Supplementary information:
Antiferromagnetic domain wall dynamics in rotating magnetic fields engineered by bending and twisting

Yelyzaveta A. Borysenko,[1, 2, 3, *] Kostiantyn V. Yershov,[2, 4, †] and Denis D. Sheka[1, ‡]

[1] *Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine*
[2] *Leibniz-Institut für Festkörper- und Werkstoffforschung, IFW Dresden, 01171 Dresden, Germany*
[3] *Department of Physics, University of Konstanz, 78457 Konstanz, Germany*
[4] *Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 03143 Kyiv, Ukraine*

Here, we provide details of the derivation of the Lagrangian for the continuous model in the exchange approximation.

I. LAGRANGIAN AND RAYLEIGH DISSIPATIVE FUNCTION FOR THE DOMAIN WALL IN THE HELIX-SHAPED GEOMETRY

In the limit case of small magnetization $|\boldsymbol{m}| \ll 1$, dynamics of the Néel vector can be described within the Lagrange formalism [1, 2]. The Lagrangian L and Rayleigh dissipative function R are

$$\begin{aligned} L &= \frac{M_s^2}{\gamma_0^2\Lambda}\int\limits_{-\infty}^{\infty}\left[\partial_t\boldsymbol{n}+\boldsymbol{n}\times\gamma_0\boldsymbol{H}\right]^2\mathrm{d}s - E, \quad R = \frac{M_s^2}{\gamma_0^2\Lambda}\frac{\eta}{\zeta}\int\limits_{-\infty}^{\infty}\left(\partial_t\boldsymbol{n}\right)^2\mathrm{d}s,\\ E &= \int\limits_{-\infty}^{\infty}\left\{A\left(\partial_s\boldsymbol{n}\right)^2 + K\left[1-\left(\boldsymbol{n}\cdot\boldsymbol{e}_{\mathrm{T}}\right)^2\right]\right\}\mathrm{d}s, \end{aligned} \tag{S.1}$$

where γ_0 is the gyromagnetic ratio, η is a damping coefficient, Λ is the uniform exchange constant, A is the exchange stiffness constant, K is the anisotropy constant. The model (S.1) is valid for a strong exchange field, i.e. $H_{\mathrm{A}}/H_{\mathrm{X}} = K/\Lambda = \zeta^2 \ll 1$.

A. Energy in the rotated ψ-frame

First, we consider a curvilinear AFM wire, which can be modelled by the 3D curved $\boldsymbol{\gamma} \subset \mathbb{R}^3$. The easy-tangential anisotropy is spatially dependent. To describe the Néel vector distribution in such systems, it is convenient to use a curvilinear Frenet–Serret (TNB) parametrization of the curve $\boldsymbol{\gamma}$:

$$\boldsymbol{e}_{\mathrm{T}} = \partial_s\boldsymbol{\gamma}, \qquad \boldsymbol{e}_{\mathrm{N}} = \frac{\partial_s\boldsymbol{e}_{\mathrm{T}}}{|\partial_s\boldsymbol{e}_{\mathrm{T}}|}, \qquad \boldsymbol{e}_{\mathrm{B}} = \boldsymbol{e}_{\mathrm{T}}\times\boldsymbol{e}_{\mathrm{N}}$$

with $\boldsymbol{e}_{\mathrm{T}}$ being the tangent, $\boldsymbol{e}_{\mathrm{N}}$ being the normal, and $\boldsymbol{e}_{\mathrm{B}}$ being the binormal to $\boldsymbol{\gamma}$ and s being the arc length. In this case, we can use the TNB parametrization of the Néel vector [3],

$$\boldsymbol{n} = \left(n_{\mathrm{T}}, n_{\mathrm{N}}, n_{\mathrm{B}}\right)^T \tag{S.2}$$

with components n_α. Here and below Greek indices α, β numerate curvilinear coordinates (TNB-coordinates) and curvilinear components of vector fields. The energy E in (S.1) can be presented as follows [4]

$$\begin{aligned} &E = \sqrt{AK}\int\mathscr{E}\mathrm{d}\xi, \qquad \mathscr{E} = \mathscr{E}_{\mathrm{x}} + \mathscr{E}_{\mathrm{a}},\\ &\mathscr{E}_{\mathrm{x}} = \mathscr{E}_{\mathrm{x}}^0 + \mathscr{E}_{\mathrm{x}}^{\mathrm{D}} + \mathscr{E}_{\mathrm{x}}^{\mathrm{A}}, \quad \mathscr{E}_{\mathrm{x}}^0 = n'_\alpha n'_\alpha,\\ &\mathscr{E}_{\mathrm{x}}^{\mathrm{D}} = \hat{\mathbb{F}}_{\alpha\beta}\left(n_\alpha n'_\beta - n'_\alpha n_\beta\right), \quad \mathscr{E}_{\mathrm{x}}^{\mathrm{A}} = \hat{\mathbb{K}}_{\alpha\beta}n_\alpha n_\beta,\\ &\mathscr{E}_{\mathrm{a}} = -n_{\mathrm{T}}^2, \end{aligned} \tag{S.3}$$

* borysenko.yelyzaveta@uni-konstanz.de
† k.yershov@ifw-dresden.de
‡ sheka@knu.ua

where the Einstein notation is used for summation. Here and below, the prime denotes the derivative with respect to the dimensionless coordinate $\xi = s/\ell$ with $\ell = \sqrt{A/K}$ being a magnetic length. The first term in the exchange energy $\mathscr{E}_{\text{x}}^{0}$ describes the common inhomogeneous exchange interaction, which has formally the same form as for the straight system. The second term $\mathscr{E}_{\text{x}}^{\text{D}}$ in the exchange energy functional is a geometry-induced effective Dzyaloshinskii-Moriya interaction (DMI), which is linear with respect to curvature and torsion. The term $\mathscr{E}_{\text{x}}^{\text{A}}$ describes an effective anisotropy interaction, where the components of the tensor $\hat{\mathbb{K}}_{\alpha\beta} = \hat{\mathbb{F}}_{\alpha\nu}\hat{\mathbb{F}}_{\beta\nu}$ are bilinear with respect to the curvature and the torsion. Explicit form of $\hat{\mathbb{F}}$ and $\hat{\mathbb{K}}$ is written as [4]

$$\hat{\mathbb{F}} = \begin{bmatrix} 0 & \varkappa & 0 \\ -\varkappa & 0 & \sigma \\ 0 & -\sigma & 0 \end{bmatrix}, \quad \hat{\mathbb{K}} = \begin{bmatrix} \varkappa^2 & 0 & -\varkappa\sigma \\ 0 & \varkappa^2 + \sigma^2 & 0 \\ -\varkappa\sigma & 0 & \sigma^2 \end{bmatrix}.$$

Here $\varkappa = \kappa\ell$ and $\sigma = \tau\ell$ are the dimensionless curvature and torsion, respectively, with κ being the curvature and τ being the torsion.

The energy of effective anisotropy

$$\mathscr{E}_{\text{eff}}^{\text{A}} = \mathscr{E}_{\text{an}} + \mathscr{E}_{\text{ex}}^{\text{A}} = \hat{\mathbb{K}}_{\alpha\beta}^{\text{eff}} n_\alpha n_\beta, \quad \hat{\mathbb{K}}_{\alpha\beta}^{\text{eff}} = \hat{\mathbb{K}}_{\alpha\beta} - \delta_{\alpha,1}\delta_{\beta,1}$$

has a form typical for biaxial systems. The tensor of effective anisotropy coefficients $\mathcal{K}_{\alpha\beta}^{\text{eff}}$ has non-diagonal components. This means that the homogeneous distribution of the Néel vector is not oriented along the TNB basis. One can easily diagonalize it, by using a unitary transformation (rotation in a local rectifying plane) of the vector $\boldsymbol{n}$ (S.2)

$$\boldsymbol{n} = \hat{\mathbb{U}}\,\tilde{\boldsymbol{n}}, \quad \tilde{\boldsymbol{n}} = \hat{\mathbb{U}}^{-1}\boldsymbol{n}, \quad \tilde{\boldsymbol{n}} = \left(n_1, n_2, n_3\right)^T, \quad \hat{\mathbb{U}} = \begin{bmatrix} \cos\psi & 0 & -\sin\psi \\ 0 & 1 & 0 \\ \sin\psi & 0 & \cos\psi \end{bmatrix}.$$

By choosing the rotation angle ψ as follows

$$\psi = \arctan\frac{2\sigma\varkappa}{1+\sigma^2-\varkappa^2+\mathscr{K}_1}, \quad \mathscr{K}_1 = \sqrt{(1-\varkappa^2+\sigma^2)^2 + 4\varkappa^2\sigma^2}, \tag{S.4}$$

one can reduce the anisotropy energy $\mathscr{E}_{\text{eff}}^{\text{A}}$ to the form

$$\mathscr{E}_{\text{eff}}^{\text{A}} = -\mathscr{K}_1 n_1^2 + \mathscr{K}_2 n_2^2, \quad \mathscr{K}_2 = \frac{1+\varkappa^2+\sigma^2-\mathscr{K}_1}{2}. \tag{S.5}$$

Here, the coefficient $\mathscr{K}_1$ characterizes the strength of the effective easy-axis anisotropy while $\mathscr{K}_2$ gives the strength of the effective easy-surface anisotropy. The direction of effective easy axis is determined by $\boldsymbol{e}_1$ and the hard axis by $\boldsymbol{e}_2$:

$$\boldsymbol{e}_1 = \boldsymbol{e}_{\text{T}}\cos\psi + \boldsymbol{e}_{\text{B}}\sin\psi, \quad \boldsymbol{e}_3 = -\boldsymbol{e}_{\text{T}}\sin\psi + \boldsymbol{e}_{\text{B}}\cos\psi.$$

One has to note that for any finite ψ the effective anisotropy direction $\boldsymbol{e}_1$ deviates from the magnetic anisotropy direction $\boldsymbol{e}_{\text{T}}$. Note that such a deviation vanishes for wires with zero torsion ($\sigma = 0$).

In the same time, the curvature and torsion show up in the effective DMI, see Eq. (S.3). In the new rotated frame of reference (ψ-frame) the effective DMI energy reads(S.6)

$$\begin{aligned} \mathscr{E}_{\text{ex}}^{\text{D}} &= \mathscr{D}_1\left(n_2 n_3' - n_3 n_2'\right) + \mathscr{D}_2\left(n_1 n_2' - n_2 n_1'\right), \\ \mathscr{D}_1 &= 2\sigma\cos\psi + 2\varkappa\sin\psi = 2\sigma\frac{\mathscr{K}_0+\varkappa^2}{\sqrt{\mathscr{K}_0^2+\sigma^2\varkappa^2}}, \\ \mathscr{D}_2 &= 2\varkappa\cos\psi - 2\sigma\sin\psi = 2\varkappa\frac{\mathscr{K}_0-\sigma^2}{\sqrt{\mathscr{K}_0^2+\sigma^2\varkappa^2}}, \end{aligned} \tag{S.6}$$

where $\mathscr{K}_0 = \left(1+\sigma^2-\varkappa^2+\mathscr{K}_1\right)/2$.

Finally we get the energy in the following form of Eq. (2) of the main text

$$\mathscr{E} = n_\alpha' n_\alpha' - \mathscr{K}_1 n_1^2 + \mathscr{K}_2 n_2^2 + \mathscr{D}_1\left(n_2 n_3' - n_3 n_2'\right) + \mathscr{D}_2\left(n_1 n_2' - n_2 n_1'\right). \tag{2}$$

B. Lagrangian and Rayleigh dissipative function in the rotated ψ-frame

We consider domain wall dynamics in helix-shaped geometry driven by the rotating magnetic field in the xy-plane $\boldsymbol{H} = H\left(\hat{\boldsymbol{x}}\cos\omega t + \hat{\boldsymbol{y}}\sin\omega t\right)$ with frequency ω and field amplitude H. In the ψ-frame, this field can be presented as a sum of three fields that rotate in different

$$\begin{aligned}
\boldsymbol{H} =& H\left(\boldsymbol{h}_{23} + \boldsymbol{h}_{13} + \boldsymbol{h}_{12}\right),\\
\boldsymbol{h}_{23} =& -\cos\xi\sqrt{\varkappa^2+\sigma^2}\left[\boldsymbol{e}_2\cos\omega t + \boldsymbol{e}_3\frac{\varkappa\sin\psi+\sigma\cos\psi}{\sqrt{\sigma^2+\varkappa^2}}\sin\omega t\right],\\
\boldsymbol{h}_{12} =& -\sin\xi\sqrt{\varkappa^2+\sigma^2}\left[\boldsymbol{e}_1\frac{\varkappa\cos\psi-\sigma\sin\psi}{\sqrt{\sigma^2+\varkappa^2}}\cos\omega t + \boldsymbol{e}_2\sin\omega t\right],\\
\boldsymbol{h}_{13} =& \boldsymbol{e}_1\frac{\varkappa\cos\psi-\sigma\sin\psi}{\sqrt{\sigma^2+\varkappa^2}}\cos\xi\sqrt{\varkappa^2+\sigma^2}\cos\omega t + \boldsymbol{e}_3\frac{\varkappa\sin\psi+\sigma\cos\psi}{\sqrt{\sigma^2+\varkappa^2}}\sin\xi\sqrt{\varkappa^2+\sigma^2}\sin\omega t.
\end{aligned} \tag{S.7}$$

Substituting the field (S.7) into the Lagrangian (S.1) one can write the Lagrangian in the form

$$L = \sqrt{AK}\int\limits_{-\infty}^{\infty}\left\{\dot{\boldsymbol{n}}^2 - 2h\,\dot{\boldsymbol{n}}\cdot\left[\left(\boldsymbol{h}_{23}+\boldsymbol{h}_{13}+\boldsymbol{h}_{12}\right)\times\boldsymbol{n}\right] - h^2\left[\boldsymbol{n}\cdot\left(\boldsymbol{h}_{23}+\boldsymbol{h}_{13}+\boldsymbol{h}_{12}\right)\right]^2\right\}\mathrm{d}\xi - E, \tag{S.8}$$

where overdot indicates the derivative with respect to dimensionles time $\bar{t} = \omega_0 t$ with $\omega_0 = \gamma_0\sqrt{\Lambda K}/M_s$ being the frequency of uniform AFM resonance, $h = H/H_{\text{sf}}$ in dimensionless magnetic field amplitude with $H_{\text{sf}} = \sqrt{\Lambda K}/M_s$ being spin-flop field.

To get an effective Lagrangian and Rayleigh dissipative function for the domain wall, we substitute the domain wall ansatz (3) [from the main text] into the (S.8) and integrate over the arc length coordinate ξ. The effective Lagrangian, normalized by $\sqrt{AK}$, reads $\mathcal{L}^{\text{DW}} = \sum_{\nu=0}^{2} h^\nu \mathscr{L}_\nu - \mathcal{E}^{\text{DW}}$, where

$$\begin{aligned}
\mathcal{E}^{\text{DW}} =& \frac{1+a^2\Delta^2}{\Delta} + \mathscr{K}_1\Delta + \frac{\mathscr{K}_2\Delta}{2}\left[1 + a\pi\Delta\frac{\cos 2\Phi}{\sinh(a\pi\Delta)}\right] + a\mathscr{D}_1\Delta + p\mathscr{D}_2\frac{\pi}{2}\left(1+a^2\Delta^2\right)\frac{\cos\Phi}{\cosh(a\pi\Delta/2)},\\
\mathscr{L}_0 =& \int_{-\infty}^{+\infty}\left(\dot{\boldsymbol{n}}^{\text{DW}}\right)^2\mathrm{d}\xi, \quad \mathscr{L}_1 = 2\int_{-\infty}^{+\infty}\dot{\boldsymbol{n}}^{\text{DW}}\cdot\left[\boldsymbol{n}^{\text{DW}}\times\left(\boldsymbol{h}_{23}+\boldsymbol{h}_{13}+\boldsymbol{h}_{12}\right)\right]\mathrm{d}\xi, \quad \mathscr{L}_2 = -\int_{-\infty}^{+\infty}\left[\boldsymbol{n}^{\text{DW}}\cdot\left(\boldsymbol{h}_{23}+\boldsymbol{h}_{13}+\boldsymbol{h}_{12}\right)\right]^2\mathrm{d}\xi,
\end{aligned} \tag{S.9}$$

where $\boldsymbol{n}^{\text{DW}}$ is Néel vector distribution for the ansatz (3) [from the main text].

In the same way, one can obtain an effective Rayleigh dissipative function

$$\mathcal{R}^{\text{DW}} = \tilde{\eta}\mathscr{L}_0 = \tilde{\eta}\int_{-\infty}^{+\infty}\left(\dot{\boldsymbol{n}}^{\text{DW}}\right)^2\mathrm{d}\xi = 2\tilde{\eta}\Delta\left(\frac{1+a^2\Delta^2}{\Delta^2}\dot{q}^2 - 2a\dot{q}\dot{\Phi} + \dot{\Phi}^2\right), \tag{S.10}$$

where $\tilde{\eta} = \eta/\zeta$ is normalized damping.

The explicit form of the Lagrangian parts $\mathcal{L}_i$ can be found in Supplemental files `L0_term.m`, `L1_term.m`, and `L2_term.m`.

II. RIGID MOTION MODE

The effective equations of motion for the domain wall are the Euler–Lagrange–Rayleigh equations

$$\frac{\partial\mathcal{L}^{\text{DW}}}{\partial X_i} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}^{\text{DW}}}{\partial\dot{X}_i} = \frac{\partial\mathcal{R}^{\text{DW}}}{\partial\dot{X}_i}, \quad X_i = \{q, \varPhi\}. \tag{5}$$

Substituting Lagrangian $\mathcal{L}^{\text{DW}}$ and Rayleigh dissipative function $\mathcal{R}^{\text{DW}}$ into the (5) results in set (7) of main text

$$\begin{aligned}
&\hat{\mathbb{M}}\cdot\begin{bmatrix}\ddot{q}\\ \ddot{\Phi}\end{bmatrix} + \left(\hat{\mathbb{R}} + \tilde{\eta}\hat{\mathbb{M}}\right)\cdot\begin{bmatrix}\dot{q}\\ \dot{\Phi}\end{bmatrix} = \boldsymbol{F}, \quad \boldsymbol{F} = \begin{bmatrix}F_q\\ F_\Phi\end{bmatrix},\\
&\hat{\mathbb{M}} = 4\Delta\begin{bmatrix}-\frac{1+a^2\Delta^2}{\Delta^2} & a\\ a & -1\end{bmatrix}, \quad \hat{\mathbb{R}} = \begin{bmatrix}R_q & R_{q\Phi}\\ -R_{q\Phi} & 0\end{bmatrix},
\end{aligned} \tag{7}$$

where R_i and F_i are functions of domain wall position, phase, geometrical parameters, and external field parameters.

Here, we are interested in the description of *rigid motion mode*. So, we consider the curvature and torsion as small parameters within a low-frequency regime with $\dot{q} = v$ and $\Phi = \Phi_0 + \varphi$, where $\varphi \ll 1$ is a small deviation from the equilibrium state. We expand in series set (7), and save terms which are quadratic with respect to small parameters (i.e. $\varkappa$, σ, φ, and ϖ) and integrate it with respect to time $\bar{t} \in [0, 2\pi/\varpi]$. As a result, we obtain equations of motion in the form

$$\begin{gathered}
-\tilde{\eta}v\left(1+\sigma^2\right) + h^2\left[\sigma\varphi + v\frac{\pi}{\varpi}\left(2\varkappa^2+\sigma^2\right)\right] + \frac{h}{\sqrt{\varkappa^2+\sigma^2}}\left[\sigma\varpi\left(\varkappa + p\mathscr{C}\frac{\pi}{2}\right) - \pi h\left(2\varkappa^2+\sigma^2\right)\right] = 0,\\
\tilde{\eta}v\sigma - \varkappa\varphi p\mathscr{C}\frac{\pi}{2} + h\left[v\varkappa - vp\mathscr{C}\frac{\pi}{2}\left(\frac{3-2\pi^2}{3} + \varkappa^2\frac{8-\pi^2}{8}\right) - \frac{\varkappa\varpi}{\sqrt{\varkappa^2+\sigma^2}}\left(1 - \varkappa p\mathscr{C}\frac{\pi}{2}\right)\right]\\
+h^2\left(1-\varkappa p\mathscr{C}\frac{\pi}{2}\right)\left(\frac{\pi\sigma}{\sqrt{\varkappa^2+\sigma^2}} - v\sigma\frac{\pi}{\varpi} - \varphi\right) = 0,
\end{gathered} \tag{S.11}$$

where $\mathscr{C} = \cos\Phi_0$. The solution of set (S.11) results in

$$\begin{aligned}
&v = v_0 + \delta v, \quad v_0 = \varpi/\sqrt{\varkappa^2+\sigma^2}, \quad \delta v \approx \frac{\tilde{\eta}\varpi^2}{\left[\pi h^2\left(2\varkappa^2+\sigma\right) - \tilde{\eta}\varpi\right]\sqrt{\varkappa^2+\sigma^2}},\\
&\varphi = \varphi_0 + \delta\varphi, \quad \varphi_0 = 2h\varpi\varkappa\frac{\left(\pi^2-1\right)\sqrt{\kappa^2+\sigma^2}}{\left(2\kappa^2+\sigma^2\right)^2}, \quad \delta\varphi \approx -p\mathscr{C}\frac{2\tilde{\eta}^2\omega^2}{\pi^2h^2\varkappa\sqrt{\varkappa^2+\sigma^2}\left(2\varkappa^2+\sigma^2\right)^2}.
\end{aligned} \tag{S.12}$$

III. DW WIDTH AND SLOPE DURING FIELD-INDUCED MOTION

DW driven by rotating magnetic field experience width and slope alterations from the equilibrium values (10) defined in main text. Amplitudes of deviations from Δ_0, a_0 in the rigid motion mode are curvature-dependent, see Fig S1(a). In the simulations we got deviation up to 12% for DW slope and up to 3% for DW width. In the rigid motion mode, Δ and a reach their new equilibrium values during motion and afterwards are constant in time, see Fig. S1(b). While in oscillating motion mode their values oscillate near the equilibrium values, see Fig. S1(c).

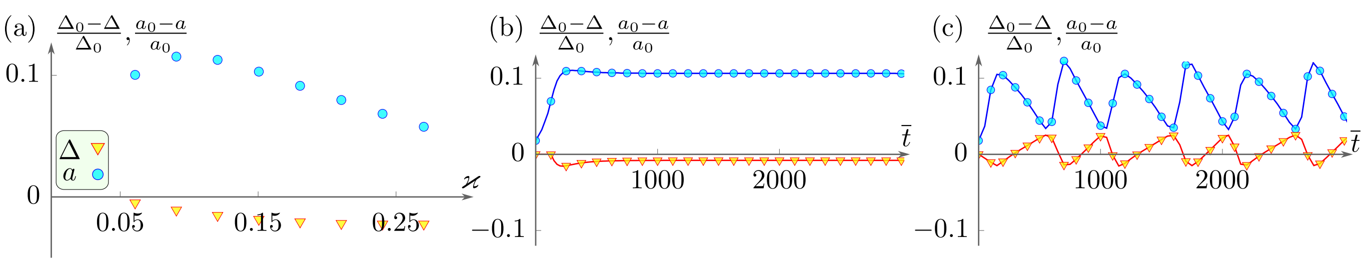

FIG. S1. (a) Average DW slope and width as functions of helix curvature for $\sigma = 0.1$, $\varpi = 0.001$, $h = 0.2$. (b) and (c) are time evolution of the DW slope and width for rigid ($\varpi = 0.004$) and oscillating ($\varpi = 0.008$) motion modes, respectively, for the helix with $\varkappa = 0.12$, $\sigma = 0.1$ and external magnetic field amplitude $h = 0.2$. All symbols are extracted from spin-lattice simulations; lines in (b) and (c) are guides to the eye.

[1] I. V. Baryakhtar and B. A. Ivanov, Nonlinear waves in antiferromagnets, Solid State Communications **34**, 545 (1980).
[2] A. M. Kosevich, B. A. Ivanov, and A. S. Kovalev, Magnetic solitons, Physics Reports **194**, 117 (1990).
[3] Here and below we utilize the assumption that the length of $\boldsymbol{n}$ is constant.
[4] D. D. Sheka, V. P. Kravchuk, and Y. Gaididei, Curvature effects in statics and dynamics of low dimensional magnets, Journal of Physics A: Mathematical and Theoretical **48**, 125202 (2015).