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HIGH ACCURACY NUMERICAL METHOD OF THIN-FILM PROBLEMS IN MICROMAGNETICS*[1)]

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Dedicated to the 80th birthday of Professor Zhou Yulin

Abstract

In this paper, a new high accuracy numerical method for the thin-film problems of micron and submicron size ferromagnetic elements is proposed. For the computation of stray field, we use the finite element method(FEM) by introducing a semi-discrete artificial boundary condition [1, 2]. In our numerical experiments about the domain patterns and their movement, we can see that the results are accordant to that of experiments and other numerical methods. Our method are very convenient to deal with arbitrary shape of thin films such as a polygon with high accuracy.

Key words: Thin-film, Micromagnetics, stray field, Semi-discrete artificial boundary condition.

1. Introduction

Micromagnetism of micron and submicron scale patterned thin-film has become an area of great scientific and technological interest in recent years[3, 4, 5, 6, 7]. Because of the important applications of ferromagnetic thin-film to magnetic information storage technology and the potential of the semiconductor microelectronics technology, there has been a rising interest in studying the efficient numerical methods for the thin-film problems in the world[5, 6, 7].

One can simulate the magnetization processes by combining the classic micromagnetic theory with dynamic descriptions of magnetization orientations. Micromagnetic theory considers the free energy in the ferromagnetic material, which in general includes the following energy terms (here we omit the *magnetoelastic energy*)

1. the *magnetic anisotropy energy*, which acts as a local constraint on the magnetization orientation,
2. the *exchange energy*, which tends to keep adjacent spins parallel,
3. the *magnetostatic (or Self-Induced) energy*,
4. the *magnetic potential energy* due to external magnetic fields,

By the simulation of the dynamic process in Micromagnetic modelling, not only we can get the remanence domain configurations in a ferromagnetic element, but also we can get the transient pictures that demonstrate how a complex domain structure forms. From the Micromagnetic Model we know that the complex magnetization domain patterns and the detailed spin structures within the domain boundaries are the results of minimizing the total free energy. That is, the different domain patterns correspond to different local energy minima. If an external field

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is applied with sufficient magnitude that the energy minimum disappears, the corresponding magnetization domain pattern will change, following the dynamic equation until a new energy minimum is reached.

In this paper, we provide a method which mixed the finite element method and integral method to get the numerical solution of the ferromagnetic thin-film problem. First, we rewrite the solution of an initial-boundary problem with the Landau-Lifshitz equation in integral formula, we can reduce the computation of the most singular part of the integral to a Poisson problem on an infinite domain in two dimensional (2D) [7]. After that, we can design a semi-discrete artificial boundary condition [1, 2] to get the numerical solution by finite element method (FEM).

2. Thin-film problem

One class of ferromagnetic thin films that has been studied extensively by micromagnetic modelling are the magnetic thin films used for data storage in hard-disk drives. In general, these thin films are a few tens of nanometers thick and less than a micron long. Therefore, we will focus on the micron and sub-micron size thin-films with tens nanometers thickness in this paper. Certainly, our method can deal with more general thin-film problems.

First, let's recall the full micromagnetic model [5, 7, 8]. Consider a ferromagnetic material contained in a domain $V_\delta = \Omega \times [-\delta, \delta] \subset \mathbb{R}^3$, where $\delta << diam(\Omega)$, $\Omega \subset \mathbb{R}^2$ is supposed to have a piecewise smooth boundary, for example, a polygon (then we can define the out normal vector on $\partial\Omega$ except a finite number of points). As we mentioned, the free-energy functional of micromagnetics can be written as

$$\begin{aligned} E(\mathbf{m}) &= \frac{\mathcal{A}}{2}\int_{V_\delta} |\nabla \mathbf{m}|^2 dx + \frac{\mathcal{K}_\mu}{2}\int_{V_\delta} \phi(\mathbf{m})\, dx + \frac{M_s^2}{2\mu_0}\int_{\mathbb{R}^3} |\mathbf{h}_{str}|^2 dx - \frac{M_s^2}{\mu_0}\int_{V_\delta} \mathbf{h}_{ext}\cdot \mathbf{m}\, dx \\ &\equiv E_{exc} + E_{ani} + E_{sta} + E_{ext}, \end{aligned} \tag{2.1}$$

where E_{exc}, E_{ani}, E_{sta} and E_{ext} represent *exchange energy*, *anisotropy energy*, *static energy*, and *external field energy* respectively. Here M_s is saturation magnetization, $\mathbf{m}$ is the normalized magnetization (= the magnetization $\mathbf{M}/M_s$), a unit vector field defined on the film V_δ. Moreover, $\mathcal{A}$ (dimension J/m) is the exchange stiffness constant, measures the strength of the exchange energy relative to that of dipolar interactions, $\mathcal{K}_\mu$ (dimension J/m^3) is the quality factor measuring the relative strength of the magnetic anisotropy ϕ, $\mathbf{h}_{str}$ is the normalized stray field, whose norm squared gives the magnetostatic energy density, $\mathbf{h}_{ext}$ is the applied field, which we assume to be uniform.

The effective magnetic field $\mathbf{h}_{eff}$ at a position inside the ferromagnetic material is defined by

$$\mathbf{h}_{eff} = -\frac{\delta E}{\delta \mathbf{m}}. \tag{2.2}$$

The magnetization orientation follows the Landau-Lifshitz equation[8],

$$\frac{d\mathbf{m}}{dt} = -\gamma \mathbf{m}\times \mathbf{h}_{eff} - \alpha\gamma \mathbf{m}\times(\mathbf{m}\times \mathbf{h}_{eff}), \tag{2.3}$$

where γ is the electron gyromagnetic ratio and α is the damping constant. If we want to get the domain patterns or observe the movement of the domain walls, we should solve the following initial-boundary value problem

$$\frac{d\mathbf{m}}{dt} = -\gamma \mathbf{m}\times \mathbf{h}_{eff} - \alpha\gamma \mathbf{m}\times(\mathbf{m}\times \mathbf{h}_{eff}) \tag{2.4}$$

$$\mathbf{m}(0,x) = \mathbf{m}_0(x) \tag{2.5}$$

$$\frac{\partial \mathbf{m}}{\partial n}\Big|_{\partial V_\delta} = 0. \tag{2.6}$$

Sure, we can separate the effective magnetic field $\mathbf{h}_{eff}$ to four parts:

$$\mathbf{h}_{eff} = \mathbf{h}_{exc} + \mathbf{h}_{ani} + \mathbf{h}_{str} + \mathbf{h}_{ext}, \tag{2.7}$$

where $\mathbf{h}_{exc} = -\frac{\delta E_{exc}}{\delta \mathbf{m}} = \mathcal{A} \triangle \mathbf{m}$, $\mathbf{h}_{ani} = -\frac{\delta E_{ani}}{\delta \mathbf{m}} = -\mathcal{K}_\mu \phi'(\mathbf{m})$, $\mathbf{h}_{str} = -\frac{\delta E_{sta}}{\delta \mathbf{m}} = -\nabla u$ and $\mathbf{h}_{ext} = -\frac{\delta E_{ext}}{\delta \mathbf{m}}$. The difficulty of the simulation procedure is computing the global term *stray field* $\mathbf{h}_{str} = -\nabla u$. It is determined by the following problem

$$\triangle u = \operatorname{div} \mathbf{m} \quad \text{in } V_\delta, \tag{2.8}$$

$$\triangle u = 0 \quad \text{in } \overline{V}_\delta{}^c, \tag{2.9}$$

$$[u]\,|_{\partial V_\delta} = 0, \tag{2.10}$$

$$\left[\frac{\partial u}{\partial n}\right]\Big|_{\partial V_\delta} = -\mathbf{m}\cdot\nu, \tag{2.11}$$

where $[f]|_{\partial V_\delta}$ is the jump of function f on the boundary ∂V_δ. The solution to this problem is given by the Biot-Savart Law:

$$\begin{aligned} u(x) &= \int_{V_\delta} \nabla_x N(x-y)\cdot \mathbf{m}(y)dy \\ &= \int_{V_\delta} N(x-y)\operatorname{div}\mathbf{m}(y)dy - \int_{\partial V_\delta} N(x-z)\mathbf{m}\cdot\vec{n}(z)d\sigma(z) \end{aligned} \tag{2.12}$$

where $N(x) = -\frac{1}{4\pi|x|}$ is the Newtonian potential in $\mathbb{R}^3$, $\vec{n}$ is the unit exterior normal vector on $\partial\Omega$.

As we are studying the thin-film problem, we assume that the magnetization does not depend on the transversal coordinate, but only on the *in plane* coordinates. By our assumption, $\mathbf{m}$ is only a function of (x_1, x_2), we can integrate in the other coordinate in the expression for ∇u [7]:

$$\nabla' u(x_1, x_2) = \int_{-\delta}^{\delta} \nabla u(x_1, x_2, x_3)dx_3 \tag{2.13}$$

If we define:

$$\widetilde{K}_\delta(r) = \frac{1}{4\pi}\log\left(\frac{2\delta + \sqrt{4\delta^2 + r^2}}{r}\right) + \frac{1}{4\pi\delta}\left(r - \sqrt{4\delta^2 + r^2}\right), \tag{2.14}$$

and

$$W_\delta(r) = \frac{1}{4\pi\delta}\left(\frac{1}{r} - \frac{1}{\sqrt{4\delta^2 + r^2}}\right), \tag{2.15}$$

we can write the expression of ∇u as follows

$$\nabla' u(x) = -\int_\Omega \nabla'_x \otimes \nabla'_x \widetilde{K}_\delta(x-y)\cdot \mathbf{m}'(y)dy, \tag{2.16}$$

$$\frac{\partial u}{\partial x_3}(x) = \int_\Omega \mathbf{m}_3(y)\; W_\delta(x-y)dy, \tag{2.17}$$

where $\nabla' = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2})$, $\mathbf{m}' = (m_1, m_2)$ denote the *in plane* part. In what follows, a prime will always denote a two-dimensional field or operator. On the other hand, the function

$$v(x) = \int_\Omega \frac{1}{2\pi} \nabla_x \log \frac{1}{|x-y|} \cdot \mathbf{m}(y) dy$$

is the solution of the following problem

$$\triangle v = \operatorname{div} \mathbf{m} \quad \text{in } \Omega, \tag{2.18}$$

$$\triangle v = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \tag{2.19}$$

$$[v]\,|_{\partial\Omega} = 0, \tag{2.20}$$

$$\left[\frac{\partial v}{\partial n}\right]\Big|_{\partial\Omega} = -\mathbf{m} \cdot \nu. \tag{2.21}$$

Therefore, if we define

$$K_\delta(r) = \frac{1}{4\pi} \log(2\delta + \sqrt{4\delta^2 + r^2}) + \frac{1}{4\pi\delta}(r - \sqrt{4\delta^2 + r^2}), \tag{2.22}$$

we can rewrite $\nabla' u$ as follows,

$$\nabla' u(x) = \frac{1}{2}\nabla' v(x) - \int_\Omega \nabla'_x \otimes \nabla'_x K_\delta(x-y) \cdot \mathbf{m}'(y) dy \equiv \frac{1}{2}\nabla' v(x) + \nabla' \bar{u}. \tag{2.23}$$

3. Numerical Algorithm

From section , the remainder problem, also the most difficult problem, is how to compute the stray field. Because the domain in (2.18)–(2.21) is infinite (the whole space $\mathbb{R}^2$), if we want to solve this problem by FEM, we must first give an artificial boundary to bound the computational domain and give an artificial boundary condition on it. In [1, 2] we gave the discrete artificial boundary conditions for this type problems (2.18). That means, we can give a relationship between u and $\frac{\partial u}{\partial n}$ on $\partial\Omega$ by solving the external problem. Therefore, we can reduce the problem (2.18) to the following problem on a bounded domain $\Omega \subset \mathbb{R}^2$

$$\triangle v = \operatorname{div} \mathbf{m} \quad \text{in } \Omega, \tag{3.1}$$

$$\frac{\partial v}{\partial n}\Big|_{\partial\Omega} = G(v|_\Omega) + \mathbf{m} \cdot \nu \tag{3.2}$$

where $G(v)$ is a function of v given by the discrete boundary condition [1, 2]. In fact, $G(v)$ is a summation of the multiplication of function v and a kernel function on the boundary $\partial\Omega$.

Then it is very easy to get the numerical solution of problem (3.1)–(3.2) by FEM. For example, if we give a triangulation $\mathcal{T}_h$ of Ω and use the piecewise linear polynomials to construct the trial and test spaces

$$S_h = \{w_h \in C(\Omega) \Big| \; w_h \text{ is a linear polynomial on each triangle of } \mathcal{T}_h\}, \tag{3.3}$$

we obtain an approximating problem of (3.1)–(3.2) in variational form:

$$\begin{cases} \text{Find } v_h \in S_h, \text{ such that} \\ \int_\Omega \nabla' v_h \cdot \nabla' w_h dx - \int_{\partial\Omega} G(v_h)\, w_h \, ds = \int_\Omega \nabla' w_h \cdot \mathbf{m} \, dx, \forall w_h \in S_h. \end{cases} \tag{3.4}$$

We can get an approximation $\nabla' v_h$ of $\nabla' v$ with high accuracy [1, 2].

From (2.23) and (2.17) we can see that the remain part of ∇u are in terms of the convolution of K_δ and $\nabla' m$, W_δ and $\mathbf{m}$ respectively. As the integral kernel function K_δ and W_δ are smooth function or with only weak singularity, we can get a high accuracy approximations of these integrals by Gaussian numerical integral methods. For example, if we use piecewise constant approximation for $\mathbf{m}'$, from (2.23) and (2.17), we have the following formula:

$$\begin{aligned} \nabla' \bar{u}(x) &= -\int_\Omega \nabla'_x \otimes \nabla'_x K_\delta(x-y) \cdot \mathbf{m}'(y) dy \\ &= -\sum_{\Omega_h \subset \mathcal{T}_h} \int_{\Omega_h} \nabla'_x \otimes \nabla'_x K_\delta(x-y) dy \cdot \mathbf{m}'_h, \qquad (3.5) \\ \frac{\partial u}{\partial x_3}(x) &= \sum_{\Omega_h \subset \mathcal{T}_h} \int_{\Omega_h} W_\delta(x-y) dy \; \mathbf{m}_3^h. \qquad (3.6) \end{aligned}$$

If the domain is a rectangular, we can use the discrete fast Fourier transform (DFT) to reduce the computation in (3.5) and (3.6).

In summary, our algorithm can be described as follows: (for example, we use 4th Rounge-Kutta method to solve the problem (2.4)–(2.6)). In each time step, first we solve the problem (3.4) to get $\nabla' v_h$. Then we can calculate ∇u by (2.23) and (2.17). Moreover, we can get the value of $\mathbf{h}_{eff}$ from (2.7). Then the value of $\mathbf{m}$ in the next time step can be computed.

4. Numerical examples of Magnetic Domains

In this section, we give two examples of Magnetic Domains and the movement subject to an external magnetic field. We consider a thin film in volume $V_\delta = [-128, 128] \times [-128, 128] \times [-4, 4] nm$. That means, the length and width of the thin film are 256 nanometer, the thickness is 8 nanometer. The constants we used are: $\mathcal{A} = 1.3 \times 10^{-11}$, $\mathcal{K}_\mu = 500$, $M_s = 8 \times 10^5$, $\mu_0 = 4\pi \times 10^{-7}$, $\gamma = 2.21 \times 10^{-7}$, $\alpha = 0.1$.

Example 1. First, we give some classic patterns of domain walls. The results are shown in figures 1–4. We can see the different final domain patterns corresponding to different initial states.

In figures 1–4, the top two graphs show the magnetization in grey scale, the bottom ones show the magnetization field in spin structure; the left two charts show the initial state of the *in plane* magnetization $\mathbf{m}' = (m_1, m_2)$, the right two charts show the final steady state, arrows indicate the magnetization direction. From these figures we know that there are so many local minima of the energy functional $E(\mathbf{m})$ in (2.1).

Example 2. Our second example is about the movement of the domain wall subject to a external field. Figure 5 shows the predictions of our numerical scheme for a square film, subject to a field applied along the diagonal.

All these results are accordant to those in [5, 7].

5. Conclusions

In summary, in this paper, we give a high accuracy numerical method for the dynamic problems of thin film in micromagnetics. In our method, we calculate the *in plane* part stray field through solving an initial-boundary value problem in whole space $\mathbb{R}^2$. After we introduce a nature artificial boundary, we can easily give a discrete type artificial boundary condition with high accuracy on this boundary. Then we get the approximation by FEM. We use numerical quadrature method to obtain other parts of the effective magnetic field. If the domain is a rectangular, we use the fast discrete Fourier transform to reduce the computation. Furthermore, our method can extend to the problem with polygon domain easily.

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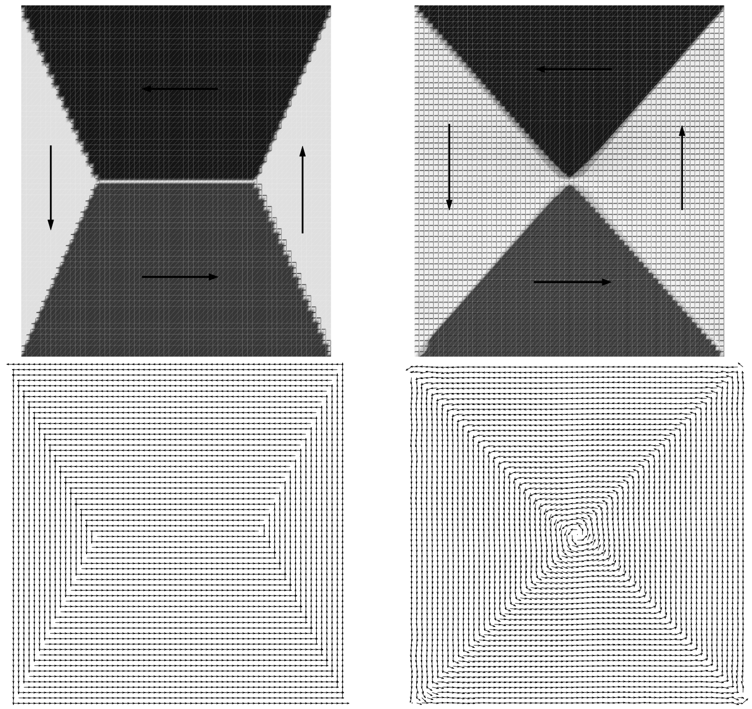

Figure 1: One vortex state.

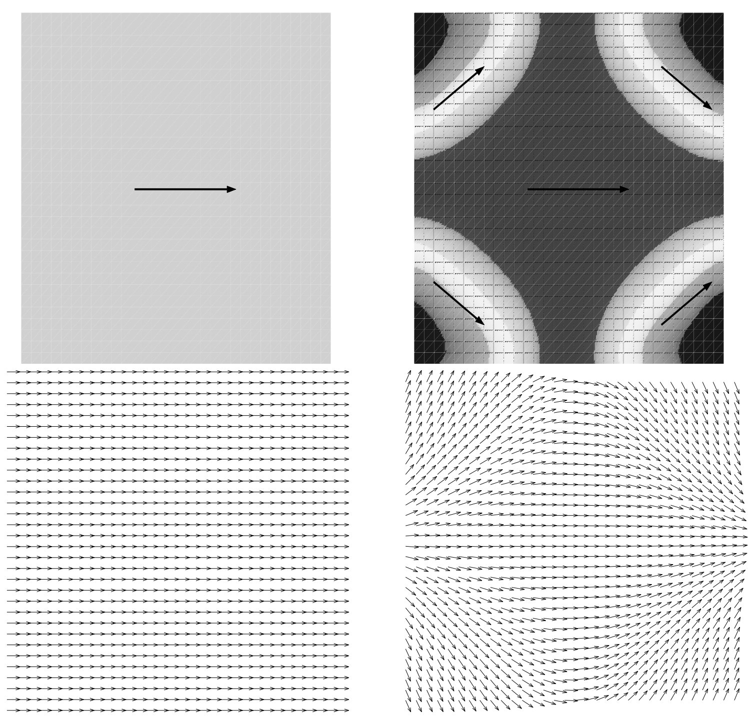

Figure 2: Flower state.

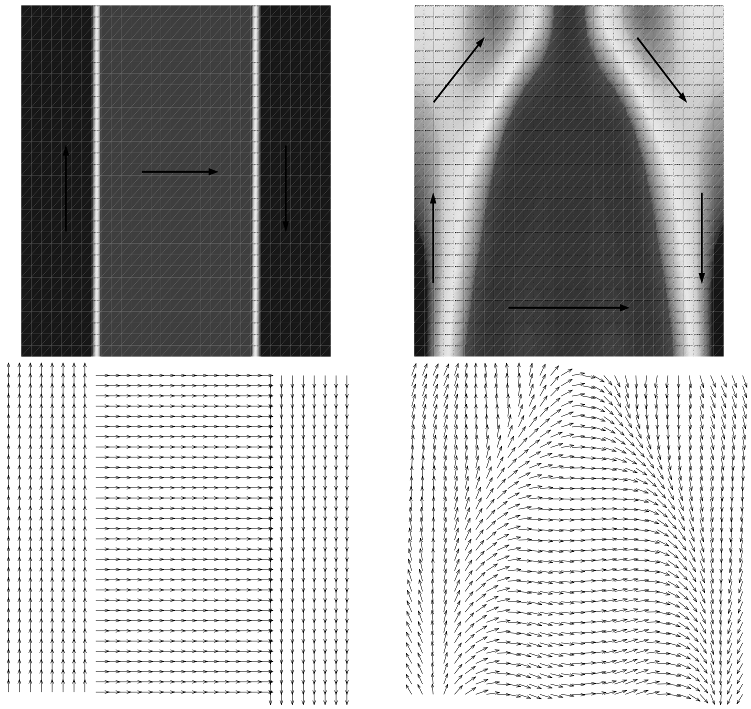

Figure 3: 'C' state.

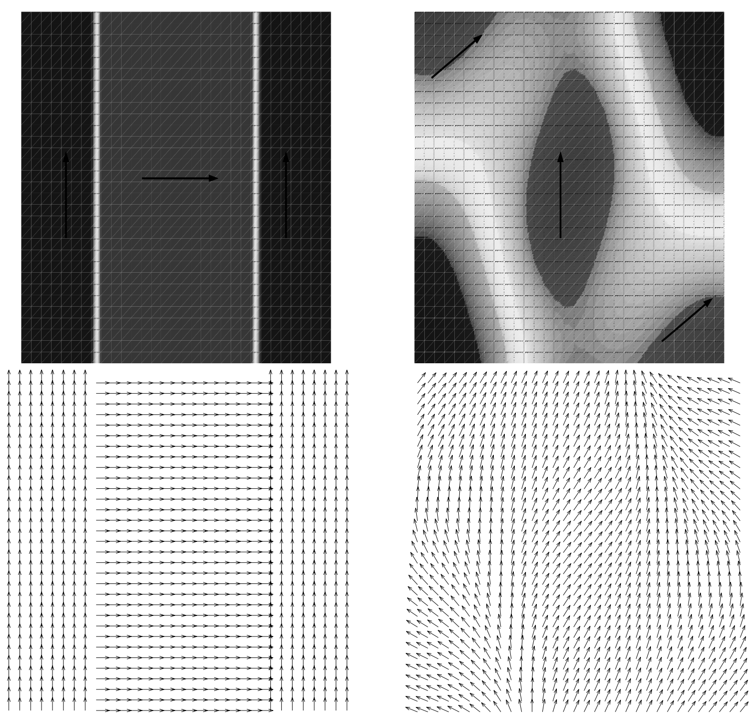

Figure 4: 'S' state.

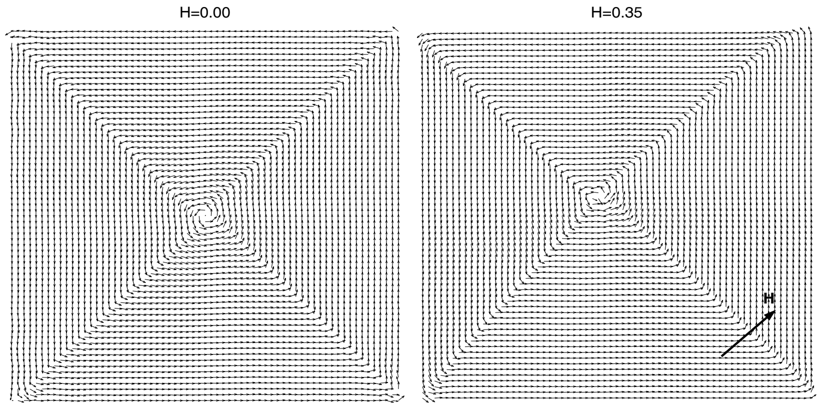

Figure 5: Plots of the vertical component $\mathbf{m}' = (m_1, m_2)$ of magnetization subject to a external field H applied along the diagonal in spin structure. If we increase the strength of H, the vortex will be more close to the top-left corner.

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