The calculations show that at wave numbers in the interval \( \sqrt{q^2+u_0-2b} < q < \sqrt{q^2+u_0+2b} \), where \( q \) is the fan vector (rotation vector of the fan), and \( b \) is the internal magnetic field of the fan, the reflection curve contains a resonance peak. This feature serves as an identification of magnetic configurations with intrinsic rotating fields. The width of the peak characterizes the uniformity of rotation and the strength of the rotating field. The analytical solutions and the numerical generalized matrix method are very useful tools for analyzing polarized neutron reflectivity data from non-collinear magnets exhibiting anisotropic exchange forces.

The time parity violation found in this model shows that observation of such an effect in some experiment must be analyzed in order to exclude the presence of magnetic fields, which may rotate in the sample space.

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