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A Lie group integrator for the Landau-Lifschitz equation

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1 Introduction

The Landau Lifschitz equation describes the magnetization of a ferromagnetic material. The magnetization is described by a time dependent vector function on $\mathcal{D} \times \mathbb{R}$, where $\mathcal{D} = \mathbb{R}^d$ for d = 1, 2 or 3, depending on the number of spatial dimensions used for the problem at hand.

The Landau-Lifschitz equation is a Hamiltonian partial differential equation with a Poisson structure [5]. Our goal is to numerically solve the Landau-Lifschitz equation given some initial conditions. When choosing such a numerical method it is desireable that conserved quantities, like the total amount of energy of the system, remain conserved as much a possible.

When it comes to choosing a time discretization, there is a strong preference for sympletic methods [5]. For Poisson systems such methods, however, are based on splitting, and they in turn rely on finding an integrable splitting. To avoid the need for finding such an integrable splitting, we will introduce an alternate formulation of the Landau-Lifschitz equation on the Lie group SO^3, the set of orthogonal 3 dimensional matrices. This structure gives rise to a canonical Hamiltonian structure.

In section 2 we will start with the formulation of a Lie-group description of the Landau-Lifschitz equation. We will start this section by introducing the Landau-Lifschitz equation in its traditional form and discuss some of the mathematical problems we can run into if we attempt to use that as a basis for a good numerical solution.

When that is done we reformulate the Landau-Lifschitz equation in terms of a description in SO^3 and derive some of its properties within this context. Before doing that we will first introduce some fundamental concepts in section 3

In section 4 we will show how a numerical method may be implemented based on this Lie group description of the equation. We will describe and derive a method to discretize both space and time, and discuss how we may solve the equations at each time step.

In our fifth section we will apply this numerical method on a so called soliton wave and provide graphs that we have generated based on the general method.

2 The traditional Landau-Lifschitz equation

2.1 The Landau-Lifschitz equation

In this section we will be focussing on the Landau Lifschitz equation. Because we work in a one dimensional domain we will define a function $m : \mathbb{R} \times \mathbb{R} \to \mathbb{R}^3$, where $m(x, t)$ gives the magnetization at position x and time t. Because we are mostly interested in the orientation of the magnetization, we will assume the strength of the magnetization to be identical, and we may as well take it to be constant. Therefore throughout this thesis we will assume that $|m(x, t)| = 1$.

As said in the introduction we will represent the magnetization of a ferromagnetic material by a time dependent vector function $m : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^3$, with d the number of physical dimensions under consideration. This magnetization must obey the Landau-Lifschitz equation [6], that is given by:

$$\frac{\partial m(x,t)}{\partial t} = m \times \Delta m(x,t) + m(x,t) \times Dm(x,t)$$

where Δ is the Laplace operator over the spatial dimensions and D is a 3×3 diagonal matrix with non negative elements. This equation is an example of a Hamiltonian partial differential equation with Poisson structure. The total energy of such a system is given in terms of it's Hamiltonian, the hamiltionian of this system is given by[reference]:

$$\mathcal{H}(m) = \frac{1}{2} \int_{\mathcal{D}} |\nabla m(x,t)|^2 - m(x,t) \cdot Dm(x,t)$$

And the Poisson structure is given by:

$$\frac{\partial m(x,t)}{\partial t} = -m(x,t) \times \frac{\delta \mathcal{H}}{\delta m}$$

where $\frac{\delta}{\delta m}$ refers to the variational derivative with respect to m. Note that this implies the conservation of energy:

$$\frac{d}{dt}\mathcal{H} = 0$$

as one would expect. Another conserved quantity is the total magnetization, as it can be seen that:

$$\frac{d}{dt}\frac{1}{2}\int_D |m(x,t)|^2 dt = 0$$

2.2 The spatially discrete Landau-Lifschitz equation

Now we will discretize this system.

We begin by discretizing space. For our purposes we will work in one dimension and will assume a periodic domain of length L with N points, with $\Delta x = L/N$ as the distance between them. One could visualize this system as a grid of points where each point has a vector associated to it that tells us about the magnetization at that point, and this vector also changes in time. As such we consider the discrete set of magnetization vectors $m_i(t) = m(x_i, t)$.

Before constructing a discrete version of the Landau-Lifschitz equation we will examine what the second derivative looks like within this discrete context. For any differentiable function in one variable the derivative is simply defined as:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

In similar fashion we take the derivative at m_i with respect to x to be the difference between m_{i+1} and m_i divided over the length of the interval between them. That gives us:

$$m_i' = \frac{m_{i+1} - m_i}{\Delta x},$$

and this gives us a set of first derivatives for i from 1 to N-1. For the second derivative we apply a variation of this formula to obtain:

$$m_i'' = \frac{m_i' - m_{i-1}'}{\Delta x} = \frac{m_{i+1} - 2m_i + m_{i-1}}{\Delta x^2}.$$

Substituting this into the Landau-Lifschitz equation then gives us:

$$\frac{dm_i}{dt} = m_i \times \frac{m_{i+1} - 2m_i + m_{i-1}}{\Delta x^2} - m_i \times Dm_i$$

Using this discretization, we can also reformulate the Hamiltonian and the total magnetization in a spatially discrete form. For the Hamiltonian this gives us:

$$\mathcal{H} = \sum_{i=1}^{N} \frac{1}{2} |\frac{m_{i+1} - m_i}{\Delta x}|^2 + m_i \cdot Dm_i.$$

If we would also like to discretize time we need a sympletic method, but for Hamiltonian systems with Poisson structure(like this one), the only available sympletic methods are based on splitting and that requires us to find an integrable splitting. Such splittings are known [4], however we will introduce the alternate formulation of the Landau-Lifschitz where we write the system in canonical form on SO^3 to make it accessible to standard symplectic Runga-Kutta methods.

And the total magnetization:

$$\mathcal{C} = \frac{1}{2} \sum_{i=1}^{N} ||m_i||^2$$

3 The Landau-Lifschitz equation in SO^3

3.1 Matrix calculus, Lie algebra's and Lie groups

In order to properly derive the Landau-Lifschitz equations, some preliminary results are required. This section will be devoted to establishing these results. In order to do this we must establish some terminology.

In the next sub section we will be working with matrices, and specifically orthonormal matrices. An orthonormal matrix is a square matrix satisfying the condition $A^T A = I$. These matrices form a group under matrix multiplication. This group contains a subgroup SO^n called the special orthogonal group. [9]

A Lie group is a group consisting of a set that is also a smooth manifold, to interpret SO^3 as a manifold we interpret each 3×3 matrix as a 9 dimensional vector, and thus consider SO^3 as a subspace of $\mathbb{R}^9$ with the standard metric, topology and smooth structure.

Because the determinant defines a polynomial function and all polynomials are smooth, SO^3 is a smooth manifold on the set of all 3×3 matrices and therefore a group.

Another important notion we will use is the notion of a Lie Algebra. We will devote some space to introduce this concept, as it will be important for our treatment of the Landau-Lifschitz equation later on.

In the theory of smooth manifolds and Lie groups it's well established that every Lie group has a unique associated Lie Algebra [7]. For the group SO^3 the corresponding Lie algebra is the algebra $so(3)$, the set of skew symmetric matrices, equipped with the commutator operation with $[A, B] = AB - BA$. One of the reasons our formulation in SO^3 will turn out to be so powerful is because this Lie Algebra is isomorphic to $\mathbb{R}^3$ equipped with the cross product!

To see how consider the isomorphism $\widehat{\ }: \mathbb{R}^3 \to so(3)$:

$$\widehat{r} = \begin{bmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{bmatrix}$$

With $r = (x, y, z)^T$. From this we can see that:

$$[r, r'] = rr' - r'r = \begin{bmatrix} 0 & x'y - y'x & x'z - z'x \\ y'x - x'y & 0 & y'z - z'y \\ z'x - x'z & z'y - y'z & 0 \end{bmatrix} = \widehat{r \times r'}$$

In the next section we will use this expression to replace the cross product with matrix notation. But in order to make sense of the Landau-Lifschitz equation in terms of matrices we should first establish how to interpret certain derivatives in the context of a matrix. In the simplest case the matrix is a function of one real variable and we just interpret the derivative with respect to this variable as the matrix that results from evaluating the derivative at every entry. In that case we have:

$$M : \mathbb{R} \to \mathbb{R}^{n\times m}$$

The derivative of M is obtained by differentiating all entries in M with respect to, say, t. In that case $\frac{dM}{dt}_{i,j} = \frac{dM_{i,j}}{dt}$. We will, however, encounter another kind of derivative [1]. As we will see in the next section, some of our expressions will involve the trace of a matrix, and it will be convenient to assign a derivative to these functions, this time with respect to a matrix.

What does it even mean to differentiate with respect to a matrix? Let's consider a function $F : \mathbb{R}^{n\times m} \to \mathbb{R}$. One can interpret this function as a function from an nm dimensional space to $\mathbb{R}$. As such one can consider the partial derivative $\frac{\partial F}{\partial M_{i,j}}$ of such a function. Taken over all i, j, this set of derivatives is used to define a new matrix in $\mathbb{R}^{n\times m}$.

Now we can make sense of derivatives with respect to a particular matrix entry, we have a clear way of assigning a meaning to a derivative with respect to a matrix. In the case of a general function $F : \mathbb{R}^{n\times n} \to \mathbb{R}$ this interpretation gives:

$$\frac{\partial F}{\partial A} = \begin{bmatrix} \frac{\partial F}{\partial A_{1,1}} & \cdots\cdots\cdots & \frac{\partial F}{\partial A_{1,n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial F}{\partial A_{n,1}} & \cdots\cdots & \frac{\partial F}{\partial A_{n,n}} \end{bmatrix}$$

To illustrate this consider the function $F : SO^n \to \mathbb{R}$ with $F(A) = \text{tr}(AB)$. Using the definition of the trace and matrix manipulation we obtain:

$$F(A)_{i,j} = \sum_{l=1}^{n}\sum_{k=1}^{n} A_{l,k}B_{l,j}$$

Differentiating this with respect to $A_{i,j}$ gives:

$$\frac{\partial}{\partial A_{i,j}} \text{tr}(AB) = B_{j,i}$$

Using this definition we can clearly see that:

$$\frac{\partial}{\partial A} tr(AB) = B^T,$$

and by extension:

$$\frac{\partial}{\partial A} tr(A^T B) = B.$$

The expression $\text{tr}(A^T B)$ is also known as the natural inner product on matrices, giving rise to the so called Frobenius norm [2]. This expression will be used in our next section, in order to derive an alternate expression for the Landau-Lifschitz equation.

3.2 Obtaining the Landau-Lifschitz equation

Here we introduce a different point of view. Instead of using a vector centred description of the magnetization we will use a matrix formulation. In the vector centred notation the function $m(x, t)$ told us the magnetization at position x and time t. Alternatively, we can look for a matrix description.

In this section we will derive a matrix form for the Landau-Lifschitz equation. The exact relation between this matrix form and the magnetization vector as described before will be clarified as we develop the theory. Our first order of business is to make sense of the cross product in terms of matrixes.

Let us recall the Landau-Lifschitz equation:

$$\frac{\partial m(x,t)}{\partial t} = m(x,t) \times \Delta m(x,t) + m(x,t) \times Dm(x,t) = m(x,t) \times (\Delta + D)m(x,t)$$

In the previous section we worked out an expression for the cross product in terms of $so(3)$, using this isomorphism we see that the Landau-Lifschitz equation is equivalent to:

$$\frac{\partial \widehat{m}(x,t)}{\partial t} = [\hat{m}(x,t), \hat{v}(x,t)],$$

With $v(x, t) = (\Delta + D)m(x, t)$. Before discretizing this equation, we will reformulate the Landau-Lifschitz equation in yet another form. In order to do this we introduce two quantities, the Langrangian and the Hamiltonian. The action integral is:

$$\mathcal{L} = \frac{1}{2} \int \int_D \text{tr}((q^{-1}\dot{q})\mathcal{A}(q^{-1}\dot{q})^T) dxdt,$$

Where $q(x, t) \in SO^3$ for all $x \in D$ and all $t \in \mathbb{R}$.

We proceed formally to show that the Landau Lifschitz equation arises as a specific case of the action integral where $\mathcal{A}$ is a symmetric operator. Specifically we want this equation to be defined such that the associated Euler-Langrange equations become equivalent to the Landau-Lifschitz equation.

Let the Langrangian L denote the integrand of $\mathcal{L}$. We now formally introduce the quantity:

$$p = \frac{\partial L}{\partial \dot{q}} = (\mathcal{A}(q^{-1}\dot{q})^T q^{-1})^T.$$

Using the expression for the derivative of the trace derived in the previous section and the chain rule, we now define the Hamiltonian via the Legendre transformation:

$$H(q,p) = \frac{1}{2}\int \mathrm{tr}(p^T\dot{q}) - L(q, \dot{q}(q,p))dx$$

And Hamiltons equations then aretaylor2005classical:

$$\dot{q} = \frac{\partial H}{\partial p} = q\mathcal{A}^{-1}q^T p$$
$$\dot{p} = -\frac{\partial H}{\partial q} = -(\mathcal{A}^{-1}(q^T p)^T p^T)^T$$

By manipulating the first equation and using the fact that $q \in SO^3$ we obtain:

$$\frac{\partial}{\partial t}(q^T q) = \dot{q}^T q + q^T \dot{q} = \mathcal{A}^{-1}(p^T q)q^T q + q^T q\mathcal{A}^{-1}(q^T p) = \mathcal{A}^{-1}(p^T q) + \mathcal{A}^{-1}(q^T p) = 0$$

If $\mathcal{A}$ preserves skew symmetry it follows that $p^T q$ must be skew symmetric. From Hamilton's equations we obtain:

$$\frac{\partial}{\partial t}(p^T q) = p^T\dot{q} + \dot{p}^T q = p^T q\mathcal{A}^{-1}q^T p - \mathcal{A}^{-1}(p^T q)^T p^T q = -[p^T q, \mathcal{A}^{-1}q^T p]$$

And this is again equivalent to the Landau-lifschitz equation if we take $\hat{m} = p^T q$ and $\mathcal{A}^{-1} = \Delta + D$. Now the relation between the magnetization vector as established before and our matrices q and p have been clarified. We have now established the theoretical framework necessary for discretizing the Landau-Lifschitz equation within this SO^3 context.

4 A sympletic discretization

In this section we will discretize the Landau-Lifschitz equation as derived in the previous section. We will make a few symplifying assumptions here, throughout this section we will assume that $D = 0$, so $\mathcal{A}^{-1}$ becomes identical to the Laplace operator, and in our case where we study one dimension, it becomes the second derivative operator.

In order to discretize this function we will be using the midpoint rule. Given a differential equation of the form

$$\frac{dy}{dt} = f(y)$$

this gives us a discretization:

$$\frac{y_{n+1} - y_n}{\Delta t} = f(\frac{y_{n+1} + y_n}{2})$$

When we define the shorthand:

$$y_{n+1/2} = \frac{y_{n+1} + y_n}{2}$$

and apply the midpoint rule to the system of differential equations that is equivalent to the Landau-Lifschitz equation we obtain:

$$\begin{cases} \frac{q_{n+1}-q_n}{\Delta t} = q_{n+1/2}\mathcal{A}^{-1}(p^T_{n+1/2}q_{n+1/2})^T \\ \frac{p_{n+1}-p_n}{\Delta t} = -(\mathcal{A}(p^T_{n+1/2}q_{n+1/2})^T p^T_{n+1/2})^T \end{cases}$$

One of the favourable properties of this discretization is that it automatically preserves any quadratic first integral of the equation, and this is a property shared by all Gauss-Legendre collocation methods [3], a class of methods to which the mid point rule is the lowest order member.

Now suppose $I(y) = y^T Ay$ is a quadratic conserved quantity. This would imply that:
$\frac{d}{dt}I(y) = y^T Af(y) = 0$
Inserting $y_{n+1/2}$ in the second equality gives:

$$y_{n+1/2}Af(y_{n+1/2}) = y_{n+1/2}A\frac{y_{n+1} - y_n}{\Delta t} = 0$$

Expanding the right hand side gives:

$$(\frac{y_{n+1} + y_n}{2})^T A(\frac{y_{n+1} - y_n}{\Delta t}) = \frac{y^T_{n+1}Ay_{n+1}}{2\Delta t} - \frac{y^T_n Ay_n}{2\Delta t} =$$

$$\frac{I(y_{n+1}) - I(y_n)}{2\Delta t} = 0$$

As we observed in the previous section $q^T q = I$ and $p^T q$ is skew-symmetric, provided the operator $\mathcal{A}^{-1}$ preserves skew symmetry, witch the partial differential operator to x clearly does. From there we can easily see that this implies that if $q_n^T q_n = I$ then $q_{n+1}^T q_{n+1} = I$ as well. Whenever we start with $q_0 \in SO^3$ we will remain on this manifold. We have seen that $q^T p$ is skew symmetric and the function $f(q,p) = q^T p + p^T q = 0$ is therefore a quadratic first integral of the equations 1-2. Because the midpoint rule is an example of a Gauss-Legendre collocation method, it preserves this quantity, and therefore

$$q_n^T p_n + p_n^T q_n = q_{n+1}^T p_{n+1} + p_{n+1}^T q_{n+1} = 0$$

hence, $q_{n+1} p_{n+1}$ is skew symmetric whenever $q_n^T p_n$ is.

If we take $\widehat{m_n} = p^T q$ we obtain:

$$\frac{\hat{m}_{n+1} - \hat{m}_n}{\Delta t} = [\hat{m}_{n+1/2}, \mathcal{A}^{-1} \hat{m}_{n+1/2}^T]$$

the same expression one would get when applying the midpoint rule directly to the Landau-Lifschitz equation.

In our next section we will apply the numerical method discussed here to an interesting example.

5 Numerical illustration

In this section we will apply the numerical method above to a concrete example, in particular we will look at the behaviour of a so called soliton, also known as a solitary wave [8]. In order to apply the theory we need to construct some initial conditions. We assume D = 0, so the operator $\mathcal{A}^{-1}$ just becomes the Laplacian and this in turn is just the second derivate operator $\frac{\partial^2}{\partial x^2}$ as we work in one dimension.

In our discretization of space we will use a spatial domain of length 30, centred around $x = 0$. So we will be working with the interval $[-15, 15]$, this will be cut into 1000 discrete points, giving us a spatial discretization of length $\Delta x = \frac{30}{1000} = 3 * 10^{-2}$. For the time discretization we will take time steps equal to $\tau = 2 * 10^{-3}$. We will let the time vary between $t = 0$ and $t = 2$, giving us 1000 time steps.

In order to know how our system will evolve in time, it is necessary to give an initial condition at time $t = 0$. As our initial condition we will have some function of x, we will start by specifying the function $m(x, 0)$ and then look for a suitable way to translate this into an initial condition on the matrices p_0 and q_0. In order to make sure that $||m(x, 0)|| = 1$ we will use a parametrization of the unit circle in SO^3 and write down seperate functions of x based on the 2 angle parameters, θ and ϕ.

A parametrization of the unit circle is given by:

$$S(\theta, \phi) = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), cos(\theta))^T$$

Where θ varies from 0 to π and ϕ from 0 to 2π. We will now start defining some functions that will be used to define the initial conditions.

We use the following set of functions to define our initial conditions [8]:

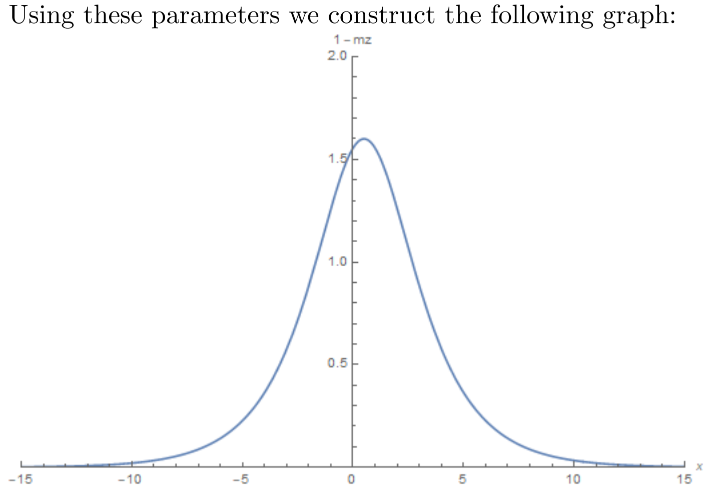
$$\begin{cases} \omega = \frac{V^2}{1-b^2} \\ \eta = x - x_0 \\ \theta = \arccos(1 - 2b^2 \operatorname{sech}(b\sqrt{\omega}\eta)) \\ \phi = 0.5V(x - x_0) + \operatorname{sign}(V) \arctan(\sqrt{(}\omega)\eta) \\ m(x,0) = S(\theta, \phi) \end{cases}$$

This now defines our initial condition. Now we have formulated the initial magnetization it is time to translate this into the language of SO^3, in order to do so we need to define initial matrices $q_0(x)$ and $p_0(x)$ that may depend on x. As long as $p_0^T q_0 = \widehat{m(x,0)}$, as we saw in the previous section this will guarantee that q remains on SO^3 and $p^T q$ remains in so^3. At any point in time we may construct $p^T q = \widehat{m}$ to reconstruct the magnetization vector.

For our purposes we will choose $q_0 = I(3)$, the 3×3 identity matrix and $p_0 = \widehat{m(x,0)}$. With these initial conditions we will use the equations derived from the midpoint rule to evaluate the magnetization at later times. It may be instructive to use this as a basis for plotting the equation.

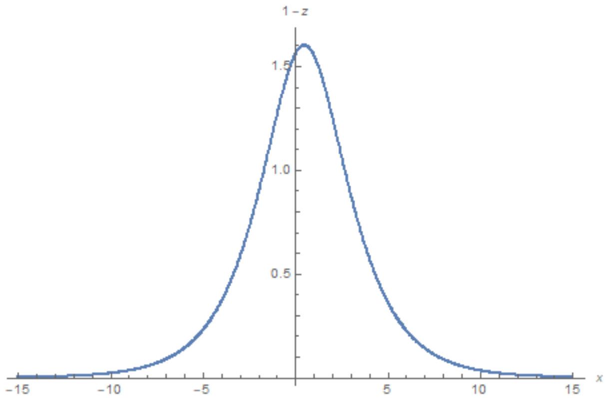
When evaluating the equation we will further assume that $x_0 = 10, V = 0.5, b = 0.8$.

Using these parameters we construct the following graph:

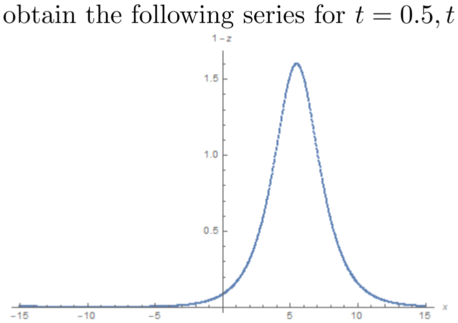


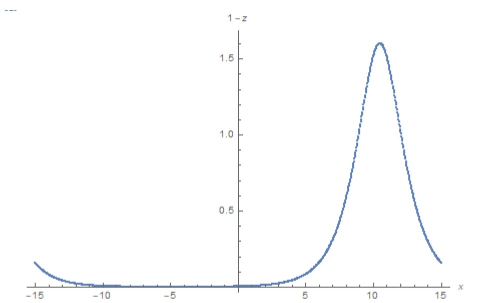
In this graph we have plotted $1 - m_z$ as a function of x, m_z being the z component of the magnetization vector. As we see in this picture this magnetization vector takes the form of a wave. This graph has been made with mathematica using the initial conditions as described.

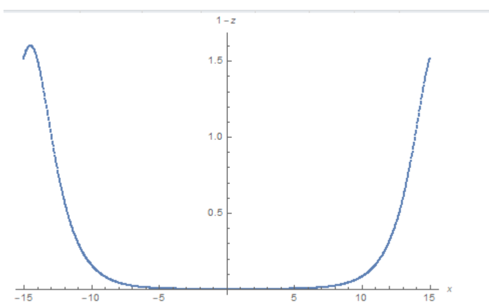
One can also obtain a discrete version of this graph:



As can be seen it is almost identical to the continiuous case, this is a listplot consisting of 1000 data points, each spread apart by $\Delta x = 3 * 10^{-2}$. When numerically evaluating this function for other times, using the midpoint method, we obtain the following series for $t = 0.5, t = 1$ and $t = 1.5$ respectively:







As can be seen in these graphs, the evolution of the function surprisingly acts like a standing wave. This example demonstrates the usefullness of the developed method. The initial condition used here has a relatively simple solution, and there are other methods capable of reproducing this text.

6 Conclusion

In this thesis we have constructed a way of numerically evaluating the Landau-Lifschitz equation based on an SO^3 interpretation of these equations. The reason our method was worth persuing is because the numerical method we used preserved quadratic first integrals of the differential equation. We have applied this method to a soliton wave and we saw this wave never change shape, it merely moved to the right by what seemed to be a constant speed, a result one wouldn't immediately suspect.

By no means has this thesis provided an exhaustive analysis of the Landau-Lifschitz equations in SO^3. We could have applied the method to a system with a different initial condition, what comes to mind is how our method would apply to a set of 2 solitons moving toward one another. One could also investigate the influence the diagonal matrix D would have on the dynamics of such systems, or perhaps introduce more than one spatial dimension and consider dynamical systems in a 2 or 3 dimensional space of magnetization vectors.

This thesis was like a proof of concept, an investigation into SO^3 to see if it could contribute anything usefull to the study of the Landau-Lifschitz equation. The method worked quite succesfully on the example we constructed, it would be interesting to see if we could push this further.

References

[1] Randal J Barnes. Matrix differentiation. *Springs Journal*, pages 1–9, 2006.

[2] Stephen Boyd and Lieven Vandenberghe. *Introduction to Applied Linear Algebra: Vectors, Matrices, and Least Squares*. Cambridge university press, 2018.

[3] Jason Frank. First integrals. `http://www.staff.science.uu.nl/~frank011/Classes/numwisk/ch14.pdf`.

[4] Jason Frank. Geometric space–time integration of ferromagnetic materials. *Applied numerical mathematics*, 48(3-4):307–322, 2004.

[5] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*, volume 31. Springer Science & Business Media, 2006.

[6] LD Landau and EM Lifshitz. On the theory of the dispersion of magnetic permeability in ferromagnetic bodies. z. sowjetunion, 8 (1935), reproduced in collected papers of ld landau, 1965.

[7] John M Lee. *Introduction to smooth manifolds*. Springer, 2001.

[8] J Tjon and Jon Wright. Solitons in the continuous heisenberg spin chain. *Physical Review B*, 15(7):3470, 1977.

[9] Christopher Triola. *Special orthogonal groups and rotations*. PhD thesis, Ph. D. dissertation, University of Mary Washington, 2009.