BFO-ator Manual

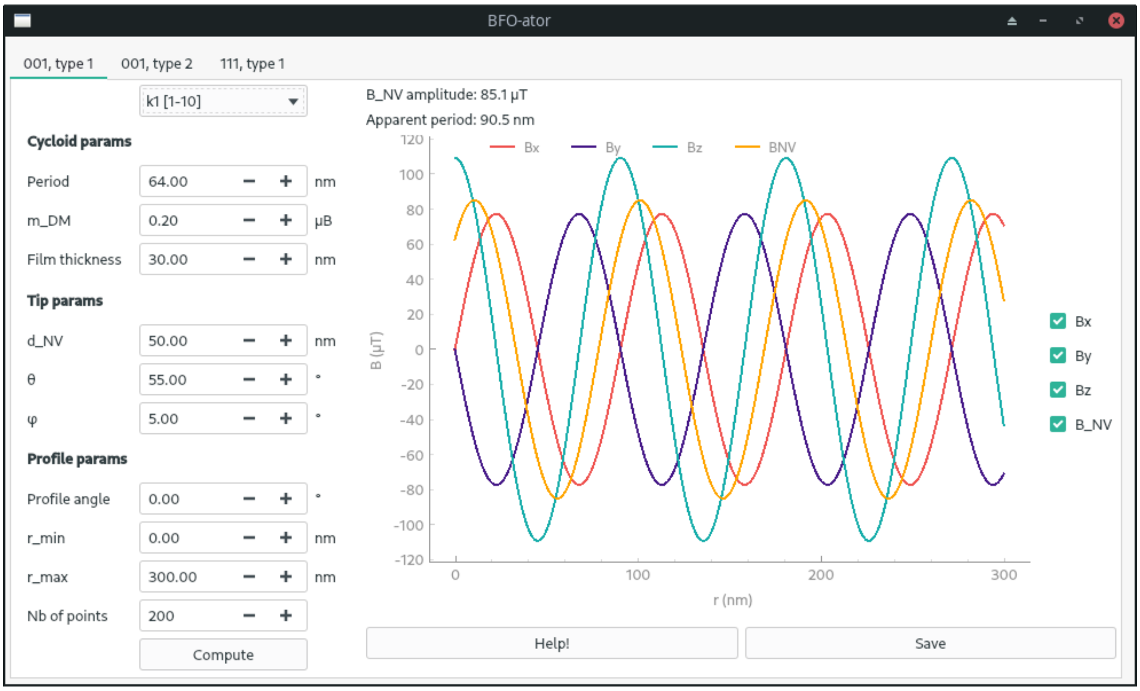
Aurore Finco
aurore.finco@umontpellier.fr
Laboratoire Charles Coulomb, CNRS and University of Montpellier, France

December 13, 2021

This program computes the stray field profile from the cycloid in $BiFeO_3$, as it is measured with NV center magnetometry. Three cases are considered, and correspond to the three available tabs:

- The type 1 (bulk-like) cycloid in (001)-oriented $BiFeO_3$, with P along [111]
- The type 2 (exotic) cycloid in (001)-oriented $BiFeO_3$, with P along [111]
- The type 1 (bulk-like) cycloid in (111)-oriented $BiFeO_3$, with P along [111]
- The type 1 (bulk-like) cycloid in (111)-oriented $BiFeO_3$, with P along $[11\bar{1}]$

In each tab, you can enter the parameters in the left section on the window. These parameters are detailed in the following sections. In the right part of the window, the corresponding profiles are plotted. You can select which magnetic field components you would like to plot with the tick boxes. With the save button, you can export these profiles in .txt format. To save the graphs, right-click on the plot and select "Export . . . ". Above the plots, the amplitude and apparent period indicated correspond to the B_{NV} component.



1 Tab 001, type 1

1.1 Geometry and parameters

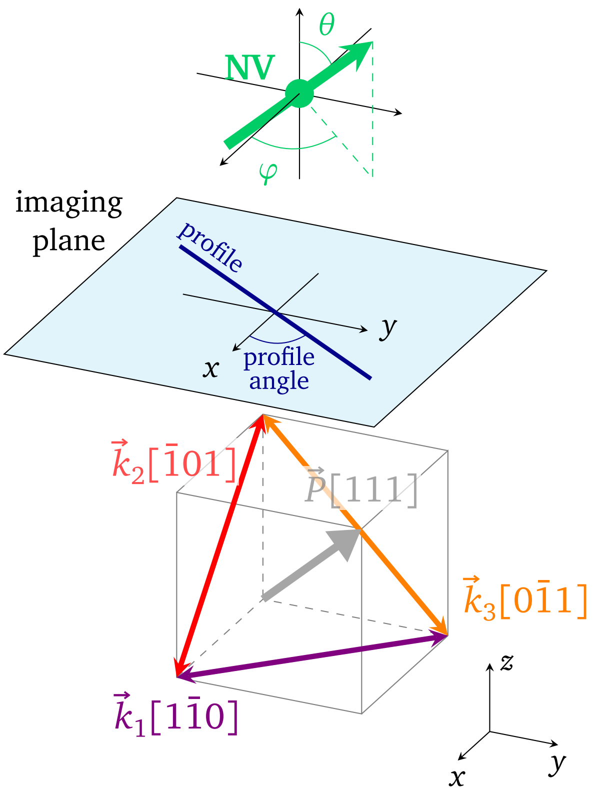


Figure 1: Geometry of the considered type 1 cycloid in (001)-oriented $BiFeO_3$

Parameters:

- Cycloid parameters
  - Period: cycloid period in nm, **not** projected onto the imaging plane, usually around 64 nm
  - m_DM: canted magnetic moment, in μ_B
  - Film thickness: in nm
- Tip parameters
  - d_NV: distance between the NV center and the surface, in nm
  - θ: polar angle of the NV orientation, in °
  - φ: azimuthal angle of the NV orientation, in °
- Profile parameters
  - Profile angle: direction of the measured profile, in °
  - r_min, r_max: start and stop coordinates of the profile, in nm
  - Nb of points: Number of data points along the profile

1.2 Analytical expression

1.2.1 Cycloid propagating along $\vec{k}_1$

$$\begin{cases} B_x = \dfrac{\mu_0\, m_{\mathrm{DM}}}{\sqrt{3}V} e^{-kd_{\mathrm{NV}}} \dfrac{1-e^{-kt}}{1-e^{-ka}} \sinh\left(\dfrac{ka}{2}\right) \sin\left(\dfrac{k}{\sqrt{2}}(x-y)\right) \\ B_y = -\dfrac{\mu_0\, m_{\mathrm{DM}}}{\sqrt{3}V} e^{-kd_{\mathrm{NV}}} \dfrac{1-e^{-kt}}{1-e^{-ka}} \sinh\left(\dfrac{ka}{2}\right) \sin\left(\dfrac{k}{\sqrt{2}}(x-y)\right) \\ B_z = \sqrt{\dfrac{2}{3}} \dfrac{\mu_0\, m_{\mathrm{DM}}}{V} e^{-kd_{\mathrm{NV}}} \dfrac{1-e^{-kt}}{1-e^{-ka}} \sinh\left(\dfrac{ka}{2}\right) \cos\left(\dfrac{k}{\sqrt{2}}(x-y)\right) \end{cases}$$

where a is the $BiFeO_3$ lattice parameter and t the film thickness.

1.2.2 Cycloid propagating along $\vec{k}_2$

$$\begin{cases} B_x = -\dfrac{A}{\sqrt{2}}\left(\mathrm{Re}\{S\} - \mathrm{Im}\{S\}\right) \\ B_y = 0 \\ B_z = \sqrt{2}\, A\mathrm{Re}\{S\} \end{cases}$$

with:

$$A = \frac{\mu_0 m_{\mathrm{DM}}}{\sqrt{3}V}\sinh\left(\frac{ka}{2\sqrt{2}}\right)$$

$$S = e^{-kd_{\mathrm{NV}}/\sqrt{2}} e^{ik(x-d_{\mathrm{NV}})/\sqrt{2}}\ \frac{1-e^{-kt(1+i)/\sqrt{2}}}{1-e^{-ka(1+i)/\sqrt{2}}}$$

where a is the $BiFeO_3$ lattice parameter and t the film thickness.

1.2.3 Cycloid propagating along $\vec{k}_3$

$$\begin{cases} B_x = 0 \\ B_y = -\dfrac{A}{\sqrt{2}}\left(\mathrm{Re}\{S\} - \mathrm{Im}\{S\}\right) \\ B_z = \sqrt{2}\, A\mathrm{Re}\{S\} \end{cases}$$

with

$$A = \frac{\mu_0 m_{\mathrm{DM}}}{\sqrt{3}V}\sinh\left(\frac{ka}{2\sqrt{2}}\right)$$

$$S = e^{-kd_{\mathrm{NV}}/\sqrt{2}} e^{ik(y-d_{\mathrm{NV}})/\sqrt{2}}\ \frac{1-e^{-kt(1+i)/\sqrt{2}}}{1-e^{-ka(1+i)/\sqrt{2}}}$$

where a is the $BiFeO_3$ lattice parameter and t the film thickness.

2 Tab 001, type 2

2.1 Geometry and parameters

If the cycloid propagates along $\vec{k}'_3[11\bar{2}]$, the canted magnetic moments are in the surface plane and therefore the cycloid does not produce stray field. Hence the introduction of the deviation angle α.

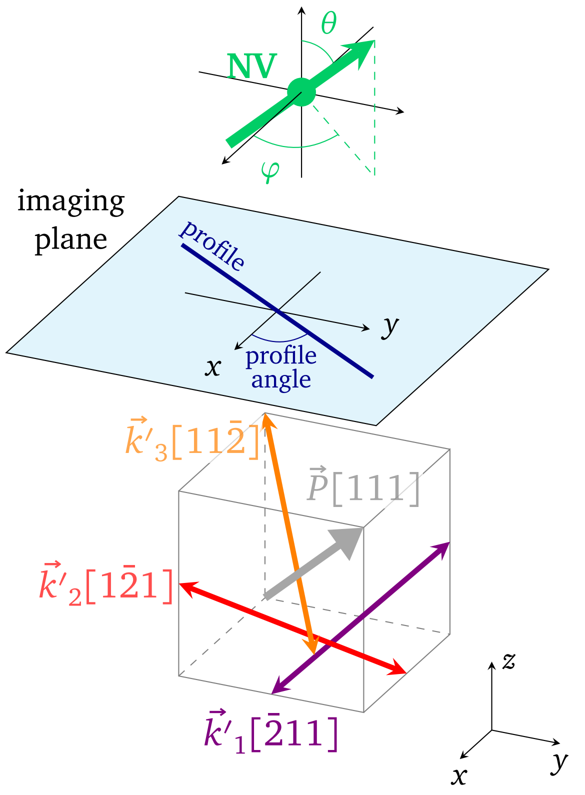


Figure 2: Geometry of the considered type 2 cycloid in (001)-oriented $BiFeO_3$

Parameters:

- Cycloid parameters
  - Period: cycloid period in nm, **not** projected onto the imaging plane.
  - m_DM: canted magnetic moment, in μ_B
  - Film thickness: in nm
  - α deviation: only if you select $\vec{k}'_3$, small deviation angle between the actual $\vec{k}'_3$ and the $[11\bar{2}]$ direction, in the plane perpendicular to $\vec{P}$
- Tip parameters
  - d_NV: distance between the NV center and the surface, in nm
  - θ: polar angle of the NV orientation, in °
  - φ: azimuthal angle of the NV orientation, in °
- Profile parameters
  - Profile angle: direction of the measured profile, in °
  - r_min, r_max: start and stop coordinates of the profile, in nm
  - Nb of points: Number of data points along the profile

2.2 Analytical expression

2.2.1 Cycloid propagating along $\vec{k}'_1$

$$\begin{cases} B_x = \sqrt{\frac{2}{5}}A\left(\frac{1}{\sqrt{5}}\mathrm{Re}\{S\} + \mathrm{Im}\{S\}\right) \\ B_y = \frac{A}{\sqrt{10}}\left(\frac{1}{\sqrt{5}}\mathrm{Re}\{S\} + \mathrm{Im}\{S\}\right) \\ B_z = \frac{A}{\sqrt{10}}\left((\frac{1}{\sqrt{5}} + \sqrt{5})\mathrm{Re}\{S\}\right) \end{cases}$$

with:

$$A = \frac{\mu_0 m_{\mathrm{DM}}}{V} \sinh\left(\sqrt{\frac{5}{6}} \frac{ka}{2} \right)$$

$$S = e^{-\sqrt{\frac{5}{6}} k d_{\mathrm{NV}}} e^{\frac{ik}{\sqrt{6}}(-2x+y+d_{\mathrm{NV}})} \; \frac{1 - e^{-\frac{kt}{\sqrt{6}}(\sqrt{5}-i)}}{1 - e^{-\frac{ka}{\sqrt{6}}(\sqrt{5}-i)}}$$

where a is the $BiFeO_3$ lattice parameter and t the film thickness.

2.2.2 Cycloid propagating along $\vec{k'}_2$

$$\begin{cases} B_x = \dfrac{A}{\sqrt{10}} \left(\dfrac{1}{\sqrt{5}} \operatorname{Re}\{S\} + \operatorname{Im}\{S\} \right) \\ B_y = \sqrt{\dfrac{2}{5}} A \left(\dfrac{1}{\sqrt{5}} \operatorname{Re}\{S\} + \operatorname{Im}\{S\} \right) \\ B_z = -\dfrac{A}{\sqrt{10}} \left(\left(\dfrac{1}{\sqrt{5}} + \sqrt{5}\right) \operatorname{Re}\{S\} \right) \end{cases}$$

$$A = \frac{\mu_0 m_{\mathrm{DM}}}{V} \sinh\left(\sqrt{\frac{5}{6}} \frac{ka}{2} \right)$$

$$S = e^{-\sqrt{\frac{5}{6}} k z} e^{\frac{ik}{\sqrt{6}}(x-2y+z)} \; \frac{1 - e^{-\frac{kt}{\sqrt{6}}(\sqrt{5}-i)}}{1 - e^{-\frac{ka}{\sqrt{6}}(\sqrt{5}-i)}}$$

where a is the $BiFeO_3$ lattice parameter and t the film thickness.

2.2.3 Cycloid propagating along $\vec{k'}_3$

No stray field if no deviation from $\vec{k'}_3$! With a deviation α:

$$\begin{cases} B_x = A \dfrac{\sin\alpha \, (\cos\alpha - \sqrt{3}\sin\alpha)}{\sqrt{\cos^2\alpha + 3\sin^2\alpha}} \operatorname{Im}\{S\} \\ B_y = A \dfrac{\sin\alpha \, (\cos\alpha + \sqrt{3}\sin\alpha)}{\sqrt{\cos^2\alpha + 3\sin^2\alpha}} \operatorname{Im}\{S\} \\ B_z = -A \sin\alpha \left(-\operatorname{Re}\{S\} + \dfrac{2\cos\alpha}{\sqrt{\cos^2\alpha + 3\sin^2\alpha}} \operatorname{Im}\{S\} \right) \end{cases}$$

with:

$$A = \frac{2\mu_0 m_{\mathrm{DM}}}{\sqrt{6} V} \sinh\left(\frac{ka}{2\sqrt{6}} \sqrt{\cos^2\alpha + 3\sin^2\alpha} \right)$$

$$S = e^{-\frac{k d_{\mathrm{NV}}}{\sqrt{6}} \sqrt{\cos^2\alpha + 3\sin^2\alpha}} e^{\frac{ik}{\sqrt{6}}[\cos\alpha \, (x+y-2d_{\mathrm{NV}}) - \sqrt{3}\sin\alpha \, (x-y)]} \; \frac{1 - e^{-\frac{kt}{\sqrt{6}}(\sqrt{\cos^2\alpha+3\sin^2\alpha} + 2i\cos\alpha)}}{1 - e^{-\frac{ka}{\sqrt{6}}(\sqrt{\cos^2\alpha+3\sin^2\alpha} + 2i\cos\alpha)}}$$

where a is the $BiFeO_3$ lattice parameter and t the film thickness.

3 Tab 111, type 1, P oop

3.1 Geometry and parameters

The three possible k directions are completely equivalent, so there is no choice between them in this case. $\vec{k}$ is set along the x direction (like $\vec{k}_1$ in the figure). There is in principle an odd/even effect on the number of unit cell in the layer thickness, therefore the thickness parameter is set in layers and not in nm.

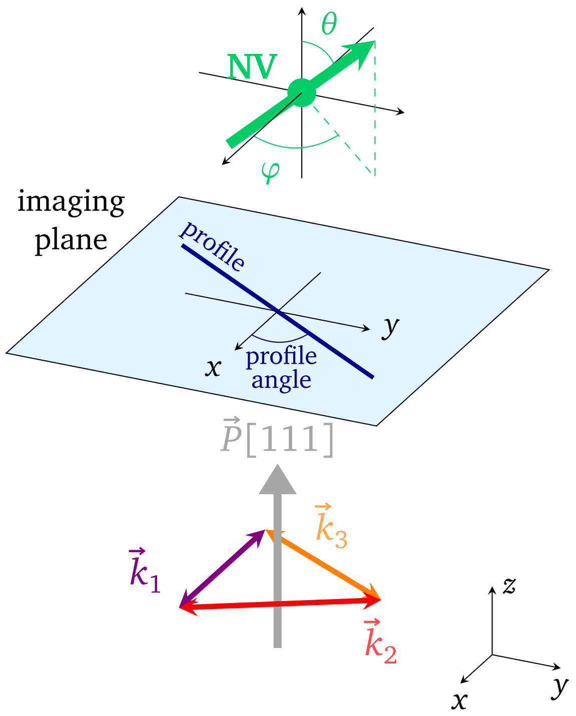


Figure 3: Geometry of the considered type 1 cycloid in (111)-oriented $BiFeO_3$

Parameters:

- Cycloid parameters
  - Period: cycloid period in nm
  - m_S: Fe magnetic moment, in μ_B
  - Film thickness: number of unit cells in the layer thickness
- Tip parameters
  - d_NV: distance between the NV center and the surface, in nm
  - θ: polar angle of the NV orientation, in °
  - φ: azimuthal angle of the NV orientation, in °
- Profile parameters
  - Profile angle: direction of the measured profile, in °
  - r_min, r_max: start and stop coordinates of the profile, in nm
  - Nb of points: Number of data points along the profile

3.2 Analytical expression

$$\begin{cases} B_x = 2\mu_0 \dfrac{m_s}{V} e^{-kz} \sinh\left(\dfrac{ka\sqrt{3}}{6}\right)\left(\dfrac{1-(-e^{-\frac{ka\sqrt{3}}{3}})^N}{1+e^{-\frac{ka\sqrt{3}}{3}}}\right)\cos(kx) \\ B_y = 0 \\ B_z = -2\mu_0 \dfrac{m_s}{V} e^{-kz} \sinh\left(\dfrac{ka\sqrt{3}}{6}\right)\left(\dfrac{1-(-e^{-\frac{ka\sqrt{3}}{3}})^N}{1+e^{-\frac{ka\sqrt{3}}{3}}}\right)\sin(kx) \end{cases}$$

where a is the $BiFeO_3$ lattice parameter and N the number of unit cells in the layer thickness.

4 Tab 111, type 1, P ip

4.1 Geometry and parameters

In this case both the cycloid and the spin density wave are contributing to the magnetic field, so we need to considering the dephasing between them. In addition, there is an odd/even effect on the number of unit cell in the layer thickness, therefore the thickness parameter is set in layers and not in nm.

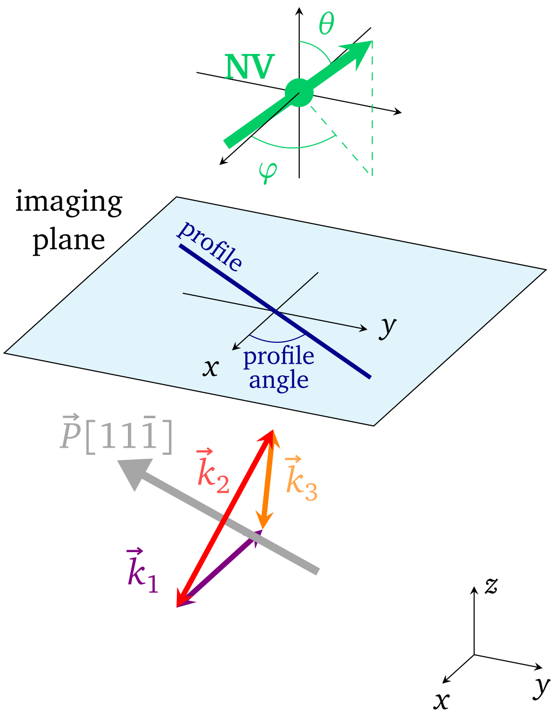


Figure 4: Geometry of the considered type 1 cycloid in (111)-oriented $BiFeO_3$

Parameters:

- Cycloid parameters
  - Period: cycloid period in nm
  - m_S: Fe magnetic moment, in μ_B
  - m_DM: canted magnetic moment, in μ_B
  - Phase: dephasing between the cycloid and the spin density wave, in $^\circ$
  - Rotational sense: for the cycloid part, exchanging it corresponds to $\vec{P} \rightarrow -\vec{P}$
  - Film thickness: number of unit cells in the layer thickness
- Tip parameters
  - d_NV: distance between the NV center and the surface, in nm
  - θ: polar angle of the NV orientation, in $^\circ$
  - φ: azimuthal angle of the NV orientation, in $^\circ$
- Profile parameters
  - Profile angle: direction of the measured profile, in $^\circ$
  - r_min, r_max: start and stop coordinates of the profile, in nm
  - Nb of points: Number of data points along the profile

4.2 Analytical expression

4.2.1 Cycloid propagating along $\vec{k}_1$

$$\begin{cases} B_x = \dfrac{\mu_0}{V} e^{-kz} \sinh\left(\dfrac{ka\sqrt{3}}{6}\right) \left[m_s(1-\dfrac{\varepsilon}{3}) \left(\dfrac{1-(-e^{-\frac{ka\sqrt{3}}{3}})^N}{1+e^{-\frac{ka\sqrt{3}}{3}}} \right) \cos(kx) \right. \\ \qquad\qquad \left. + \dfrac{2\sqrt{2}}{3} m_{\mathrm{DM}} \left(\dfrac{1-e^{-\frac{kaN\sqrt{3}}{3}}}{1-e^{-\frac{ka\sqrt{3}}{3}}} \right) \sin(kx+\Phi) \right] \\ B_y = 0 \\ B_z = -\dfrac{\mu_0}{V} e^{-kz} \sinh\left(\dfrac{ka\sqrt{3}}{6}\right) \left[m_s(1-\dfrac{\varepsilon}{3}) \left(\dfrac{1-(-e^{-\frac{ka\sqrt{3}}{3}})^N}{1+e^{-\frac{ka\sqrt{3}}{3}}} \right) \sin(kx) \right. \\ \qquad\qquad \left. - \dfrac{2\sqrt{2}}{3} m_{\mathrm{DM}} \left(\dfrac{1-e^{-\frac{kaN\sqrt{3}}{3}}}{1-e^{-\frac{ka\sqrt{3}}{3}}} \right) \cos(kx+\Phi) \right] \end{cases}$$

where a is the $BiFeO_3$ lattice parameter and N the number of unit cells in the layer thickness.

4.2.2 Cycloid propagating along $\vec{k}_2$

$$\begin{cases} B_x = \dfrac{\sqrt{3}\,A}{2}\left[m_s(\sqrt{3}+\varepsilon)\left(\mathrm{Re}\{S_1\}-\sqrt{2}\,\mathrm{Im}\{S_1\}\right)+\sqrt{2}\;m_{\mathrm{DM}}\left(\sqrt{2}\,\mathrm{Re}\{S_2\}+\mathrm{Im}\{S_2\})\}\right)\right] \\ B_y = \dfrac{A}{2}\left[m_s(\sqrt{3}+\varepsilon)\left(\mathrm{Re}\{S_1\}-\sqrt{2}\,\mathrm{Im}\{S_1\}\right)+\sqrt{2}\;m_{\mathrm{DM}}\left(\sqrt{2}\,\mathrm{Re}\{S_2\}+\mathrm{Im}\{S_2\})\}\right)\right] \\ B_z = A\left[3\;m_s(\sqrt{3}+\varepsilon)\,\mathrm{Im}\{S_1\}-\sqrt{2}\;m_{\mathrm{DM}}(2\sqrt{2}\,\mathrm{Im}\{S_2\}+\mathrm{Re}\{S_2\}\right] \end{cases}$$

with

$$A = \frac{\mu_0}{3V}\sinh\left(\frac{ka}{6}\right)e^{-\frac{kz}{\sqrt{3}}}$$

and

$$S_1 = e^{i\vec{k}_2\cdot\vec{r}}\;\frac{1-(-1)^N e^{-\frac{kNa}{3}(1-i\sqrt{2})}}{1+e^{-\frac{ka}{3}(1-i\sqrt{2})}},\quad S_2 = e^{i(\vec{k}_2\cdot\vec{r}+\Phi)}\;\frac{1-e^{-\frac{kNa}{3}(1-i\sqrt{2})}}{1-e^{-\frac{ka}{3}(1-i\sqrt{2})}}$$

where a is the $BiFeO_3$ lattice parameter and N the number of unit cells in the layer thickness.

4.2.3 Cycloid propagating along $\vec{k}_3$

$$\begin{cases} B_x = \dfrac{\sqrt{3}\,A}{2}\left[m_s(\sqrt{3}+\varepsilon)\left(\mathrm{Re}\{S_1\}+\sqrt{2}\,\mathrm{Im}\{S_1\}\right)-\sqrt{2}\;m_{\mathrm{DM}}\left(\sqrt{2}\,\mathrm{Re}\{S_2\}-\mathrm{Im}\{S_2\})\}\right)\right] \\ B_y = -\dfrac{A}{2}\left[m_s(\sqrt{3}+\varepsilon)\left(\mathrm{Re}\{S_1\}+\sqrt{2}\,\mathrm{Im}\{S_1\}\right)-\sqrt{2}\;m_{\mathrm{DM}}\left(\sqrt{2}\,\mathrm{Re}\{S_2\}-\mathrm{Im}\{S_2\})\}\right)\right] \\ B_z = A\left[3\;m_s(\sqrt{3}+\varepsilon)\,\mathrm{Im}\{S_1\}-\sqrt{2}\;m_{\mathrm{DM}}(2\sqrt{2}\,\mathrm{Im}\{S_2\}-\mathrm{Re}\{S_2\})\right] \end{cases}$$

with

$$A = \frac{\mu_0}{3V}\sinh\left(\frac{ka}{6}\right)e^{-\frac{kz}{\sqrt{3}}}$$

and

$$S_1 = e^{i\vec{k}_3\cdot\vec{r}}\;\frac{1-(-1)^N e^{-\frac{kNa}{3}(1+i\sqrt{2})}}{1+e^{-\frac{ka}{3}(1+i\sqrt{2})}},\quad S_2 = e^{i(\vec{k}_3\cdot\vec{r}+\Phi)}\;\frac{1-e^{-\frac{kNa}{3}(1+i\sqrt{2})}}{1-e^{-\frac{ka}{3}(1+i\sqrt{2})}}$$

where a is the $BiFeO_3$ lattice parameter and N the number of unit cells in the layer thickness.