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A simple formula of the magnetic potential and of the stray field energy induced by a given magnetization

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The primary aim of this paper is the derivation and a proof of a simple and tractable formula for the stray field energy in micromagnetic problems. The formula is based on an expansion in terms of a special family of recently discovered functions. It remains valid even if the magnetization is not of constant magnitude or if the sample is not geometrically bounded. The paper continues with a direct and important application which consists in a fast summation technique of the stray field energy. The convergence of this method is established, and its efficiency is proved by various numerical experiments.

KEYWORDS

Landau–Lifshitz equation, micromagnetics, special functions, stray field

MSC CLASSIFICATION

35J47, 35J15, 35C10, 35C20

1 | INTRODUCTION

The description and the understanding of magnetic microstructures are often based on the theory of Landau and Lifshitz [1] (see also Brown [2]) which consists in minimizing of the total free energy (see, e.g., earlier studies [3–5] and Miyazaki and Jin [6]):

$$E_{tot}(M) = \alpha \int_\Omega |\nabla M|^2 dx + \int_\Omega \phi(M) dx - \frac{1}{2}\int_\Omega H_d \cdot J dx - \int_\Omega H_{ex} \cdot J dx + E_s, \tag{1}$$

where Ω is the sample (or the magnetic body), α is the exchange stiffness (positive) constant, ϕ is a function describing structural anisotropies, H_{ex} is an external field, H_d is the stray (or demagnetizing) field generated by the magnetic body itself, and E_s is the sum of the remaining energies (like magnetostrictive self-energy and magneto-elastic interaction energy). The magnetic polarization J is given by the formula $J = \mu_0 M$, while the stray field H_d is related to M by the equations:

$$\text{curl } H_d = 0 \text{ in } \mathbb{R}^3, \ \text{div } (\mu_0(H_d + M\chi_\Omega)) = 0 \text{ in } \mathbb{R}^3, \tag{2}$$

where μ_0 denotes the vacuum permeability and χ_Ω is the characteristic function of the sample.

The magnetization M is often subject to the Heisenberg–Weiss constraint

$$|M| = M_s \text{ a. e. in } \Omega, \tag{3}$$

where M_s is the spontaneous saturation magnetization which is assumed to be constant (and generally depending on the temperature).

In the literature, much attention is paid to the calculation of the stray field energy resulting from the demagnetizing field H_d:

$$\mathcal{E}_{sf}(M) := -\frac{\mu_0}{2}\int_\Omega H_d \cdot M dx. \tag{4}$$

In view of Equation (2), H_d is curl free and can be written into the form

$$H_d = -\nabla U, \tag{5}$$

(see Girault & Raviart [7]), where U is the magnetic potential which is solution of the Poisson equation in *the whole space*:

$$\Delta U = \text{div}\,(M\chi_\Omega) \text{ in } \mathbb{R}^3. \tag{6}$$

The stray field energy can be expressed as

$$\mathcal{E}_{sf}(M) = \frac{\mu_0}{2}\int_{\mathbb{R}^3} |\nabla U|^2 dx = \frac{\mu_0}{2}\int_{\mathbb{R}^3} |H_d|^2 dx. \tag{7}$$

Computing the stray field energy (7) is one of the most challenging issues in micromagnetics (see, e.g., Hubert & Schäfer [3] and Prohl [4]). The difficulty is mainly due to its nonlocal nature. There are several methods for the effective calculation of this energy. Some of these methods are based on solving the elliptic partial differential Equation (6) using finite differences method (see, e.g., previous research [8–10]) or finite elements method (see, e.g., earlier studies [11–14]). Other methods are based on the calculation of U from the integral formula (see, e.g., previous research [15–20]):

$$U(x) = \frac{1}{4\pi}\int_\Omega \frac{(y-x)\cdot M(y)}{|y-x|^3} dy. \tag{8}$$

We can also mention truncation-free methods for solving second-order elliptic PDEs that could be used to solve (6), such as the infinite element method which relies on the use of adequate shape functions in the radial direction (see, e.g., earlier works [21–26]) or inverted finite elements method which is based on applying a polygonal inversion to an unbounded component of the domain [27–32]. For instance, the latter method was successfully used by the author and a co-author in a recent work (see Boulmezaoud & Kaliche [33]).

The primary aim of this work is to establish the following formula

$$\mathcal{E}_{sf}(M) = \frac{\mu_0}{2}\sum_{k=0}^{\infty} \frac{4}{4(k+1)^2-1}\sum_{\alpha\in\Lambda_k}\left(\int_\Omega M.\nabla \mathcal{W}_\alpha dx\right)^2, \tag{9}$$

where $(\mathcal{W}_\alpha)_\alpha$ designates a special family of multidimensional functions introduced in Arar and Boulmezaoud [34] and in Boulmezaoud et al. [35] (these functions will be presented along with their properties in Section 2). The index sets Λ_k, $k \geqslant 0$, are defined hereafter by (16).

We also prove the following formula for the magnetic potential

$$U = \sum_{k=0}^{\infty} \frac{4}{4(k+1)^2-1}\sum_{\alpha\in\Lambda_k}\left(\int_\Omega M\cdot\nabla \mathcal{W}_\alpha dx\right)\mathcal{W}_\alpha. \tag{10}$$

Formulas (9) and (10) are valid for any domain Ω, not necessarily bounded, and any (measurable) vector field M satisfying

$$\int_\Omega |M|^2 dx < +\infty.$$

Nevertheless, the latter condition is obviously fulfilled when the sample Ω has a finite volume and M satisfying the Heisenberg-Weiss constraint (3).

Another by-product, as we shall see, concerns approximation of the stray-field energy (7). More precisely, truncating formula (9) gives the approximation

$$\mathscr{E}_{sf}^N(M) = \frac{\mu_0}{2} \sum_{k=0}^{N} \frac{4}{4(k+1)^2 - 1} \sum_{\alpha \in \Lambda_k} \left(\int_\Omega M.\nabla \mathscr{W}_\alpha dx \right)^2, \tag{11}$$

where N is a discretization parameter intended to tend to infinity. We will show that

$$\lim_{N \to +\infty} \mathscr{E}_{sf}^N(M) = \mathscr{E}_{sf}(M). \tag{12}$$

Moreover, when $\text{div}\, M \in L^2(\Omega)$ and $M \cdot n = 0$ on the boundary of Ω, n being the outward unit normal vector, we establish the estimate

$$0 \leqslant \mathscr{E}_{sf}(M) - \mathscr{E}_{sf}^N(M) \leqslant CN^{-2} \|\text{div}\, M\|_{L^2(\Omega)}. \tag{13}$$

The rest of the paper is organized as follows. In Section 2, we present the special functions introduced in Arar and Boulmezaoud [34] and which are the key ingredient of this paper. Their most useful properties are listed. These properties are essentially known, and no originality is claimed in Section 2. The formulas that form the main output of this paper are presented and proved in Section 3. In Section 4, a new method for calculating the energy resulting from these formulas is proposed and analyzed. In particular, the convergence of the method is established. In Section 5, focus is on computational tests through several examples. The last section is devoted to a conclusion.

2 | A FAMILY OF SPECIAL FUNCTIONS. AN OVERVIEW

In Arar and Boulmezaoud [34], Arar and the author introduced a family of multidimensional rational and quasi-rational functions ($\mathscr{W}_\alpha$) which turned out to be particularly appropriate for solving second order elliptic equations in unbounded regions of space (see Boulmezaoud et al. [35]). This is primarily due to their completeness, their orthogonal properties, and their behavior at large distances.

The definition of these functions in $\mathbb{R}^3$ necessitates the use of spherical harmonics on the unit sphere of $\mathbb{R}^4$ and the stereographic projection (four-dimensional spherical harmonics are less encountered than those on $\mathbb{S}^2$ the unit sphere of $\mathbb{R}^3$).

For each integer $k \geqslant 0$, $\mathbb{H}_k$ will be the space of spherical harmonics of degree k over the unit sphere (see, e.g., earlier studies [36–40]):

$$\mathbb{S}^3 := \{x \in \mathbb{R}^4 \,|\, |x| = 1\}.$$

(spherical harmonics of degree k on $\mathbb{S}^3$ are restrictions to $\mathbb{S}^3$ of harmonic homogeneous polynomials of degree k on $\mathbb{R}^4$). We know that

$$\dim \mathbb{H}_k = (k+1)^2 \text{ for all } k \geqslant 0. \tag{14}$$

In order to construct an orthogonal basis of $\mathbb{H}_k$, we set

$$\Lambda = \{(i, \ell, m) \in \mathbb{N}^2 \times \mathbb{Z} \mid 0 \leqslant \ell \leqslant i \text{ and} - \ell \leqslant m \leqslant \ell\}, \tag{15}$$

and for each integer $k \geqslant 0$,

$$\begin{aligned} \Lambda_k &= \{(i, \ell, m) \in \Lambda \mid i = k\}, \\ \Lambda_k^\star &= \bigcup_{i=0}^k \Lambda_i. \end{aligned} \tag{16}$$

If $\alpha = (k, \ell, m)$, $\beta = (k', \ell', m') \in \Lambda$, then $\delta_{\alpha,\beta}$ denotes the usual Kronecker symbol of α, β, that is, $\delta_{\alpha,\beta} = \delta_{k,k'}\delta_{\ell,\ell'}\delta_{m,m'}$. Define the spherical coordinates for $\mathbb{S}^3$ as the triplet (ϕ, θ, χ) such that $0 \leqslant \phi < 2\pi$, $0 \leqslant \theta \leqslant \pi$, $0 \leqslant \chi \leqslant \pi$ and

$$\xi = (\sin\theta \cos\phi \sin\chi, \sin\theta \sin\phi \sin\chi, \cos\theta \sin\chi, \cos\chi). \tag{17}$$

Spherical harmonics on $\mathbb{S}^3$ are defined by the following:

$$\mathscr{Y}_\alpha(\xi) = \frac{1}{\sqrt{a_{k,\ell}}}(\sin\chi)^\ell T_{k+1}^{(\ell+1)}(\cos\chi)Y_{\ell,m}(\phi,\theta), \text{for } \alpha = (k,\ell,m) \in \Lambda. \tag{18}$$

Here,

- $(T_k)_{k\geqslant 0}$ designate Chebyshev polynomials of the first kind satisfying

$$\cos(k\theta) = T_k(\cos\theta) \text{ for } \theta \in \mathbb{R},$$

- $(Y_{\ell,m})_{\ell,m}$ are the usual real spherical harmonics on $\mathbb{S}^2$:

$$Y_{\ell,m}(\phi,\theta) = \eta_\ell K_\ell^{|m|}(\cos\theta)y_m(\phi), \tag{19}$$

where

$$y_m(\phi) = \begin{cases} \cos(m\phi) & \text{if } m \geqslant 1, \\ \frac{1}{\sqrt{2}} & \text{if } m = 0, \\ \sin(|m|\phi) & \text{if } m \leqslant -1, \end{cases} \tag{20}$$

$$\eta_\ell = \sqrt{\frac{2\ell+1}{2\pi}}, \tag{21}$$

and

$$K_\ell^m(x) = (-1)^m \sqrt{\frac{(\ell-m)!}{(\ell+m)!}} P_\ell^m(x), \quad \text{for } -\ell \leqslant m \leqslant \ell. \tag{22}$$

(thus, $K_\ell^{-m} = (-1)^m K_\ell^m$). Here $(P_\ell^m)_{\ell,m}$ designate the associated Legendre functions defined as follows:

$$P_\ell^m(t) = \frac{(-1)^m}{2^\ell \ell!}(1-t^2)^{m/2}\frac{d^{\ell+m}}{dt^{\ell+m}}(t^2-1)^\ell, -\ell \leqslant m \leqslant \ell$$

(some authors omit the $(-1)^m$ factor, commonly referred to as the Condon-Shortley phase, or append it in the definition of $Y_{\ell,m}$). We also adopt the convention $P_\ell^m = 0$ and $K_\ell^m = 0$ when $|m| > \ell$.
- $(a_{k,\ell})$ are normalization constants given by

$$a_{k,\ell} = \frac{(k+1)\pi}{2}\frac{(k+\ell+1)!}{(k-\ell)!}. \tag{23}$$

The following properties hold true

- For all $k \geqslant 0$, $(\mathscr{Y}_\alpha)_{\alpha\in\Lambda_k}$ is a basis of $\mathbb{H}_k$.
- For all $\alpha, \beta \in \Lambda$

$$\int_{\mathbb{S}^3} \mathscr{Y}_\alpha(\xi)\mathscr{Y}_\beta(\xi)dS(\xi) = \delta_{\alpha,\beta}. \tag{24}$$

- For all $k \geqslant 0$ and $\alpha \in \Lambda_k$,

$$-\Delta_S \mathscr{Y}_\alpha = k(k+2)\mathscr{Y}_\alpha,$$

where Δ_S is the Laplace–Beltrami operator over the unit sphere $\mathbb{S}^3$. In terms of spherical coordinates, this operator is given by

$$\frac{1}{\sin^2\chi}\left\{\frac{\partial}{\partial\chi}\left(\sin^2\chi\frac{\partial}{\partial\chi}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}.$$

In the three-dimensional situation (the only one that interests us here), special functions we need here are defined as follows (see Arar & Boulmezaoud [34] and Boulmezaoud et al. [35]): for any $\alpha \in \Lambda$

$$\mathscr{W}_\alpha(x) = \left(\frac{2}{|x|^2+1}\right)^{\frac{1}{2}} \mathscr{Y}_\alpha(\pi^{-1}(x)). \tag{25}$$

Here, π denotes the stereographic projection defined on $\mathbb{S}^3_\star = \mathbb{S}^3 - \{(0,\cdots,0,1)\}$ by

$$\begin{aligned} \pi : \mathbb{S}^3_\star &\to \mathbb{R}^3 \\ \xi &\mapsto \left(\frac{\xi_1}{1-\xi_4}, \frac{\xi_2}{1-\xi_4}, \frac{\xi_3}{1-\xi_4}\right). \end{aligned}$$

Its inverse is given by

$$\begin{aligned} \pi^{-1} : \mathbb{R}^3 &\to \mathbb{S}^3_\star \\ x &\mapsto \left(\frac{2x_1}{|x|^2+1}, \frac{2x_2}{|x|^2+1}, \frac{2x_3}{|x|^2+1}, \frac{|x|^2-1}{|x|^2+1}\right). \end{aligned}$$

Functions $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$ were discovered by Arar and Boulmezaoud [34] in studying spectrum of weighted Laplacians in $\mathbb{R}^n$. These functions exist in all dimensions and not only the dimension three used here. One can consult Arar and Boulmezaoud [34] and Boulmezaoud et al. [35] for higher dimensions and for $n = 1$ or $n = 2$.

In Table B1 of Appendix B, the expressions of the first functions $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$ are given explicitly (when $n = 3$). One may observe that these functions have a rational or quasi-rational nature. This is a general property as it is announced in the following proposition which summarizes some useful properties of the functions $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$. We refer to Arar and Boulmezaoud [34] and Boulmezaoud et al. [35] for the proofs.

Proposition 2.1. *Let $k \geqslant 0$ be an integer and $\alpha \in \Lambda_k$. Then,*

– *we have*

$$-\Delta\mathscr{W}_\alpha = \frac{(2k+1)(2k+3)}{(|x|^2+1)^2}\mathscr{W}_\alpha, \tag{26}$$

– *there exists $k+1$ polynomial functions $p_0, \cdots, p_k$ such that:*

$$\mathscr{W}_\alpha(x) = \sum_{i=0}^{k} \frac{p_i(x)}{(|x|^2+1)^{i+1/2}}, \tag{27}$$

where for each $i \leqslant \ell$, p_i is of degree less than or equal to i,

– *for all $\beta \in \Lambda$*

$$\int_{\mathbb{R}^3} \frac{\mathscr{W}_\alpha(x)\mathscr{W}_\beta(x)}{(|x|^2+1)^2} dx = \frac{1}{4}\delta_{\alpha,\beta}, \tag{28}$$

$$\int_{\mathbb{R}^3} \nabla\mathscr{W}_\alpha(x)\cdot\nabla\mathscr{W}_\beta(x) dx = \frac{(2k+1)(2k+3)}{4}\delta_{\alpha,\beta}. \tag{29}$$

The orthogonality identities (28) and (29) are among the most important properties of the functions $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$. These relations will be the cornerstone of the formula given in this paper and of the resulting numerical approximation.

Here ends this first enumeration of the properties of functions $(\mathscr{W}_\alpha)$. We will need other properties later on, in particular for the calculation of gradients (see paragraph 5.1).

3 | THE FIRST MAIN RESULT: THE FORMULAS

The objective here is to prove formulas (9) and (10) announced in Section 1. These formulas will be used in the next section to propose a new method for computing stray-field energy. However, before stating the first main result, it is appropriate to give some basics concerning the underlying functional framework we use here. In particular, we show the well-posed nature of Equation (6) (see also Praetorius [41]).

Here and subsequently, we assume that

($\mathscr{H}_1$) the material fills a Lipschitz domain $\Omega \subset \mathbb{R}^3$,
($\mathscr{H}_2$) the magnetization field M is defined and measurable over Ω and satisfies

$$\int_\Omega |M|^2 dx < \infty, \tag{30}$$

that is, $M \in L^2(\Omega)^3$.

Assumption ($\mathscr{H}_2$) is obviously fulfilled when $|M|$ satisfies the Heisenberg–Weiss constraint (3) and $|\Omega| < \infty$ since

$$\|M\|^2_{L^2(\Omega)^3} = \int_\Omega |M|^2 dx = |M|^2 |\Omega| < +\infty.$$

Despite this, we assume neither that Ω is bounded nor that $|M|$ is satisfying the Heisenberg–Weiss constraint (3). Only assumptions ($\mathscr{H}_1$) and ($\mathscr{H}_2$) are needed here.

We now introduce some weighted function spaces. For all integers $\ell \in \mathbb{Z}$ and $m \geqslant 0$, $W^m_\ell(\mathbb{R}^3)$ stands for the space of functions v satisfying

$$\forall |\lambda| \leqslant m, \; (1+|x|^2)^{(\ell+|\lambda|-m)/2} D^\lambda v \in L^2(\mathbb{R}^3).$$

This space is equipped with the norm

$$\|v\|_{W^m_\ell(\mathbb{R}^3)} = \left(\sum_{|\lambda| \leqslant m} \int_{\mathbb{R}^3} (|x|^2+1)^{|\lambda|+\ell-m} |D^\lambda v|^2 dx \right)^{1/2}. \tag{31}$$

When $m \geqslant 1$, the following inclusions hold:

$$W^m_\ell(\mathbb{R}^3) \hookrightarrow W^{m-1}_{\ell-1}(\mathbb{R}^3) \hookrightarrow \cdots \hookrightarrow W^1_{\ell-m+1}(\mathbb{R}^3) \hookrightarrow W^0_{\ell-m}(\mathbb{R}^3).$$

The following asymptotic property holds true for any function $v \in W^m_\ell(\mathbb{R}^3)$ (see, e.g., Alliot [42])

$$\lim_{|x| \to +\infty} |x|^{\ell-m+3/2} \|v(|x|,.)\|_{L^2(\mathbb{S}^2)} = 0, \tag{32}$$

where $\mathbb{S}^2$ is the unit sphere of $\mathbb{R}^3$ and

$$\|v(|x|,.)\|^2_{L^2(\mathbb{S}^2)} = \int_{\mathbb{S}^2} |v(|x|,\sigma)|^2 d\sigma. \tag{33}$$

Let us mention the following Hardy's type inequality in $W^1_0(\mathbb{R}^3)$ (see Boulmezaoud & Kaliche [33]):

$$\forall v \in W^1_0(\mathbb{R}^3), \; \int_{\mathbb{R}^3} \frac{|v|^2}{|x|^2+1} dx \leqslant 4 \int_{\mathbb{R}^3} |\nabla v|^2 dx. \tag{34}$$

Thus, from now on, we shall consider that the Hilbert space $W^1_0(\mathbb{R}^3)$ is endowed with the scalar product

$$((v,w))_{W^1_0(\mathbb{R}^3)} = \int_{\mathbb{R}^3} \nabla v \cdot \nabla w dx,$$

and with the corresponding norm

$$|v|_{W^1_0(\mathbb{R}^3)} = |\nabla v|_{L^2(\mathbb{R}^3)},$$

which is equivalent to the norm $\|.\|_{W_0^1(\mathbb{R}^3)}$. The following lemma will play a prominent role in the sequel (see Arar & Boulmezaoud [34] and Boulmezaoud et al. [35]):

Lemma 3.1. *The family $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$ is a Hilbert basis of $W_0^1(\mathbb{R}^3)$ endowed with the norm $|.|_{W_0^1(\mathbb{R}^3)}$.*

Here, we look for a solution U of (6) satisfying

$$\int_{\mathbb{R}^3} |\nabla U|^2 dx < \infty, \tag{35}$$

The first main result of this paper is summarized as follows:

Theorem 3.2. *Assume that assumptions $(\mathscr{H}_1)$ and $(\mathscr{H}_2)$ hold true. Then (6) has a unique solution $U \in W_0^1(\mathbb{R}^3)$ which is given by*

$$U = \sum_{k=0}^{\infty} \sum_{\alpha\in\Lambda_k} \frac{4}{4(k+1)^2-1} \left(\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx \right) \mathscr{W}_\alpha, \tag{36}$$

where the series in the right-hand side converges in $W_0^1(\mathbb{R}^3)$. The corresponding stray field energy is given by

$$\mathscr{E}_{sf}(U) = \sum_{k=0}^{\infty} \frac{2\mu_0}{4(k+1)^2-1} \sum_{\alpha\in\Lambda_k} \left(\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx \right)^2. \tag{37}$$

Moreover, $U \in L^2(\mathbb{R}^3)$, $(1+|x|^2)^{1/2}\nabla U \in L^2(\mathbb{R}^3)^3$ and

$$\|(1+|x|^2)^{-1/2} U\|_{L^2(\mathbb{R}^3)} \leqslant 4\|M\|_{L^2(\Omega)}, \tag{38}$$

$$\mathscr{E}_{sf}(U) \leqslant \frac{\mu_0}{2} \|M\|^2_{L^2(\Omega)}, \tag{39}$$

$$\|U\|_{L^2(\mathbb{R}^3)} + \|(1+|x|^2)^{1/2}\nabla U\|_{L^2(\mathbb{R}^3)^3} \leqslant C_0(\Omega)\|M\|_{L^2(\Omega)}, \tag{40}$$

where $C_0(\Omega) > 0$ is a constant depending only on Ω. We also have

$$\lim_{|x|\to+\infty} |x|^{3/2} \|U(|x|,.)\|_{L^2(\mathbb{S}^2)} = 0. \tag{41}$$

Issues concerning the regularity of the solution U are postponed to the next section (see Theorem 4.4).

Proof. We can reformulate Equation (6) as follows: find $U \in W_0^1(\mathbb{R}^3)$ such that

$$\forall v \in W_0^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \nabla U \cdot \nabla v dx = \int_\Omega M \cdot \nabla v dx. \tag{42}$$

The existence and uniqueness of solutions are direct consequences of the Lax–Milgram theorem (see also Praetorius [41] for existence results in weighted L^p spaces).

Estimate (39) results from the use of Cauchy–Schwarz inequality on the right when $v = u$ in (42). Combining with Hardy inequality (34) gives (38). In view of Lemma 3.1, we have

$$\begin{aligned} U &= \sum_{\alpha\in\Lambda} \frac{((U,\mathscr{W}_\alpha))_{W_0^1(\mathbb{R}^3)}}{((\mathscr{W}_\alpha,\mathscr{W}_\alpha))_{W_0^1(\mathbb{R}^3)}} \mathscr{W}_\alpha, \\ &= \sum_{k=0}^{+\infty} \frac{4}{4(k+1)^2-1} \sum_{\alpha\in\Lambda_k} (\nabla U, \nabla \mathscr{W}_\alpha)_{L^2(\mathbb{R}^3)^3} \mathscr{W}_\alpha. \end{aligned}$$

Combining with (42) and (29) gives (36). Since convergence of the right-hand side holds in $W_0^1(\mathbb{R}^3)$, we also get (37). The reader can refer to Boulmezaoud and Kaliche [33] for estimate (40). Hence, $U \in W_1^1(\mathbb{R}^3)$ and (32) holds true with $\ell = m = 1$. This gives (41). □

4 | THE SECOND MAIN RESULT: A NEW METHOD FOR CALCULATING THE STRAY-FIELD ENERGY

The main purpose of this section is to show that from the two formulas (36) and (37) results a very efficient and easy to implement numerical method for calculating the stray field energy. This numerical method could be seen as a spectral method in an unbounded domain. However, unlike the usual spectral methods in a bounded domain and which use polynomial functions or trigonometric functions, here we use (quasi)-rational functions guaranteeing a decay of the solution at large distances. Indeed, in view of Proposition 2.1, the functions $(\mathscr{W}_\alpha)_\alpha$ are rationals up to a multiplicative factor.

4.1 | The method

In view of (37), the energy $\mathscr{E}_{sf}(U)$ can be reasonably approximated by truncating the sum. For this end, we set for each $N \geqslant 1$

$$\mathscr{E}_{sf}^N(U) = \sum_{k=0}^{N} \sum_{\alpha \in \Lambda_k} \frac{2\mu_0}{4(k+1)^2 - 1} \left(\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx \right)^2. \tag{43}$$

We observe that

$$\mathscr{E}_{sf}^N(U) = \frac{\mu_0}{2} \int_{\mathbb{R}^3} |\nabla U_N|^2 dx, \tag{44}$$

where

$$U_N = \sum_{\ell=0}^{N} \sum_{\alpha \in \Lambda_k} \frac{4}{4(k+1)^2 - 1} \left(\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx \right) \mathscr{W}_\alpha. \tag{45}$$

Let us give another interpretation of U_N. Define the family of finite dimensional spaces $(H_N)_{N \geqslant 0}$ as follows: for $N \geqslant 0$, H_N is the space of functions of the form

$$v(x) = \sum_{k=0}^{N} \frac{p_k(x)}{(|x|^2 + 1)^{k+1/2}}, \; x \in \mathbb{R}^3, \tag{46}$$

where, for each $k \leqslant N$, p_k is a polynomial of degree less than or equal to k. Obviously,

$$H_0 \subset H_1 \subset H_2 \subset \cdots \subset H_N \subset \cdots \tag{47}$$

The following inclusion holds for $N \geqslant 0$:

$$H_N \hookrightarrow W_0^1(\mathbb{R}^3). \tag{48}$$

It can be easily proved that (see, e.g., Arar & Boulmezaoud [34])

$$\dim H_N = \binom{3+N}{3} + \binom{N+2}{3} = \frac{(N+1)(N+2)(2N+3)}{6}. \tag{49}$$

Since

$$|\Lambda_k| = (k+1)^2 \text{ for } k \geqslant 0$$

($|\Lambda_k|$ designates the cardinal of the set Λ_k), we deduce the identity

$$\dim H_N = \sum_{k=0}^{N} |\Lambda_k| = |\Lambda_N^\star|. \tag{50}$$

On the other hand, in view of Proposition 2.1, we have for all $N \geqslant 0$,

$$(\alpha \in \Lambda_\ell \text{ for some } \ell \leqslant N) \Rightarrow \mathscr{W}_\alpha \in H_N.$$

In other words,

$$\{\mathscr{W}_\alpha;\ \alpha \in \Lambda_N^\star\} \subset H_N.$$

Combining the latter with (50) and with orthogonality properties (28) and (29) gives

Lemma 4.1. *For all $N \geqslant 1$, the family $(\mathscr{W}_\alpha)_{\alpha\in\Lambda_N^\star}$ is a basis of H_N.*

Now, we state this.

Proposition 4.2. *The function U_N given by formula (45) is also the unique solution of the well-posed discrete problem*

$$\forall v_N \in H_N,\quad \int_{\mathbb{R}^3} \nabla U_N \cdot \nabla v_N dx = \int_\Omega M \cdot \nabla v_N dx. \tag{51}$$

In addition, U_N is the projection of U on H_N with respect to the inner product $((.,.))_{W_0^1(\mathbb{R}^3)}$.

One could therefore consider that the approximation (45) is none other than the solution of the discrete problem (51) which consists to approximate the original problem (6) by a spectral method using the functions of H_N. The use of the family $(\mathscr{W}_\alpha)_{\alpha\in\Lambda_N^\star}$ as a basis of H_N reduces the discrete problem (51) to a simple *diagonal linear system*

$$DX = B \tag{52}$$

with D the diagonal matrix

$$D = \operatorname{diag}\left(\frac{4}{3}, \underbrace{\frac{4}{15}, \cdots, \frac{4}{15}}_{4 \text{ coefficients}}, \cdots, \underbrace{\frac{4}{4(N+1)^2-1}, \cdots, \frac{4}{4(N+1)^2-1}}_{(N+1)^2 \text{ coefficients}}\right).$$

Here X contains the components of U_N with respect to the basis $(\mathscr{W}_\alpha)_{\alpha\in\Lambda_N^\star}$ and B covers the integrals $\int_\Omega M \cdot \nabla\mathscr{W}_\alpha dx$. Thus, the solution of (51) is obviously given by formula (36). This is a significant observation which demonstrates the benefits of using functions $(\mathscr{W}_\alpha)_\alpha$.

4.2 | Convergence of the method and error estimate

The focus now is on convergence when $N \to +\infty$. We have the following:

Theorem 4.3. *Assume that $(\mathscr{H}_1)$ and $(\mathscr{H}_2)$ are fulfilled. Then,*

$$\mathscr{E}_{sf}(U) - \mathscr{E}_{sf}(U_N) = \frac{\mu_0}{2}|U - U_N|^2_{W_0^1(\mathbb{R}^3)}, \tag{53}$$

and

$$\lim_{N\to+\infty} \mathscr{E}_{sf}^N(U_N) = \mathscr{E}_{sf}(U). \tag{54}$$

Proof. We first observe that (54) is a direct consequence of (36). Indeed, in view of (42) and (51), we get

$$\int_{\mathbb{R}^3} (\nabla U - \nabla U_N) \cdot \nabla U_N dx = 0,$$

and (53) follows immediately. □

Theorem 4.4. *Assume that $(\mathscr{H}_1)$ and $(\mathscr{H}_2)$ are fulfilled. Assume also that Ω is bounded, div $M \in L^2(\Omega)$ and $M \cdot n = 0$ on $\partial\Omega$. Then, $U \in W_2^2(\mathbb{R}^3)$ and there exists a constant C_1 depending only on Ω such that*

$$\|U - U_N\|_{W_0^1(\mathbb{R}^3)} \leqslant \frac{C_1}{N}\|div\ M\|_{L^2(\Omega)}, \tag{55}$$

$$0 \leqslant \mathcal{E}_{sf}(U) - \mathcal{E}_{sf}(U_N) \leqslant \frac{C_1^2}{N^2}\|div\ M\|^2_{L^2(\Omega)}. \tag{56}$$

If in addition div $M \in H_0^{k-1}(\Omega)$ *for some integer* $k \geqslant 2$ *and if*

$$\int_\Omega M.\nabla q dx = 0 \ \text{ for all } \ q \in \mathbb{P}^\Delta_{k-1}, \tag{57}$$

then $U \in W^{k+1}_{2k}(\mathbb{R}^3)$ *and there exists a constant* C_k *depending only on* k *and* Ω *such that*

$$\|U - U_N\|_{W_0^1(\mathbb{R}^3)} \leqslant C_k N^{-k}\|div\ M\|^2_{H^{k-1}(\Omega)}, \tag{58}$$

$$0 \leqslant \mathcal{E}_{sf}(U) - \mathcal{E}_{sf}(U_N) \leqslant C_k^2 N^{-2k}\|div\ M\|^2_{H^{k-1}(\Omega)}. \tag{59}$$

Here, the usual Sobolev space $H_0^{k-1}(\Omega)$ designates the closure of $\mathcal{C}_0^\infty(\Omega)$ in the usual Sobolev space $H^{k-1}(\Omega)$.

Remark 1. The estimates (55)–(59) show that the method superconverges when $M \cdot n = 0$. In the case $M \cdot n \neq 0$, these estimates do not seem to be valid, although convergence occurs according to Theorem 4.3. We have no estimate of the speed of convergence when $M \cdot n \neq 0$. Nevertheless, the numerical results established in Section 5.2 suggest convergence as $N^{-1/2}$ for $\|U - U_N\|_{W_0^1(\mathbb{R}^3)}$ and as N^{-1} for the energy error when $M \cdot n \neq 0$.

Proof. Firstly, we adopt the following notation: given a function f defined over Ω, we denote by $\tilde{f}$ its extension to $\mathbb{R}^3$ defined as

$$\tilde{f} = \begin{cases} f & \text{in } \ \Omega, \\ 0 & \text{in } \ \mathbb{R}^3\backslash\Omega. \end{cases}$$

The following lemma is due to Giroire [43] :

Lemma 4.5. *Let* $m \geqslant 1$ *and* $\ell \geqslant 1$ *be two integers. Then, the Laplace operator* Δ *defined by*

$$\Delta : \ W^{1+m}_{\ell+m}(\mathbb{R}^3) \to W^{-1+m}_{\ell+m}(\mathbb{R}^3) \perp \mathbb{P}^\Delta_{\ell-1},$$

is an isomorphism. Here $\mathbb{P}^\Delta_{\ell-1} = \{p \in \mathbb{P}_{\ell-1} \mid \Delta p = 0\}$ *and*

$$W^{-1+m}_{\ell+m}(\mathbb{R}^3) \perp \mathbb{P}^\Delta_{\ell-1} = \left\{ f \in W^{-1+m}_{\ell+m}(\mathbb{R}^3) \mid \int_{\mathbb{R}^3} f q dx = 0 \ \text{ for all } \ q \in \mathbb{P}^\Delta_{\ell-1} \right\}.$$

Assume now that div $M \in L^2(\Omega)$ and $M \cdot n = 0$ on $\partial\Omega$. Then, U is solution of the problem

$$\Delta U = \widetilde{\text{div}\ M} \text{ in } \mathbb{R}^3. \tag{60}$$

Since

$$\int_{\mathbb{R}^3} (1 + |x|^2)|\widetilde{\text{div}\ M}|^2 dx = \int_\Omega (1 + |x|^2)|\text{div}\ M|^2 dx \leqslant c(\Omega)\|\text{div}\ M\|^2_{L^2(\Omega)},$$

we deduce that $\widetilde{\text{div}\ M} \in W_2^0(\mathbb{R}^3)$. We also have

$$\int_{\mathbb{R}^3} \widetilde{\text{div}\ M} dx = \int_\Omega \text{div}\ M dx = 0.$$

In view of condition (57) and Lemma 4.5, we deduce that $U \in W_2^2(\mathbb{R}^3)$. If in addition div $M \in H_0^{k-1}(\Omega)$ for some $k \geqslant 1$ and if M satisfies condition (57) when $k \geqslant 2$, then $\widetilde{\text{div}\ M} \in W_s^{k-1}(\mathbb{R}^3)$ for any real number s (since $\widetilde{\text{div}\ M}$ vanishes outside Ω). In particular, $\widetilde{\text{div}\ M} \in W^{k-1}_{2k}(\mathbb{R}^3)$. By Green's formula, we also have

$$\forall q \in \mathbb{P}^\Delta_{k-1}, \ \int_{\mathbb{R}^3} \widetilde{\text{div}\ M} q dx = \int_\Omega \text{div}\ M q dx = -\int_\Omega M \cdot \nabla q dx = 0.$$

Hence, $U \in W^{k+1}_{2k}(\mathbb{R}^3)$, thanks to Lemma 4.5. Moreover, there exists a constant C_k depending only on k such that

$$\|U\|_{W^{k+1}_{2k}(\mathbb{R}^3)} \leqslant C_k \|\widetilde{\text{div } M}\|_{W^{k-1}_{2k}(\mathbb{R}^3)} \leqslant \tilde{C}_k \|\text{div } M\|_{H^{k-1}(\Omega)}. \tag{61}$$

Let π_N be the orthogonal projector on H_N with respect to the scalar product associated to the norm $|.|_{W^1_0(\mathbb{R}^3)}$. The following result is due to Boulmezaoud et al. [35]:

Lemma 4.6. *Assume that* $v \in W^{k+1}_{2k}(\mathbb{R}^3)$ *for some integer* $k \geqslant 0$. *Then,*

$$\|\nabla v - \nabla(\pi_N v)\|_{L^2(\mathbb{R}^3)^3} \leqslant C^\star_k N^{-k} \|v\|_{W^{k+1}_{2k}(\mathbb{R}^3)}, \tag{62}$$

where $C^\star_k$ *is a constant which depends neither on* N *nor on* v.

We know that $U_N = \pi_N U$. The inequalities (55) and (56) result from (62) and (61) with $k = 1$ and from (34). The inequalities (58) and (59) are deduced in a similar way. □

Remark 2. Assumption $M \cdot n = 0$ on $\partial\Omega$ means that the effective magnetic charges are zero. One can easily see that if $M \cdot n \neq 0$ on $\partial\Omega$ then U does not belong to $W^2_2(\mathbb{R}^3)$. Indeed, Equation (6) can be rewritten as

$$\begin{cases} \Delta u = \text{div } M & \text{in } \Omega, \\ \Delta u = 0 & \text{in } \mathbb{R}^3 \backslash \overline{\Omega}, \\ [u] = 0 & \text{on } \partial\Omega, \\ \left[\frac{\partial u}{\partial n}\right] = -M \cdot n & \text{on } \partial\Omega, \end{cases}$$

where n is the exterior normal on $\partial\Omega$. Thus, $\left[\frac{\partial u}{\partial n}\right] \neq 0$ on $\partial\Omega$ and $U \notin W^2_2(\mathbb{R}^3)$.

5 | IMPLEMENTATION AND COMPUTATIONAL TESTS

The first purpose of this section is to examine the numerical results obtained after implementation of the method suggested in the previous section and to check whether the theoretical error estimates are confirmed numerically and whether they are optimal. Another goal is to give some additional details regarding the implementation of the method, including the calculation of integrals. It is worth noting at this early stage that despite the three-dimensional nature of the problem, and despite the fact that it is posed in an open domain, the implementation of the method remains rather easy and fast.

5.1 | Additional details about gradients of the functions $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$

Formulas in Theorem 3.2 as well as the approximation method proposed in Section 4.1 involve functions $(\mathscr{W}_\alpha)_\alpha$ by their gradients, particularly in the integral coefficients

$$\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx. \tag{63}$$

In practice, during the implementation of the method, the precise calculation of these gradients could be of great importance. It is consequently preferable to compute them by exact analytical expressions and not by discretization of the differentiation operators. Of course, one can use Green's formula in (63) to make these gradients disappear:

$$\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx = -\int_\Omega (\text{div } M)\mathscr{W}_\alpha dx + \langle M \cdot n, \mathscr{W}_\alpha \rangle_{\partial\Omega}, \tag{64}$$

($\langle ., . \rangle_{\partial\Omega}$ designates the duality pairing between $H^{1/2}(\partial\Omega)$ and $H^{-1/2}(\partial\Omega)$). However, this requires a little more regularity on the magnetization vector field M (e.g., that div $M \in L^2(\Omega)$), and moreover, it makes surface integrals appear unless $M \cdot n = 0$ on $\partial\Omega$. Apart from the latter case, where formula (64) may be used, we prefer to calculate the integrals (63) directly, without any additional assumptions on M. It will therefore not be useless to spell out the gradients $(\nabla \mathscr{W}_\alpha)_\alpha$.

Actually, in view of (18) and (25), these gradients are not quite easy to calculate, especially because of the special functions that appear in their formulas (i.e., Chebyshev polynomials and associated Legendre functions of Legendre).

In this paragraph, we deduce simpler and exact expressions to the gradients of the functions $(\mathscr{W}_\alpha)_\alpha$, in order to facilitate the computation of magnetic potential and the stray-field energy by formulas (45) and (43).

The starting point is the following proposition

Proposition 5.1. *For $\alpha \in \Lambda$ and $x \in \mathbb{R}^3$:*

$$\nabla \mathscr{W}_\alpha(x) = (1-\xi_4)^{1/2}(\mathscr{V}_\alpha(\xi) - \frac{1}{2}\mathscr{Y}_\alpha(\xi)\hat{\xi}), \tag{65}$$

where $\xi = (\xi_1, \xi_2, \xi_3, \xi_4) = \pi^{-1}(x) \in \mathbb{S}^3$, $\hat{\xi} = (\xi_1, \xi_2, \xi_3)$, (ϕ, θ, χ) are the spherical coordinates of ξ (see (17)) and

$$\mathscr{V}_\alpha(\xi) = (1-\cos\chi)\begin{pmatrix} -\sin\phi & \cos\phi\cos\theta & -\cos\phi\sin\theta \\ \cos\phi & \sin\phi\cos\theta & -\sin\phi\sin\theta \\ 0 & -\sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} \frac{1}{\sin\theta\sin\chi}\frac{\partial\mathscr{Y}_\alpha}{\partial\phi}(\xi) \\ \frac{1}{\sin\chi}\frac{\partial\mathscr{Y}_\alpha}{\partial\theta}(\xi) \\ \frac{\partial\mathscr{Y}_\alpha}{\partial\chi}(\xi) \end{pmatrix}. \tag{66}$$

By the sake of simplicity, proof of Proposition 5.1 is postponed to Appendix A.

Remark 3. In Proposition 5.1, $\frac{\partial\mathscr{Y}_\alpha}{\partial\phi}$, $\frac{\partial\mathscr{Y}_\alpha}{\partial\theta}$, and $\frac{\partial\mathscr{Y}_\alpha}{\partial\chi}$ designate (abusively) the derivatives of $\mathscr{Y}_\alpha$ considered as a function of θ, ϕ, and χ.

At this stage, all that remains is the calculation of the partial derivatives

$$\frac{\partial\mathscr{Y}_\alpha}{\partial\phi}, \ \frac{\partial\mathscr{Y}_\alpha}{\partial\theta} \text{ and } \frac{\partial\mathscr{Y}_\alpha}{\partial\chi}.$$

In view of formula (18), the first two ones can be easily expressed in terms of derivatives of spherical harmonics on $\mathbb{S}^2$. For example, if $\alpha = (k, \ell, m)$, then

$$\begin{aligned} \frac{\partial\mathscr{Y}_\alpha}{\partial\phi}(\xi) &= \frac{1}{\sqrt{a_{k,\ell}}}(\sin\chi)^\ell T_{k+1}^{(\ell+1)}(\cos\chi)\frac{\partial Y_{\ell,m}}{\partial\phi}(\phi,\theta), \\ &= -\frac{m}{\sqrt{a_{k,\ell}}}(\sin\chi)^\ell T_{k+1}^{(\ell+1)}(\cos\chi) Y_{\ell,-m}(\phi,\theta). \end{aligned} \tag{67}$$

In order to avoid division by zero in (66) (when $\sin\theta = 0$), which is useless, one can employ in the definition (19) of $Y_{\ell,-m}$ the recurrence relation concerning associated Legendre functions:

$$2mK_\ell^m(\cos\theta) = \sin\theta\left(\tau_{\ell,m}K_{\ell+1}^{m+1}(\cos\theta) + \tau_{\ell,-m}K_{\ell+1}^{m-1}(\cos\theta)\right), \tag{68}$$

with

$$\tau_{\ell,m} = \sqrt{(\ell+m+2)(\ell+m+1)} \text{ for } -\ell \leqslant m \leqslant \ell.$$

Thus, for $m \neq 0$, we have

$$\begin{aligned} \frac{2|m|}{\sin\theta}\frac{\partial\mathscr{Y}_\alpha}{\partial\phi}(\xi) = &-m\frac{\eta_\ell}{\sqrt{a_{k,\ell}}}(\sin\chi)^\ell T_{k+1}^{(\ell+1)}(\cos\chi) y_{-m}(\phi) \\ &\left(\tau_{\ell,|m|}K_{\ell+1}^{|m|+1}(\cos\theta) + \tau_{\ell,-|m|}K_{\ell+1}^{|m|-1}(\cos\theta)\right). \end{aligned} \tag{69}$$

Similarly, we have

$$\begin{aligned} \frac{\partial\mathscr{Y}_\alpha}{\partial\phi}(\xi) = &\frac{\eta_\ell}{\sqrt{a_{k,\ell}}}(\sin\chi)^\ell T_{k+1}^{(\ell+1)}(\cos\chi) \\ &\left(c_{\ell,-|m|}K_\ell^{|m|-1}(\cos\theta) - c_{\ell,|m|}K_\ell^{|m|+1}(\cos\theta)\right) y_m(\phi), \end{aligned} \tag{70}$$

where

$$c_{\ell,m} = \frac{1}{2}\sqrt{(\ell - m)(\ell + m + 1)} \text{ for } \ell \geqslant 0 \text{ and } -\ell \leqslant m \leqslant \ell. \tag{71}$$

Note that we used the following recurrence relation:

$$(\sin\theta)(K_\ell^m)'(\cos\theta) = c_{\ell,m}K_\ell^{m+1}(\cos\theta) - c_{\ell,-m}K_\ell^{m-1}(\cos\theta). \tag{72}$$

(and with the convention $K_\ell^j = 0$ when $|j| > \ell$). Hence,

$$\begin{aligned}\frac{\partial \mathcal{Y}_\alpha}{\partial\theta}(\xi) = &\frac{\eta_\ell}{\sqrt{a_{k,\ell}}}(\sin\chi)^\ell T_{k+1}^{(\ell+1)}(\cos\chi)\\ &\left(c_{\ell,-|m|}K_\ell^{|m|-1}(\cos\theta) - c_{\ell,|m|}K_\ell^{|m|+1}(\cos\theta)\right) y_m(\phi).\end{aligned} \tag{73}$$

Finally, we also have

$$\frac{\partial \mathcal{Y}_\alpha}{\partial\chi}(\xi) = \frac{(\sin\chi)^{\ell-1}}{\sqrt{a_{k,\ell}}}Y_{\ell,m}(\phi,\theta)\left(\ell\cos(\chi)T_{k+1}^{(\ell+1)}(\cos\chi) - (\sin\chi)^2 T_{k+1}^{(\ell+2)}(\cos\chi)\right), \tag{74}$$

for all $\alpha = (k, \ell, m) \in \Lambda$.

By using these expressions of partial derivative of functions $(\mathcal{Y}_\alpha)$ in (65), we obtain a complete formula which is readily available for practical use and for implementation.

5.2 | Computational tests and numerical validation

In this section, the focus is on some numerical results that allow to assess the practical usability of formulas (36) and (37) and the performances of the resulting numerical method outlined in Section 3. Three different examples are investigated in the following. In the first example, we deal with nonhomogeneously magnetized spherical domain for which we have an error estimate by Theorem 4.4. In the two last examples, the domain is homogeneously magnetized. In the three cases, we derive expressions of the exact stray field, to which the numerical solution is compared. In all these computational tests, we set $\mu_0 = 1$.

5.3 | Example 1: A nonhomogeneously magnetized sphere with $M.n = 0$

We prefer starting numerical experiments with the case of a nonhomogeneously magnetized spherical sample, that is,

$$\Omega = \{x \in \mathbb{R}^3 \mid |x| < r_0\}$$

and

$$M = (\cos\theta)e_\varphi + (\sin\theta)e_\theta \text{ in } \Omega. \tag{75}$$

It may be noted that M is complying with Heisenberg–Weiss constraint (3) since $|M| = 1$ in Ω. Besides, M is tangential on the boundary of Ω since $M \cdot n = 0$ on $\partial\Omega$ (here $n(x) = x/|x|$). We are able to give an analytical expression of the exact solution (see earlier studies [32, 33]). More precisely,

$$U(x) = \begin{cases} -\frac{2z}{9} + \frac{2z}{3}\ln\left(\frac{|x|}{r_0}\right) & \text{if } |x| \leqslant r_0,\\ -\frac{2{r_0}^3 z}{9|x|^3} & \text{if } |x| \geqslant r_0.\end{cases} \tag{76}$$

The exact stray-field energy is given by

$$\mathcal{E}_{sf}(U) = \frac{\mu_0}{2}\int_{\mathbb{R}^3}|\nabla U|^2 dx = \frac{16}{81}\pi {r_0}^3. \tag{77}$$

TABLE 1 The exact and the approximate stray-field energy due to a nonhomogeneously magnetized sphere (Example 1).

N	$\mathscr{E}_{sf}(\boldsymbol{u})$	$\mathscr{E}_{sf}(\boldsymbol{u_N})$	$\frac{\lvert\mathscr{E}_{sf}(\boldsymbol{u})-\mathscr{E}_{sf}(\boldsymbol{u_N})\rvert}{\mathscr{E}_{sf}(\boldsymbol{u})}$	$\boldsymbol{e_0(H_d)}$
10	0.07757018	0.07696625	7.78E-3	8.82E-2
20	-	0.07750001	9.03E-4	3.00E-2
30	-	0.07754315	3.48E-4	1.86E-2
40	-	0.07756016	1.29E-4	1.13E-2
50	-	0.07756414	7.79E-5	8.82E-3
60	-	0.07756708	4.00E-5	6.32E-3
The log. slope			−2.90	−1.45

Here, we choose $r_0 = 1/2$. In Table 1, we outline the computed stray-field energy (43) for several values of N (considered as a discretization parameter). We also outline the relative L^2 error on the stray field $H_d = -\nabla U$ defined by

$$e_0(H_d) = \frac{|U_N - U|_{W_0^1(\mathbb{R}^3)}}{|U|_{W_0^1(\mathbb{R}^3)}}.$$

We can then observe that the error $e_0(H_d)$ decreases in as $N^{-1.45}$. This is in accordance with Proposition 4.3 in which it is forecasted that

$$|U - U_N|_{W_0^1(\mathbb{R}^3)} \leqslant CN^{-1}\|\text{div } M\|_{L^2(\Omega)}.$$

Actually, the solution u belongs $W_2^2(\mathbb{R}^3)$ since div $M \in L^2(\Omega)$ and $M \cdot n = 0$ on $\partial\Omega$. There is even a superconvergence with respect to this estimate. Note also that the error on the stray field energy decreases as $N^{-2.90}$ (in agreement with the identity $|\mathscr{E}_{sf}(U) - \mathscr{E}_{sf}(U_N)| = |U - U_N|^2_{W_0^1(\mathbb{R}^3)^3}$).

5.4 | Example 2: A homogeneously magnetized sphere

In this second benchmark test, we consider a spherical sample

$$\Omega = \{x \in \mathbb{R}^3 \mid |x| < r_0\}$$

with a constant magnetization $M = M_0$. It is easy to prove that the exact solution of (6) is given by the formula:

$$U(x) = \begin{cases} \frac{1}{3}M_0 \cdot x & \text{if } |x| < r_0, \\ \frac{r_0{}^3}{3}\frac{M_0 \cdot x}{|x|^3} & \text{if } |x| \geqslant r_0. \end{cases} \tag{78}$$

The exact energy is

$$\mathscr{E}_{sf}(U) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla U|^2 dx = -\frac{1}{2}\int_{\Omega} M_0 \cdot h dx = \frac{2\pi|M_0|^2}{9} r_0{}^3. \tag{79}$$

Here, we choose $M_0 = (0, 0, 1)$ and $r_0 = 0.5$. Thus,

$$\mathscr{E}_{sf}(u) = \frac{\pi}{36} = 0.08726646.$$

It may be observed that $\left[\frac{\partial U}{\partial n}\right] = -M_0.n \neq 0$ on $\partial\Omega$. Thus, $U \notin W_2^2(\mathbb{R}^3)$ although $U_{|\Omega} \in H^2(\Omega)$ and $U_{|\mathbb{R}^3\backslash\overline{\Omega}} \in W_2^2(\mathbb{R}^3\backslash\overline{\Omega})$ (here $U_{|\Omega}$ and $U_{|\mathbb{R}^3\backslash\overline{\Omega}}$ designate the restrictions of U to Ω and to $\mathbb{R}^3\backslash\overline{\Omega}$, respectively). We are therefore not within the validity assumptions of Theorem 4.4, and the error estimates (55) and (56) are no longer necessarily true.

In Table 2, the approximate energy $\mathscr{E}_{sf}(U_N)$ is given for several values of the discretization parameter N. We also compute the relative L^2 error on the stray field $H_d = -\nabla U$. One can observe that this error decreases as $N^{-0.46}$. The error on the energy decreases as $N^{-0.93}$.

Here again, convergence of the approximate solution to the exact one holds although the normal component of $h = -\nabla U$ is not continuous across the boundary of the sample.

TABLE 2 The exact and the approximate stray-field energy due to a homogeneously magnetized sphere (Example 2).

N	$\mathscr{E}_{sf}(u)$	$\mathscr{E}_{sf}(u_N)$	$\frac{\lvert\mathscr{E}_{sf}(u)-\mathscr{E}_{sf}(u_N)\rvert}{\mathscr{E}_{sf}(u)}$	$e_0(H_d)$
10	0.08726646	0.07845252	10.10E-2	0.3153
20		0.08252939	5.42E-2	0.2322
30	-	0.08402011	3.72E-2	0.1924
40	-	0.08479348	2.83E-2	0.1680
50	-	0.08526692	2.29E-2	0.1511
60	-	0.08558669	1.92E-2	0.1385
The log. slope			−0.93	−0.46

TABLE 3 The exact and the approximate stray-field energy due to an homogeneously magnetized cube (Example 3).

N	$\mathscr{E}_{sf}(u)$	$\mathscr{E}_{sf}(u_N)$	$\frac{\lvert\mathscr{E}_{sf}(u)-\mathscr{E}_{sf}(u_N)\rvert}{\mathscr{E}_{sf}(u)}$	$e_0(H_d)$
10	0.16666666	0.14711046	0.1173	0.3397
20	-	0.15617466	6.3E-2	0.2499
30	-	0.15951131	4.2E-2.	0.2066
40	-	0.16123614	3.2E-2	0.180
50	-	0.16229007	2.62E-2	0.1618
60	-	0.16300181	2.19E-2	0.1481
The log. slope			−0.94	−0.47

5.5 | Example 3: Homogeneously magnetized cube.

In this last test, we change the geometry of the sample, and we consider a homogeneously magnetized cubic rod $\Omega =]-\gamma, \gamma[^3$, with $\gamma = 1/2$, and $M = (0, 1, 0)$. The stray-field energy in this case is (see, e.g., Abert et al. [44])

$$\mathscr{E}_{sf}(U) = \frac{1}{6}. \tag{80}$$

The exact analytical expression of the demagnetizing field is (see Engel-Herbert and Hesjedal [45]):

$$\begin{aligned} H_d(x) = & \frac{1}{4\pi}\left(\sum_{k,\ell,m=1}^{2}(-1)^{k+\ell+m}\ln(z+(-1)^m\gamma+\varrho)\right)e_x, \\ & -\frac{1}{4\pi}\left(\sum_{k,\ell,m=1}^{2}(-1)^{k+\ell+m}\arctan\left(\frac{(x+(-1)^k\gamma)(z+(-1)^m\gamma)}{(y+(-1)^\ell\gamma)\varrho}\right)\right)e_y, \\ & +\frac{1}{4\pi}\left(\sum_{k,\ell,m=1}^{2}(-1)^{k+\ell+m}\ln(x+(-1)^k\gamma+\varrho)\right)e_z, \end{aligned}$$

where $\varrho = \sqrt{(x+(-1)^k\gamma)^2+(y+(-1)^\ell\gamma)^2+(z+(-1)^m\gamma)^2}$.

It may be observed that $M \cdot n \neq 0$ on $\partial\Omega$. Thus, $U \notin W_2^2(\mathbb{R}^3)$ (see Remark 2). The numerical results summarized in Table 3 confirm the convergence of the method and show that here too the L^2 error on the stray field H_d decreases as $N^{-0.47}$, while the error on the energy decreases like $N^{-0.97}$.

6 | CONCLUSION AND PERSPECTIVES

Formula (36), in addition to being original, has several advantages both theoretically and numerically. From a computational point of view, it has been established that the formula inspires a particularly efficient and easy to implement numerical method to calculate the demagnetizing field and the associated energy. Indeed, the numerical results show a rapid convergence of the method. When $M \cdot n = 0$ on $\partial\Omega$, the observed convergence is even faster than that predicted by the error estimate in Theorem 4.4 since the convergence in energy is of order close to $O\left(\frac{1}{N^3}\right)$. This suggests that these estimates are not optimal and could possibly be improved theoretically. In the case $M \cdot n \neq 0$, the method also converges in accordance with Theorem 4.3, but one notes that convergence of the energy is of order close to $O\left(\frac{1}{N}\right)$. This fact remains to be proven theoretically.

From a theoretical point of view, one could exploit formula (36) to give a new expression to the functional to be minimized. Actually, the total free energy can be expressed as follows:

$$\begin{aligned} E_{tot}(M) = \alpha \int_\Omega |\nabla M|^2 dx + \int_\Omega \phi(M) dx - \mu_0 \int_\Omega H_{ex} \cdot M dx \\ + \sum_{k=0}^{\infty} \frac{2\mu_0}{4(k+1)^2 - 1} \sum_{\alpha \in \Lambda_k} \left(\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx \right)^2 + E_s. \end{aligned} \tag{81}$$

It is well-known that the minimization of the functional E_{tot} with respect to the variable M under Heisenberg–Weiss constraint (3) leads to the following partial differential equation (see, e.g., Hubert & Schäfer [3] and references therein):

$$-2\alpha \Delta M + \nabla_M \phi(M) - \mu_0 (H_d + H_{ext}) = \lambda M \text{ in } \Omega, \tag{82}$$

where λ is a Lagrangian multiplier. By the sake of simplicity, we assumed here that $E_s = 0$ (the reader can refer to, e.g., Hubert & Schäfer [3] for the general equations taking into account this term).

Formula (36) simplifies system (82) and reduces it to only one equation

$$\begin{aligned} -2\alpha \Delta M + \nabla_M \phi(M) - \mu_0 H_{ext} \\ + \mu_0 \sum_{k=0}^{\infty} \sum_{\alpha \in \Lambda_k} \frac{2}{4(k+1)^2 - 1} \left(\int_\Omega M \cdot \nabla \mathscr{W}_\alpha dx \right) \nabla \mathscr{W}_\alpha = \lambda M \text{ in } \Omega. \end{aligned} \tag{83}$$

The study of this nonlocal PDE could provide new information about the best configuration minimizing the functional E_{tot}. If we truncate the series on the left-hand side, keeping only the first term, we obtain the simplified approximate nonlocal equation:

$$-2\alpha \Delta M + \nabla_M \phi(M) - \mu_0 H_{ext} + \frac{2\mu_0}{3\pi^2 (|x|^2+1)^{3/2}} \left(\int_\Omega \frac{M.x}{(|x|^2+1)^{3/2}} dx \right) x = \lambda M \text{ in } \Omega. \tag{84}$$

The study of this kind of equations is beyond the scope of this paper; it will be the subject of a forthcoming paper.

In addition, it should be pointed out that the author, together with a co-author, has introduced another fundamentally different method for solving the same problem numerically; this is the inverted finite element method (see Boulmezaoud & Kaliche [33]). Nevertheless, both methods share the same functional framework (weighted Sobolev spaces). The comparison of these methods with each other and with other existing methods in the literature will be the subject of another paper. Here, the emphasis is on the originality of formulas (9) and (10) and on their applications.

AUTHOR CONTRIBUTIONS

Tahar Zamene Boulmezaoud: Conceptualization; investigation; writing—original draft; methodology; validation; visualization; writing—review and editing; software; project administration; formal analysis; data curation; supervision; resources.

CONFLICT OF INTEREST STATEMENT

This work does not have any conflicts of interest.

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APPENDIX A: PROOF OF PROPOSITION 5.1

The objective here is to prove formula (65). Let Y be an arbitrary smooth function defined on $\mathbb{S}^3$ and set

$$W(x) = \left(\frac{2}{|x|^2+1}\right)^{1/2} Y(\pi^{-1}(x)),$$

(thus, if $Y = \mathscr{Y}_\alpha$, $\alpha \in \Lambda$, then $W = \mathscr{W}_\alpha$). In Arar and Boulmezaoud [34] and Boulmezaoud et al. [35] (formula A.9), the authors prove the following identity (linking the gradient of W to Y and its tangential derivatives on the unit sphere):

$$\nabla W(x) = (1-\xi_4)^{1/2}\left(S(\xi)\nabla_\xi Y(\xi) - \frac{1}{2}Y(\xi)\hat{\xi}\right), \quad \text{for } x \in \mathbb{R}^3, \tag{A1}$$

where $\xi = \pi^{-1}(x) \in \mathbb{S}^3$, $\hat{\xi} = (\xi_1, \xi_2, \xi_3)$ is the orthogonal projection of $\xi = (\xi_1, \xi_2, \xi_3, \xi_4)$ on $\mathbb{R}^3$, $\nabla_\xi Y$ is the tangential gradient of Y on $\mathbb{S}^3$ and $S(\xi)$ is the 3×4 rectangular matrix

$$\begin{aligned} S(\xi) &= \begin{pmatrix} 1-\xi_4 & 0 & 0 & \xi_1 \\ 0 & 1-\xi_4 & 0 & \xi_2 \\ 0 & 0 & 1-\xi_4 & \xi_3 \end{pmatrix} \\ &= \begin{pmatrix} 1-\cos\chi & 0 & 0 & \cos\phi\sin\theta\sin\chi \\ 0 & 1-\cos\chi & 0 & \sin\phi\sin\theta\sin\chi \\ 0 & 0 & 1-\cos\chi & \cos\theta\sin\chi \end{pmatrix}. \end{aligned} \tag{A2}$$

It remains to spell out the expression of the tangential gradient $\nabla_\xi Y(\xi)$ in terms of partial derivatives of Y with respect to ϕ, θ and χ, the spherical coordinates of ξ (see Section 2). We state this as follows.

Lemma .1. *If* $\sin\chi \neq 0$*, then*

$$\nabla_\xi Y(\xi) = \frac{1}{\sin\chi}\begin{pmatrix} -\sin\phi & \cos\phi\cos\theta & \cos\phi\sin\theta\cos\chi \\ \cos\phi & \sin\phi\cos\theta & \sin\phi\sin\theta\cos\chi \\ 0 & -\sin\theta & \cos\theta\cos\chi \\ 0 & 0 & -\sin\chi \end{pmatrix}\begin{pmatrix} \frac{1}{\sin\theta}\frac{\partial\tilde{Y}}{\partial\phi}(\phi,\theta,\chi) \\ \frac{\partial\tilde{Y}}{\partial\theta}(\phi,\theta,\chi) \\ \sin\chi\frac{\partial\tilde{Y}}{\partial\chi}(\phi,\theta,\chi) \end{pmatrix}, \tag{A3}$$

where $\tilde{Y}(\phi, \theta, \chi) = Y(\cos\phi \sin\theta \sin\chi, \sin\phi \sin\theta \sin\chi, \cos\theta \sin\chi, \cos\chi)$.

Proof. Consider the 0-homogeneous function F defined over $\mathbb{R}^4\backslash\{0\}$ by

$$F(y) = Y\left(\frac{y}{|y|}\right), \ y \in \mathbb{R}^4\backslash\{0\}.$$

It follows that

$$\nabla_\xi Y(\xi) = \nabla F(\xi) \ \text{for} \ \xi \in \mathbb{S}^3. \tag{A4}$$

In view of Euler's homogeneous function lemma, we have

$$\sum_{i=1}^{4} y_i \frac{\partial F}{\partial y_i}(y) = 0 \text{ for } y \in \mathbb{R}^4\backslash\{0\}. \tag{A5}$$

Since

$$\tilde{Y}(\phi, \theta, \chi) = F(\cos\phi \sin\theta \sin\chi, \sin\phi \sin\theta \sin\chi, \cos\theta \sin\chi, \cos\chi),$$

we deduce that

$$\begin{aligned}
\frac{\partial \tilde{Y}}{\partial \phi}(\phi, \theta, \chi) &= \sin\theta \sin\chi \left(-\sin\phi \frac{\partial F}{\partial y_1}(y) + \cos\phi \frac{\partial F}{\partial y_2}(y)\right), \\
\frac{\partial \tilde{Y}}{\partial \theta}(\phi, \theta, \chi) &= \cos\theta \sin\chi \left(\cos\phi \frac{\partial F}{\partial y_1}(y) + \sin\phi \frac{\partial F}{\partial y_2}(y)\right) \\
&\quad - \sin\theta \sin\chi \frac{\partial F}{\partial y_3}(y), \\
\frac{\partial \tilde{Y}}{\partial \chi}(\phi, \theta, \chi) &= \sin\theta \cos\chi \left(\cos\phi \frac{\partial F}{\partial y_1}(y) + \sin\phi \frac{\partial F}{\partial y_2}(y)\right) \\
&\quad + \cos\theta \cos\chi \frac{\partial F}{\partial y_3}(y) - \sin\chi \frac{\partial F}{\partial y_4}(y),
\end{aligned}$$

where $y = (\cos\phi \sin\theta \sin\chi, \sin\phi \sin\theta \sin\chi, \cos\theta \sin\chi, \cos\chi)$.

Completing these identities with Equation (A5) gives a square linear system in terms of the derivatives $\frac{\partial F}{\partial y_i}(y)$, $1 \leqslant i \leqslant 4$. Inverting this system gives

$$\nabla F(y) = R(\xi) \begin{pmatrix} \frac{\partial \tilde{Y}}{\partial \phi} \\ \frac{\partial \tilde{Y}}{\partial \theta} \\ \frac{\partial \tilde{Y}}{\partial \chi} \\ 0, \end{pmatrix}$$

where

$$R(\xi) = \begin{pmatrix} -\frac{\sin\phi}{\sin\theta \sin\chi} & \frac{\cos\phi \cos\theta}{\sin\chi} & \cos\phi \sin\theta \cos\chi & \cos\phi \sin\theta \sin\chi \\ \frac{\cos\phi}{\sin\theta \sin\chi} & \frac{\sin\phi \cos\theta}{\sin\chi} & \sin\phi \sin\theta \cos\chi & \sin\phi \sin\theta \sin\chi \\ 0 & -\frac{\sin\theta}{\sin\chi} & \cos\theta \cos\chi & \cos\theta \sin\chi \\ 0 & 0 & -\sin\chi & \cos\chi \end{pmatrix}$$

This ends the proof of (A3). Formula (65) is a direct consequence of (A1) and (A3). □

APPENDIX B: THE FIRST FEW THREE-DIMENSIONAL FUNCTIONS $(\mathscr{W}_\alpha)$

In this appendix, we give explicit formulas of the first few three-dimensional $(\mathscr{W}_\alpha)$ functions defined by (25). These functions are illustrated in Table B1.

TABLE B1 Explicit expressions of the first functions $(\mathscr{W}_\alpha)_{\alpha\in\Lambda}$ in $\mathbb{R}^3$.

k	ℓ	m	$\mathscr{W}_{(k,\ell,m)}(x)$
0	0	0	$\pi^{-1}(\lvert x\rvert^2+1)^{-1/2}$
1	0	0	$2\pi^{-1}(\lvert x\rvert^2-1)(\lvert x\rvert^2+1)^{-3/2}$
	1	0	$4\pi^{-1}x_3(\lvert x\rvert^2+1)^{-3/2}$
		1	$4\pi^{-1}x_1(\lvert x\rvert^2+1)^{-3/2}$
		−1	$4\pi^{-1}x_2(\lvert x\rvert^2+1)^{-3/2}$
2	0	0	$\pi^{-1}(3\lvert x\rvert^4-10\lvert x\rvert^2+3)(\lvert x\rvert^2+1)^{-5/2}$
	1	0	$4\sqrt{6}\pi^{-1}x_3(\lvert x\rvert^2-1)(\lvert x\rvert^2+1)^{-5/2}$
		1	$4\sqrt{6}\pi^{-1}x_1(\lvert x\rvert^2-1)(\lvert x\rvert^2+1)^{-5/2}$
		−1	$4\sqrt{6}\pi^{-1}x_2(\lvert x\rvert^2-1)(\lvert x\rvert^2+1)^{-5/2}$
	2	0	$4\sqrt{2}\pi^{-1}(3x_3^2-\lvert x\rvert^2)(\lvert x\rvert^2+1)^{-5/2}$
		1	$8\sqrt{6}\pi^{-1}x_1x_3(\lvert x\rvert^2+1)^{-5/2}$
		2	$4\sqrt{6}\pi^{-1}(x_1^2-x_2^2)(\lvert x\rvert^2+1)^{-5/2}$
		−1	$8\sqrt{6}\pi^{-1}x_2x_3(\lvert x\rvert^2+1)^{-5/2}$
		−2	$8\sqrt{6}\pi^{-1}x_1x_2(\lvert x\rvert^2+1)^{-5/2}$