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On symplectic and isospectral integration of the stationary Landau–Lifshitz (Neumann oscillator) equation

Saša Krešić–Jurić* and Tea Martinić–Bilać

Faculty of Science, University of Split, Rudjera Boškovića 33, HR-21 000 Split, Croatia

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Abstract. In this paper, we discuss numerical integration of the stationary Landau–Lifshitz (LL) equation. Using a Lax pair representation of the LL equation, we propose an isospectral algorithm that preserves the geometric structure of the system. The algorithm computes a discrete flow of a pair of matrices satisfying Lax–type equations and projects the flow on the phase space of the system. Since the stationary LL equation is equivalent to an integrable Hamiltonian system on the cotangent bundle of the unit sphere, we show that it can also be integrated by a symplectic method for constrained Hamiltonian systems. Comparison of the two methods demonstrates that they are similar in terms of accuracy and stability over long–time integration, but the isospectral method is much faster since it avoids solving a system of nonlinear equations required at each iteration of the symplectic algorithm.

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1. Introduction

The Landau–Lifshitz (LL) equation is an important integrable system given by the partial differential equation:

$$S_t = S \times S_{xx} + S \times JS, \quad S \in \mathbb{R}^3, \quad \|S\| = 1, \tag{1}$$

where $S = S(x,t)$ is a unit vector and $J = \mathrm{diag}(J_1, J_2, J_3)$ is a constant diagonal matrix. Equation (1) describes classical spin waves in a ferromagnetic crystal with magnetization vector S and J characterizes the interaction anisotropy [14]. In this model, the ferromagnetic crystal is assumed to have one distinguished axis (such as a stretched wire), which is the axis of easiest magnetization. The crystal consists of layers called domains, which are magnetized to saturation parallel to this axis in opposite directions. Between two domains there is an intermediate region in which the direction of the magnetic moment S changes from one domain to the next. The length of the vector S is equal to the saturation moment which is normalized to one. If the axis perpendicular to the layers is labelled by x, then the time evolution of

*Corresponding author. *Email addresses:* skresic@pmfst.hr (S. Krešić–Jurić), teamar@pmfst.hr (T. Martinić–Bilać)

S is given by (1). We note that equation (1) remains invariant if the interaction constants J_i are replaced by $J_i + C$, hence we may assume that $J_i > 0$ for $i = 1, 2, 3$.

Integrability of the Landau–Lifshitz equation has been studied extensively in the literature. We refer the reader to [9] for a comprehensive review, and mention here only a few key results. The LL equation admits a zero–curvature representation with spectral parameter lying on a torus [24, 6]. Using this representation, it was shown in [8] that the LL equation can be integrated by an analogue of the Birkhoff factorization for elliptic curves. The inverse scattering method for the LL equation was developed in [17] and [23] as a matrix Riemann problem on an elliptic curve, and a description of the n–soliton solution was given. Soliton solutions to the LL equation were obtained by a dressing procedure presented in [5, 4], and solutions in terms of theta functions were found in [2, 3]. The isotropic case $J = 0$, also known as the Heisenberg magnet equation, was studied by the inverse scattering method in [15] and [26], and a geometric description in terms of the Segal–Wilson Grassmannian was given in [13].

Although many special solutions to the LL equation have been found in the literature, there is no closed form solution to a general initial value problem. Thus, it is of interest to study numerical solutions to the LL equation. This paper is concerned with numerical integration of the stationary (time independent) equation. The stationary case of the LL equation is interesting because it is related to an integrable Hamiltonian system and it also admits a Lax pair representation. Thus it can be efficiently integrated by symplectic or isospectral methods. The stationary solutions satisfy

$$S \times (S_{xx} + JS) = 0, \quad \|S\| = 1,$$

which implies

$$S_{xx} + JS = \lambda S \tag{2}$$

for some $\lambda \in \mathbb{R}$. The multiplier λ is uniquely determined from the normalization condition $\|S\| = 1$. Differentiating $\|S\|^2 = 1$ twice with respect to x we obtain

$$\langle S_{xx}, S\rangle + \|S_x\|^2 = 0, \tag{3}$$

where $\langle \cdot\,, \cdot \rangle$ denotes the inner product in $\mathbb{R}^3$. Substituting (2) into (3) we find

$$\lambda = \langle JS, S\rangle - \|S_x\|^2,$$

hence the stationary LL equation is a nonlinear problem given by

$$S_{xx} = -JS + \left(\langle JS, S\rangle - \|S_x\|^2\right) S, \quad \|S\| = 1. \tag{4}$$

In this paper, we consider two efficient methods for integrating equation (4) based on symplectic and isospectral techniques. The symplectic method uses interpretation of (4) as a constrained Hamiltonian system, while the isospectral method employs the Lax pair representation of the equation.

The paper is organized as follows. In Section 2, we recall that the stationary Landau–Lifshitz equation is equivalent to the C. Neumann problem which describes the motion of an anisotropic harmonic oscillator constrained to the unit sphere. Using this equivalence, we devise a symplectic algorithm for the integration of the LL

equation, which exactly preserves the geometric constraints of the system. Section 3 is concerned with isospectral integration of the stationary LL equation based on a Lax pair representation of the Neumann problem with a spectral parameter $z \in \mathbb{C}$. The Lax representation reduces to a system of differential equations for matrices defined on the phase space of the system. We show that the system can be integrated by an isospectral method which leads to exact conservation of the geometric constraints of the system. In Section 4, we compare numerical results of both methods for oscillatory solutions and with a special case of an explicit solution admitting the prescribed asymptotic behaviour.

2. Symplectic integration of the Landau–Liftshitz equation

It was noted by Veselov [25] that the stationary LL equation (4) is equivalent to the C. Neumann problem, which describes the motion of a point particle with Hamiltonian

$$H(q,p) = \frac{1}{2}\|p\|^2 + \frac{1}{2}\langle Jq, q\rangle, \quad (q,p) \in \mathbb{R}^6 \tag{5}$$

constrained to the unit sphere. This allows for the application of symplectic methods to integration of (1). Let

$$X_H = \sum_{k=1}^{3} \frac{\partial H}{\partial p_k}\frac{\partial}{\partial q_k} - \frac{\partial H}{\partial q_k}\frac{\partial}{\partial p_k}$$

be the Hamiltonian vector field associated with Hamiltonian (5). The equations of motion of the Neumann problem can be derived by the method of constrained vector fields [19]. We constrain the vector field X_H to the cotangent bundle of the unit sphere $T^*S^2 = \big\{(q,p) \in \mathbb{R}^6 \mid \|q\| = 1,\ \langle q,p\rangle = 0\big\}$ by requiring that the constrained field is tangent to T^*S^2. The manifold T^*S^2 is the level set of the function $G\colon \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^2$ defined by

$$G_1(q,p) = \frac{1}{2}\big(\|q\|^2 - 1\big), \quad G_2(q,p) = \langle q,p\rangle,$$

hence we replace X_H by the vector field

$$X_H^* = X_H - \lambda_1 X_{G_1} - \lambda_2 X_{G_2},$$

where the functions $\lambda_i = \lambda_i(q,p)$ are chosen such that the flow of X_H^* lies on T^*S^2. This holds if and only if the field X_H^* satisfies the invariance condition

$$dG_i(q,p)X_H^*(q,p) = 0 \quad \forall\,(q,p) \in T^*S^2, \quad i = 1,2,$$

which is equivalent to the system of equations

$$\{G_i, H\} - \sum_{j=1}^{2} \lambda_j \{G_i, G_j\} = 0, \quad i = 1,2, \tag{6}$$

where $\{\cdot\,,\cdot\}$ is the canonical Poisson bracket $\{F,G\}=\sum_{k=1}^{3}\frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k}-\frac{\partial F}{\partial p_k}\frac{\partial G}{\partial q_k}$. One easily verifies that $\{G_1,G_2\}=1$ on T^*S^2, hence the system of equations (6) has a unique solution

$$\lambda_1(q,p)=\langle Jq,q\rangle-\|p\|^2,\quad \lambda_2=0.$$

Therefore, the constrained vector field is given by

$$X_H^*=\sum_{k=1}^{3}\frac{\partial H}{\partial p_k}\frac{\partial}{\partial q_k}-\Big(\frac{\partial H}{\partial q_k}-\lambda_1\frac{\partial G_1}{\partial q_k}\Big)\frac{\partial}{\partial p_k}.$$

The Hamiltonian equations of motion yield

$$\frac{dq_k}{dt}=X_H^*(q_k)=\frac{\partial H}{\partial p_k}=p_k, \tag{7}$$

$$\frac{dp_k}{dt}=X_H^*(p_k)=-\frac{\partial H}{\partial q_k}+\lambda_1\frac{\partial G_1}{\partial q_k}=-J_kq_k+\big(\langle Jq,q\rangle-\|p\|^2\big)q_k, \tag{8}$$

where $(q,p)\in T^*S^2$. Combining (7) and (8) we find

$$\frac{d^2q}{dt^2}=-Jq+\Big(\langle Jq,q\rangle-\Big\|\frac{dq}{dt}\Big\|^2\Big)q,\quad \|q\|=1. \tag{9}$$

We note that equation (9) is the same as equation (4) if we identify the magnetization vector S with the position vector $q\in S^2$ and the space variable x with time t. It is well known that (9) is a completely integrable Hamiltonian system. This was shown by C. Neumann using separation of variables in the Hamilton–Jacobi equation [20]. The system has constants of motion in involution found by K. Uhlenbeck (see [21]),

$$F_i=q_i^2+\sum_{k\neq i}\frac{(p_iq_k-q_ip_k)^2}{J_i-J_k},\quad \sum_{i=1}^{3}F_i=1. \tag{10}$$

Integrability of the Neumann problem has also been proved by Lie algebraic methods in [21] and by Birkhoff factorization of loops groups in [12].

The Hamiltonian structure of (9) allows the application of geometric numerical integration techniques in finding efficient and stable numerical algorithms that preserve the structure of the system under discretization. Since the phase space of the Neumann problem is the cotangent bundle T^*S^2, one should apply an algorithm that preserves the symplectic structure of the system together with geometric constraints $\|q\|=1$ and $\langle q,p\rangle=0$. Symplectic algorithms that preserve geometric constraints can be constructed in various ways. Here we consider the composition method proposed by C. Reich in [22]. Consider a free Hamiltonian

$$H(q,p)=\frac{1}{2}p^TM^{-1}p+U(q), \tag{11}$$

where M is a positive definite symmetric matrix. The equations of motion are given by

$$\dot q=\nabla_pH=M^{-1}p, \tag{12}$$

$$\dot p=-\nabla_qH=-\nabla U(q). \tag{13}$$

A widely used symplectic integrator for equations (12)–(13) is the Strömer–Verlet algorithm [11] defined by

$$p_{n+\frac{1}{2}} = \hat{p}_n - \frac{h}{2}\nabla U(\hat{q}_n), \tag{14}$$

$$\hat{q}_{n+1} = \hat{q}_n + hM^{-1}p_{n+\frac{1}{2}}, \tag{15}$$

$$\hat{p}_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2}\nabla U(\hat{q}_{n+1}). \tag{16}$$

The discrete flow $\varphi\colon (\hat{q}_n, \hat{p}_n) \mapsto (\hat{q}_{n+1}, \hat{p}_{n+1})$ given by (14)–(16) is symplectic and of order two, and it is also symmetric with respect to changing the direction of time $t \mapsto -t$ (for details see [11]).

Suppose now that the system with Hamiltonian (11) satisfies the holonomic constraint $f(q) = 0$ for some C^1 function $f\colon \mathbb{R}^d \to \mathbb{R}^m$, $m < d$. By differentiating $\frac{d}{dt}f(q) = 0$ we find that the system also satisfies the constraint $Df(q)M^{-1}p = 0$, where $Df(q)$ is the Jacobian matrix of f. Thus, the flow of the Hamiltonian vector field X_H lies on the manifold

$$\mathcal{M} = \big\{(q,p) \in \mathbb{R}^{2d} \mid f(q) = 0,\ Df(q)M^{-1}p = 0\big\}.$$

In order to take the geometric constraints into account, we want to project the discrete flow φ onto the manifold $\mathcal{M}$ such that the projection remains symplectic. This can be done using the following lemma proved in [22].

Lemma 1. *Let $\lambda\colon \mathbb{R}^{2d} \to \mathbb{R}^m$ be an arbitrary function of phase space coordinates $(q,p) \in \mathbb{R}^{2d}$. Suppose that q satisfies the holonomic constraint $f(q) = 0$ for some C^1 function $f\colon \mathbb{R}^d \to \mathbb{R}^m$. Then the map $(q,p) \mapsto (\hat{q},\hat{p})$ defined by*

$$\hat{q} = q, \tag{17}$$

$$\hat{p} = p - hDf(q)^T\lambda(q,p), \quad h \in \mathbb{R}, \tag{18}$$

preserves the symplectic form $\omega = \sum_{i=1}^d dq_i \wedge dp_i$.

The idea is to compose the map (17)–(18) by the Strömer–Verlet algorithm (14)–(16) and use freedom of choice of λ in order to satisfy the constraints defining the manifold $\mathcal{M}$. Let $\varphi_1\colon (q_n,p_n) \mapsto (\hat{q}_n,\hat{p}_n)$ denote the map (17)–(18) with step size $h/2$ and an arbitrary function $\lambda\colon \mathbb{R}^{2d} \to \mathbb{R}^m$. The composition with the Strömer–Verlet map, $\varphi \circ \varphi_1\colon (q_n,p_n) \mapsto (\hat{q}_{n+1},\hat{p}_{n+1})$, yields

$$\begin{aligned}
p_{n+\frac{1}{2}} &= p_n - \frac{h}{2}\Big[Df(q_n)^T\lambda(q_n,p_n) + \nabla U(q_n)\Big],\\
\hat{q}_{n+1} &= q_n + hM^{-1}p_{n+\frac{1}{2}},\\
\hat{p}_{n+1} &= p_{n+\frac{1}{2}} - \frac{h}{2}\nabla U(\hat{q}_{n+1}).
\end{aligned}$$

Furthermore, let $\varphi_2\colon (\hat{q}_{n+1},\hat{p}_{n+1}) \mapsto (q_{n+1},p_{n+1})$ denote the map (17)–(18) with step size $h/2$ and an arbitrary function $\mu\colon \mathbb{R}^{2d} \to \mathbb{R}^m$. Then by composing the maps

$\varphi_2 \circ \varphi \circ \varphi_1 \colon (q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$ we obtain

$$p_{n+\frac{1}{2}} = p_n - \frac{h}{2}\Big[Df(q_n)^T \lambda_n + \nabla U(q_n)\Big], \tag{19}$$

$$q_{n+1} = q_n + hM^{-1} p_{n+\frac{1}{2}}, \tag{20}$$

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2}\Big[Df(q_{n+1})^T \mu_{n+1} + \nabla U(q_{n+1})\Big], \tag{21}$$

where $\lambda_n = \lambda(q_n, p_n)$ and $\mu_{n+1} = \mu(q_{n+1}, \hat{p}_{n+1})$. Since all maps are symplectic, the composition $\varphi_2 \circ \varphi \circ \varphi_1$ is also symplectic for any choice of the functions λ and μ. Now choose λ such that

$$f(q_{n+1}) = 0. \tag{22}$$

This leads to a system of equations (19), (20) and (22) for the unknowns $q_{n+1} \in \mathbb{R}^d$ and $\lambda_n \in \mathbb{R}^m$. Similarly, we can choose μ such that

$$Df(q_{n+1}) M^{-1} p_{n+1} = 0, \tag{23}$$

which yields a system of equations (19), (21) and (23) for the unknowns $p_{n+1} \in \mathbb{R}^d$ and $\mu_{n+1} \in \mathbb{R}^m$. We note that we do not require the explicit form of λ and μ, but only their numerical values λ_n and μ_{n+1} determined by the conditions (22) and (23). Thus, if we start with initial data $(q_0, p_0) \in \mathcal{M}$, then the discrete flow $(q_n, p_n) \mapsto (q_{n+1}, p_{n+1})$ lies on the manifold $\mathcal{M}$. The algorithm (19)–(23) is known as the RATTLE algorithm. It is symplectic, time reversible and convergent of order two, and it is also explicit for separable Hamiltonians. More details about the RATTLE algorithm, including a different proof of its symplecticity, can be found in [11].

Applying the RATTLE algorithm to the Neumann problem (9) with potential $U(q) = \frac{1}{2}\langle Jq, q\rangle$ and holonomic constraint $f(q) \equiv \|q\|^2 - 1 = 0$, we find

$$q_{n+1} = q_n + hp_n - \frac{h^2}{2}\big(\lambda_n q_n + Jq_n\big), \tag{24}$$

$$p_{n+1} = p_n - \frac{h}{2}\big(\lambda_n q_n + Jq_n + \mu_{n+1} q_{n+1} + Jq_{n+1}\big), \tag{25}$$

where $J = \operatorname{diag}(J_1, J_2, J_3)$. Here, $\lambda_n, \mu_{n+1} \in \mathbb{R}$ are determined on the basis of conditions (22) and (23), i.e.,

$$\|q_{n+1}\|^2 = 1 \tag{26}$$

and

$$\langle q_{n+1}, p_{n+1}\rangle = 0. \tag{27}$$

First we show that one can always solve the sytem of equations (24) and (26).

Lemma 2. *Let $(q_n, p_n) \in T^*S^2$. Then the system of equations* (24) *and* (26) *has a unique solution $(q_{n+1}, \lambda_n) \in S^2 \times \mathbb{R}$ for a sufficiently small h.*

Proof. Writing the system of equations (24) and (26) explicitly in components, we have

$$q^i_{n+1} - hp^i_n + \frac{h^2}{2}\lambda_n q^i_n + \frac{h^2}{2} J_i q^i_n - q^i_n = 0, \quad i = 1, 2, 3, \tag{28}$$

$$\sum_{i=1}^{3} (q^i_{n+1})^2 - 1 = 0. \tag{29}$$

Introduce variables $x = h$, $y_i = q^i_{n+1}$, $i = 1, 2, 3,$, and $y_4 = h^2\lambda_n$. Then the system (28)–(29) is equivalent to $F(x, y) = 0$, where $F\colon \mathbb{R} \times \mathbb{R}^4 \to \mathbb{R}$ is given by

$$F(x,y) = \begin{bmatrix} y_1 + \frac{1}{2}q^1_n\, y_4 - xp^1_n + \frac{1}{2}x^2 J_1 q^1_n - q^1_n \\ y_2 + \frac{1}{2}q^2_n\, y_4 - xp^2_n + \frac{1}{2}x^2 J_2 q^2_n - q^2_n \\ y_3 + \frac{1}{2}q^2_n\, y_4 - xp^3_n + \frac{1}{2}x^2 J_3 q^3_n - q^3_n \\ y_1^2 + y_2^2 + y_3^2 - 1 \end{bmatrix}.$$

Note that $F(a, b) = 0$ at the point $a = 0, b = (q_n, 0)$ since $\|q_n\|^2 = 1$. The Jacobian of F with respect to y,

$$D_y F(x,y) = \begin{bmatrix} 1 & 0 & 0 & \frac{1}{2}q^1_n \\ 0 & 1 & 0 & \frac{1}{2}q^2_n \\ 0 & 0 & 1 & \frac{1}{2}q^3_n \\ 2y_1 & 2y_2 & 2y_3 & 0 \end{bmatrix},$$

has a nonvanishing determinant at (a, b), $\det D_y F(a, b) = -1 \neq 0$; hence by the Implicit Function Theorem there exists $\varepsilon > 0$ and a unique C^1 function $g\colon (-\varepsilon, \varepsilon) \to \mathbb{R}^4$ such that $g(0) = (q_n, 0)$ and $F(x, g(x)) = 0$ for all $x \in (-\varepsilon, \varepsilon)$. This implies that the equation $F(x, y) = 0$ has a unique solution $y = g(x)$ for all $|x| < \varepsilon$. Consequently, the system of equations (28)–(29) has a unique solution $q^i_{n+1} = y_i$, $i = 1, 2, 3$, and $\lambda_n = y_4/h^2$ whenever $0 < |h| < \varepsilon$. □

Now, given q_{n+1} with $\|q_{n+1}\|^2 = 1$ one finds from (25) and (27) that μ_{n+1} has the explicit form

$$\mu_{n+1} = \frac{2}{h}\langle q_{n+1}, p_n\rangle - \lambda_n\langle q_{n+1}, q_n\rangle - \langle q_{n+1}, Jq_n\rangle - \langle q_{n+1}, Jq_{n+1}\rangle. \tag{30}$$

Finally, (30) and (25) yield the momentum p_{n+1}. We summarize the algorithm for the integration of the Neumann problem as follows:

(i) given a point $(q_n, p_n) \in T^*S^2$, solve by a numerical method the system of equations (28)–(29) to obtain q_{n+1} and λ_n,

(ii) compute μ_{n+1} from (30) and then compute p_{n+1} from (25).

The obtained solution is a point $(q_{n+1}, p_{n+1}) \in T^*S^2$.

In the following section, we present an alternative method for solving numerically the Neumann problem based on a Lax pair representation, and compare it with the symplectic method discussed here.

3. Isospectral method for solving the Landau–Liftshitz equation

A number of integrable systems possess a Lax representation whereby the equations of motion can be written in the form:

$$\frac{dL}{dt} = [M, L], \quad L(0) = L_0, \tag{31}$$

where L and M are matrix functions defined on the phase space of the system possibly depending on a spectral parameter, and $[M, L] = ML - LM$ is the matrix commutator. It is well known that the solution of the Lax equation (31) is given by $L(t) = P(t)L(0)P(t)^{-1}$, where the matrix $P(t)$ satisfies the differential equation

$$\frac{dP}{dt} = MP, \quad P(0) = I.$$

Since $L(t)$ and $L(0)$ have the same spectrum, the eigenvalues of $L(t)$ are time independent, hence the flow $(t, L_0) \mapsto L(t)$ is isospectral. It is easily seen that the trace $\mathrm{Tr}L^k(t)$, $k \geq 1$, is also invariant under the flow determined by (31). Therefore, if a system of Hamilton's equations can be written in Lax form for some choice of matrices L and M, then the constants of motion can be found by algebraic methods either from the eigenvalues of $L(t)$ or from $\mathrm{Tr}L^k(t)$. This usually implies integrability of the system in the Arnold–Liouville sense provided there are sufficiently many independent integrals of motion in involution. Examples of Hamiltonian systems with Lax representation include the Kowalevski top, the Toda chain, the Calogero–Moser model [1], [18], and Euler–Arnold equation [16].

In this section, we are concerned with solving the Neumann problem numerically by discretizing (31) such that the underlying discrete flow lies on the manifold T^*S^2. For further discussion we recall the following result due to K. Uhlenbeck [21].

Lemma 3. *Define matrices $Q = q \otimes q$ and $L = p \otimes q - q \otimes p$, and let $U(z) = Jz^2 + Lz - Q$ and $M(z) = Jz + L$ be matrix polynomials in the spectral parameter $z \in \mathbb{C}$. Then equation* (9) *is equivalent to the Lax equation*

$$\frac{dU}{dt} = [M, U] \quad \textit{subject to constraints} \quad \|q\| = 1,\ \langle q, p\rangle = 0. \tag{32}$$

Proof. The Lax equation (32) is equivalent to the system of equations

$$\frac{dQ}{dt} = [L, Q], \quad \frac{dL}{dt} = -[J, Q]. \tag{33}$$

Since $Q_{ij} = q_i q_j$ and $L_{ij} = p_i q_j - q_i p_j$, the commutators $[L, Q]$ and $[J, Q]$ are given by

$$[L, Q]_{ij} = p_i\, q_j + q_i\, p_j, \quad [J, Q]_{ij} = (J_i - J_j)\, q_i\, q_j.$$

The first equation in (33) yields

$$(\dot{q}_i - p_i)q_j + (\dot{q}_j - p_j)q_i = 0,$$

which implies $\dot{q}_i = p_i$ since any two coordinates are independent. The second equation in (33) implies

$$\dot{p}_i\, q_j + p_i\, \dot{q}_j - \dot{q}_i\, p_j - q_i\, \dot{p}_j = -(J_i - J_j)\, q_i\, q_j. \tag{34}$$

Substituting $\dot{q}_i = p_i$ into (34) we find

$$\ddot{q}_i\, q_j - q_i\, \ddot{q}_j = -(J_i - J_j)\, q_i\, q_j. \tag{35}$$

Multiplying equation (35) by q_j and summing over j we obtain

$$\ddot{q}_i = -J_i\, q_i + \langle q, \ddot{q}\rangle\, q_i + \langle Jq, q\rangle\, q_i, \tag{36}$$

where we have used the constraint $\|q\| = 1$. Differentiating the condition $\langle q, p\rangle = 0$ yields $\langle \ddot{q}, q\rangle = -\|\dot{q}\|^2$, hence substituting this expression into (36) we obtain the equation of motion for the Neumann problem (9). □

As noted earlier, the constants of motion can be found from the trace $\operatorname{Tr} U^k(z)$, $k \geq 1$. For $k = 1$ we have $\operatorname{Tr} U(z) = -\|q\|^2$, which is trivially constant since $\|q\| = 1$. For $k = 2, 3$, after some algebraic manipulation we find

$$\operatorname{Tr} U^2(z) = (\operatorname{Tr} J^2)z^4 - 2\big(\langle Jq, q\rangle + L_{12}^2 + L_{13}^3 + L_{23}^2\big)z^2 + \|q\|^4, \tag{37}$$

$$\begin{aligned}\operatorname{Tr} U^3(z) = {}& (\operatorname{Tr} J^3)z^6 \\ & - 3\Big[\langle Jq, Jq\rangle + J_1(L_{12}^2 + L_{13}^2) + J_2(L_{12}^2 + L_{23}^2) + J_3(L_{13}^2 + L_{23}^2)\Big]z^4 \\ & + 3\Big[\|q\|^2\langle Jq, q\rangle + \sum_{i<j} L_{ij}^2(q_i^2 + q_j^2) + 2 \sum_{\substack{k=1 \\ k\neq i<j\neq k}}^{3} L_{ki}\, L_{kj}\, q_i\, q_j\Big]z^2 - \|q\|^6.\end{aligned} \tag{38}$$

Since each coefficient multiplying the spectral parameter z is constant, we obtain the following nontrivial integrals of motion from (37) and (38):

$$\begin{aligned}\tilde{F}_1 &= \langle Jq, q\rangle + L_{12}^2 + L_{13}^2 + L_{23}^2, \\ \tilde{F}_2 &= \langle Jq, Jq\rangle + J_1(L_{12}^2 + L_{13}^2) + J_2(L_{12}^2 + L_{23}^2) + J_3(L_{13}^2 + L_{23}^2), \\ \tilde{F}_3 &= \langle Jq, q\rangle + \sum_{i<j} L_{ij}^2(q_i^2 + q_j^2) + 2 \sum_{\substack{k=1 \\ k\neq i<j\neq k}}^{3} L_{ki}\, L_{kj}\, q_i\, q_j.\end{aligned}$$

These integrals are different from the ones given in (10). Since the Neumann problem has two degrees of freedom, only two functionally independent constants in involution are sufficient to prove its integrability. We note that the Lax equation (32) can be intepreted as a differential equation on the Lie algebra of the twisted loop group $LSO(3)$, and it can be integrated by solving a special case of the Birkhoff factorization problem on $LSO(3)$ [12].

Next, we turn to a numerical solution of the Neumann problem using the Lax equation (32). Our goal is to solve the system of differential equations (33) by an isospectral method. A solution to the Lax equation for Q in (33) can be written as

$$Q(t) = P(t)\, Q(0)\, P(t)^{-1}, \quad t \geq 0,$$

where

$$\frac{dP}{dt} = L(t)P(t), \quad P(0) = I, \quad t \geq 0. \tag{39}$$

Let us introduce a partition of the time interval $0 = t_0 < t_1 < t_2 < \cdots$. In every subinterval $[t_n, t_{n+1}]$ the matrix Q satisfies

$$Q(t_{n+1}) = P(t_{n+1})\, Q(t_n)\, P(t_{n+1})^{-1},$$

where $P(t)$ is the solution to

$$\frac{dP}{dt} = L(t)P(t), \quad t_n \leq t \leq t_{n+1}, \quad P(t_n) = I \tag{40}$$

(note that the functions $P(t)$ appearing in (39) and (40) are actually different). Since $L(t)$ is skew–symmetric, it follows from (40) that $P(t)$ is orthogonal, $P(t)^{-1} = P(t)^T$. Therefore, we can write $Q(t_{n+1}) = P(t_{n+1})\, Q(t_n)\, P(t_{n+1})^T$. Suppose that $(P_n)_{n=1}^{\infty}$ is a sequence of orthogonal matrices approximating $P(t_n)$, and define a sequence $(Q_n)_{n=0}^{\infty}$ by

$$Q_{n+1} = P_{n+1}\, Q_n\, P_{n+1}^T, \quad Q_0 = Q(0). \tag{41}$$

Recall that $Q(t) = q(t) \otimes q(t)$ is a symmetric matrix and $\operatorname{Tr} Q(t) = \|q(t)\|^2 = 1$ for all $t \geq 0$. The advantage of computing numerical approximations of $Q(t)$ by the method (41) is twofold. Since $Q_0^T = Q_0$, algorithm (41) implies that $Q_n^T = Q_n$ for all $n \geq 1$. Furthermore, the discrete flow $Q_n \mapsto Q_{n+1}$ is isospectral since $P_{n+1}^T = P_{n+1}^{-1}$, and also $\operatorname{Tr} Q_n = 1$ for all $n \geq 1$. Therefore, algorithm (41) preserves two important properties of the continuous system:

(i) symmetry of the matrix $Q(t)$, and

(ii) the geometric constraint $\|q(t)\| = 1$.

In order to compute the map $Q_n \mapsto Q_{n+1}$ using (41), we need to solve equation (40) by a method that preserves orthogonality of the matrix P. Then we can use the second equation in (33) to approximate $L(t_n)$ and obtain the phase space variables $(q_n, p_n) \in T^*S^2$.

We solve equation (40) by the implicit midpoint rule, which is a one–stage Runge–Kutta method with a Butcher tableau

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

Recall that if y satisfies the differential equation $y'(t) = f(t, y)$, the midpoint rule is defined by

$$y_{n+1} = y_n + hk_1, \tag{42}$$

$$k_1 = f\big(t_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1\big). \tag{43}$$

Applying the algorithm (42)–(43) to (40) with $f(t, P) = L(t)P$ we obtain

$$P_{n+1} = P_n + hK_1, \tag{44}$$

$$K_1 = L_{n+\frac{1}{2}}\big(P_n + \frac{1}{2}hK_1\big), \tag{45}$$

where $L_{n+\frac{1}{2}} = L(t_n + \frac{1}{2}h)$. Note that the above algorithm is explicit since K_1 can be expressed as

$$K_1 = \big(I - \frac{1}{2}hL_{n+\frac{1}{2}}\big)^{-1} L_{n+\frac{1}{2}} P_n.$$

The algorithm (44)–(45) belongs to a family of Runge–Kutta methods that preserve orthogonality of the matrix P_n [7]. We provide a simplified proof of this fact for the special case considered here.

Theorem 1. *Suppose $(P_n)_{n=1}^{\infty}$ is a sequence of matrices obtained by the algorithm (44)–(45), where $L(t)$ is a skew–symmetric matrix. If P_1 is orthogonal, then P_n is orthogonal for all $n \geq 1$.*

Proof. We prove that $P_{n+1}^T P_{n+1} = P_n^T P_n$. Define $\Phi = P_n + \frac{1}{2}hK_1$. Then

$$P_{n+1}^T P_{n+1} = (P_n + hK_1)^T (P_n + hK_1) = P_n^T P_n + h(K_1^T P_n + P_n^T K_1) + h^2 K_1^T K_1. \quad (46)$$

Furthermore,

$$K_1^T P_n + P_n^T K_1 = K_1^T \big(\Phi - \frac{1}{2}hK_1\big) + \big(\Phi - \frac{1}{2}hK_1\big)^T K_1 = K_1^T \Phi + \Phi^T K_1 - hK_1^T K_1. \quad (47)$$

Substituting (47) into (46) we find

$$P_{n+1}^T P_{n+1} = P_n^T P_n + h(K_1^T \Phi + \Phi^T K_1).$$

From (45) we have $K_1 = L_{n+\frac{1}{2}} \Phi$, which yields

$$K_1^T \Phi + \Phi^T K_1 = \Phi^T \big(L_{n+\frac{1}{2}}^T + L_{n+\frac{1}{2}}\big)\Phi = 0,$$

since $L_{n+\frac{1}{2}}$ is skew–symmmetric. Therefore, $P_{n+1}^T P_{n+1} = P_n^T P_n$. Since $P_1^T P_1 = I$, it follows by induction that $P_n^T P_n = I$ for all $n \geq 1$. The matrix P_n is regular, hence also $P_n P_n^T = I$ for all $n \geq 1$. Thus, the algorithm (44)–(45) preserves orthogonality of P_n. □

We use the method (44)–(45) to solve the differential equation (40). Since $P(t_n) = I$, the value of $P(t_{n+1})$ is approximated by $P_{n+1} = I + hK_1$, where

$$K_1 = \big(I - \frac{1}{2}hL_{n+\frac{1}{2}}\big)^{-1} L_{n+\frac{1}{2}}.$$

The value of the matrix $L_{n+\frac{1}{2}} = L(t_n + \frac{1}{2}h)$ can be easily approximated to any degree of accuracy using the Taylor series of $L(t)$ since all derivatives $L^{(k)}(t)$ can be expressed as nested commutators of the matrices $L(t)$ and $Q(t)$ by using equations (33). For example, to the second order in Δt we have

$$L(t + \Delta t) = L(t) + \Delta t\,[Q(t), J] + \frac{1}{2}(\Delta t)^2 \big[[L(t), Q(t)], J\big] + O(\Delta t^3). \quad (48)$$

Each term in the Taylor expansion of $L(t)$ is skew–symmetric, hence the above approximation does not destroy skew–symmetry of $L_{n+\frac{1}{2}}$. Now, the full algorithm

for computation of Q_{n+1} can be described as follows. For given values of Q_n and L_n compute

$$L_{n+\frac{1}{2}} = L_n + \frac{1}{2}h[Q_n, J] + \frac{h^2}{8}\big[[L_n, Q_n], J\big], \tag{49}$$

$$K_1 = \big(I - \frac{1}{2}hL_{n+\frac{1}{2}}\big)^{-1} L_{n+\frac{1}{2}}, \tag{50}$$

$$P_{n+1} = I + hK_1, \tag{51}$$

$$Q_{n+1} = P_{n+1} Q_n P_{n+1}^T. \tag{52}$$

In the final, step we approximate the value of $L(t_n + h)$ by the Taylor series (48),

$$L_{n+1} = L_n + h[Q_n, J] + \frac{1}{2}h^2\big[[L_n, Q_n], J\big]. \tag{53}$$

Approximations (49) and (53) can be computed by a higher order Taylor series, if desired. The map $(Q_n, L_n) \mapsto (Q_{n+1}, L_{n+1})$ given by (49)–(53) describes the flow of the phase space variables (q_n, p_n) on the manifold T^*S^2. Next, we show how to compute (q_n, p_n) from the given values of the matrices (Q_n, L_n).

Lemma 4. *Let Q_n and L_n, $n \geq 0$, be a sequence of matrices obtained from the algorithm (49)–(53), where $Q_0 = q_0 \otimes q_0$ and $L_0 = p_0 \otimes q_0 - q_0 \otimes p_0$ for some initial data $(q_0, p_0) \in T^*S^2$. Then for every $n \geq 1$ there exists a point $(q_n, p_n) \in T^*S^2$ such that $Q_n = q_n \otimes q_n$ and $L_n = p_n \otimes q_n - q_n \otimes p_n$.*

Proof. The characteristic polynomial of Q_0 is given by

$$\det(Q_0 - \lambda I) = \|q_0\|^2\lambda^2 - \lambda^3 = \lambda^2(1 - \lambda),$$

hence the eigenvalues of Q_0 are $\lambda_1 = 1, \lambda_2 = \lambda_3 = 0$. Since P_n is orthogonal for all $n \geq 1$, the matrix Q_n is similar to Q_0; thus Q_n has the same spectrum as Q_0. Furthermore, $Q_0^T = Q_0$ implies that $Q_n^T = Q_n$ for all $n \geq 1$. By the Spectral theorem for real symmetric matrices, Q_n can be factored as

$$Q_n = \Omega_n \, D \, \Omega_n^T, \tag{54}$$

where $D = \mathrm{diag}(1, 0, 0)$ and $\Omega_n = [\Omega_n^{ij}]$ is an orthogonal matrix. The right–hand side of (54) implies that $Q_n = q_n \otimes q_n$ for a unit vector $q_n \in \mathbb{R}^3$, where $q_n^i = \pm\Omega_n^{ii}$. The same conclusion holds for any ordering of the eigenvalues of Q_0. Decomposition (54) determines the vector q_n up to an overall sign. The correct sign is chosen by minimizing the distance $\|q_n - q_{n-1}\| = \min$. Now, given the vector q_n, there is a unique vector $p_n \in \mathbb{R}^3$ such that $L_n = p_n \otimes q_n - q_n \otimes p_n$ and $\langle q_n, p_n \rangle = 0$. It is readily verified that the components of p_n are given by

$$p_n^j = \sum_{i=1}^{3} L_n^{ji} \, q_n^i, \quad j = 1, 2, 3.$$

Therefore, the matrices Q_n and L_n yield the phase space variables (q_n, p_n) on T^*S^2. □

4. Numerical results

We compare the two methods by performing numerical simulations of the Neumann problem in the case of oscillatory and asymptotic solutions. Figure 1 shows the RATTLE and isospectral simulation of the Neumann oscillator with interaction constants $J_1 = 1$, $J_2 = 2$, $J_3 = 5$, and step size $h = 0.02$ for $N = 10000$ iterations. The initial condition is given by $q_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}}\right)$ and $p_0 = (1, -1, 0)$. We observe that numerical trajectories computed by both methods are very close and show the correct qualitative behaviour of the system. Figure 2 shows the corresponding solution $S(x)$ of the stationary Landau-Lifshitz equation obtained by mapping $q \mapsto S$ and $t \mapsto x$.

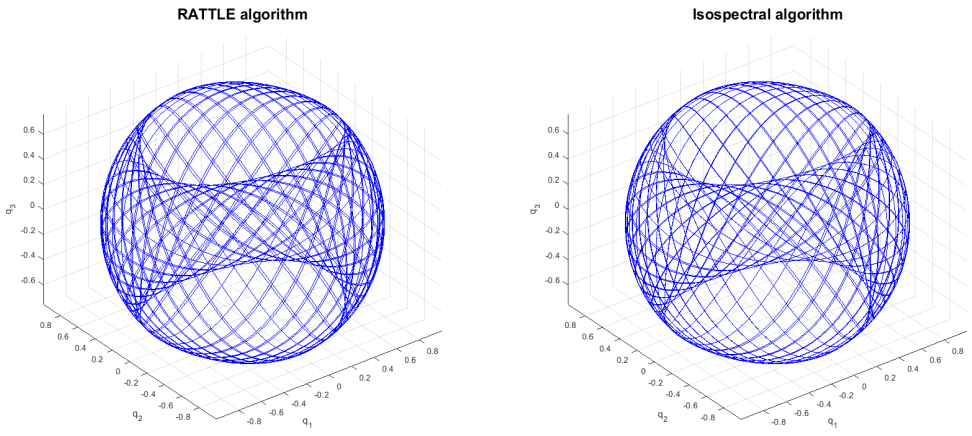

Figure 1: *Simulation of the Neumann oscillator with the RATTLE and isospectral methods with time step* $h = 0.02$ *and* $N = 10000$ *iterations*

Figure 3 compares the error in constants of motion F_i given by (10) for the RATTLE and isospectral methods. Both errors are of the same order of magnitude (i.e. 10^{-3}), but the error in F_1 and F_3 for the isospectral algorithm shows a small overall growth after a large number of iterations. The behaviour of the error for F_1, F_2 and F_3 is consistent with the fact that they are constrained by the relation $F_1 + F_2 + F_3 = 1$.

Next, we compare the two methods with the exact solution given in [10] exhibiting the asymptotic behavior $q(t) \to (0, 0, 1)$ as $t \to \infty$. Introduce the variables $x = \omega_1 t + \alpha_1$ and $y = \omega_2 t + \alpha_2$, where $\omega_1 = \sqrt{J_3 - J_1}$, $\omega_2 = \sqrt{J_3 - J_2}$, and α_1, α_2 are arbitrary real numbers. Let $k = \omega_2/\omega_1$, $k' = \sqrt{1 - k^2}$ and define

$$a(t) = \cosh(x)\cosh(y) - k\sinh(x)\sinh(y),$$
$$b(t) = \sinh(x)\sinh(y) - k\cosh(x)\cosh(y).$$

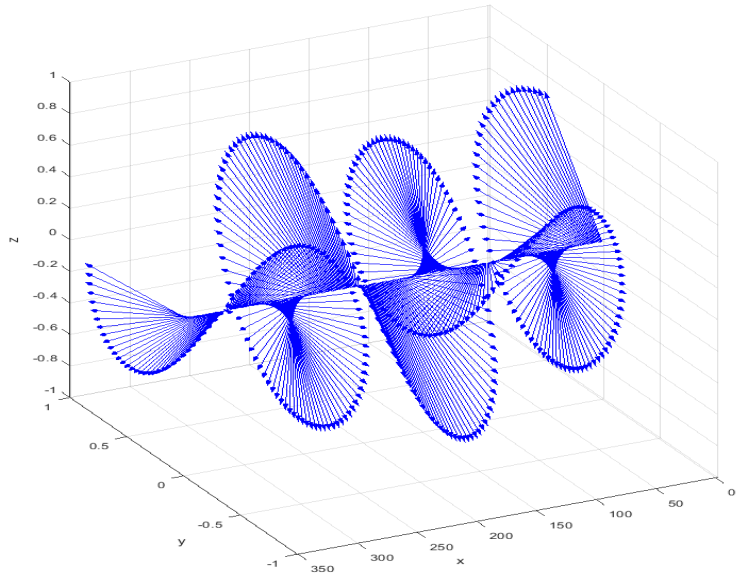

Figure 2: *Magnetization vector $S(x)$ between two domains*

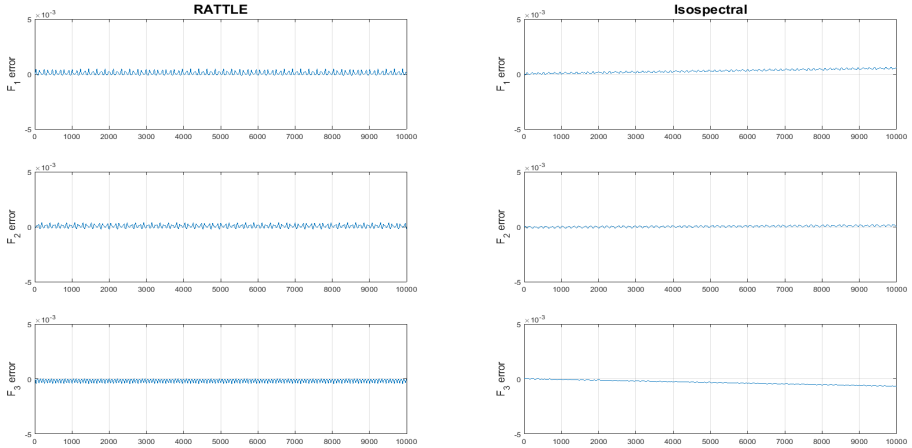

Figure 3: *Error in constants of motion* (10) *for the RATTLE and isospectral methods*

Then the vector $q = (q_1, q_2, q_3)$ given by

$$q_1(t) = \frac{k' \cosh(y)}{a(t)}, \quad q_2(t) = \frac{k' \sinh(x)}{a(t)}, \quad q_3(t) = \frac{b(t)}{a(t)}, \tag{55}$$

is a solution to (9) such that $q(t) \to (0, 0, 1)$ as $t \to \infty$. The initial position as a

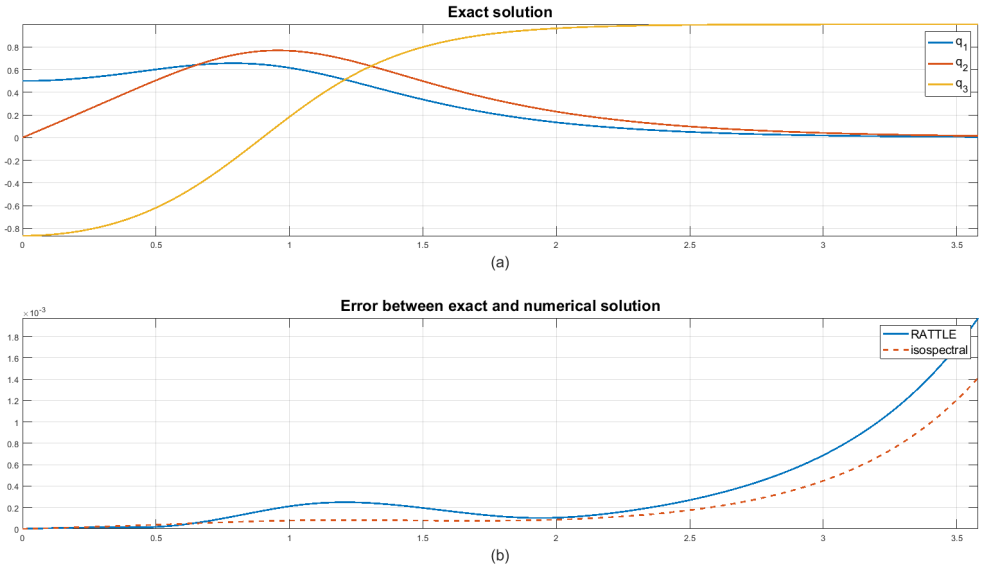

Figure 4: *(a) Exact solution with asymptotic limit $q \to (0,0,1)$. (b) L^2–error between the exact solution and numerical approximations computed by the RATTLE and isospectral algorithms*

function of the parameters $\alpha_1, \alpha_2 \in \mathbb{R}$ is given by

$$q_1(0) = \frac{k' \cosh(\alpha_2)}{a(0)}, \quad q_2(0) = \frac{k' \sinh(\alpha_1)}{a(0)}, \quad q_3(0) = \frac{b(0)}{a(0)}.$$

The initial momenta $p_i(0) = \dot{q}_i(0)$ are found to be

$$\begin{aligned} p_1(0) &= k' \frac{\omega_2 \sinh(\alpha_2) a(0) - \cosh(\alpha_2) \dot{a}(0)}{a^2(0)}, \\ p_2(0) &= k' \frac{\omega_1 \cosh(\alpha_1) a(0) - \sinh(\alpha_1) \dot{a}(0)}{a^2(0)}, \\ p_3(0) &= (k')^2 \frac{\omega_2 \cosh(\alpha_1) \sinh(\alpha_1) + \omega_1 \cosh(\alpha_2) \sinh(\alpha_2)}{a^2(0)}, \end{aligned}$$

where

$$\dot{a}(0) = (\omega_1 - k\omega_2) \sinh(\alpha_1) \cosh(\alpha_2) + (\omega_2 - k\omega_1) \cosh(\alpha_1) \sinh(\alpha_2).$$

Figure 4(a) shows the exact solution (55) corresponding to $\alpha_1 = \alpha_2 = 0$ with interaction constants $J_1 = 1$, $J_2 = 2$, $J_3 = 5$, and step size $h = 0.02$. Figure 4(b) shows the error $\|q_{ex} - q_{num}\|$ between the exact solution and numerical approximation computed by the RATTLE and isospectral methods.

We observe that the error of the isospectral method grows slower than the error of the RATTLE algorithm. Numerical experiments show that both methods exhibit similar performance in terms of accuracy, stability and preservation of geometric

constraints and constants of motion. However, measuring the execution time reveals that the isospectral method is about 80 times faster for $N = 10000$ iterations since it avoids solving a nonlinear system of equations (28)–(29) required at each iteration of the RATTLE algorithm. The difference in speed is even more evident as the number of iterations increases. This gives the proposed isospectral method a considerable advantage over the RATTLE algorithm for long–time simulations.

References

[1] O. Babelon, D. Barnard, M. Talon, *Introduction to Classical Integrable Systems*, Cambridge University Press, 2003.

[2] R. F. Bikbaev, A. I. Bobenko, *On finite-gap integration of the Landau–Lifshitz equation. XYZ case*, Preprint LOMI E–8–83, Leningrad, 1983.

[3] A. I. Bobenko, *Real algebraic–geometric solutions of the Landau–Lifshitz equation in terms of Prym theta–functions*, Funk. Anal. Prilož. **19**(1985), 6–19 (in Russian).

[4] R. F. Bikbaev, A. I. Bobenko, A. R. Its, *The Landau–Lifshitz equation. The theory of exact solutions*, Preprints Don PTI–4–6(81), Donetsk, 1984 (in Russian).

[5] A. I. Bobenko, *The Landau–Lifshitz equation. Dressing up of the solutions and elementary excitations*, in: *Differential geometry, Lie groups and mechanics*, V. Zap. Nauchn. Semin. LOMI **123**(1983), 58–66 (in Russian).

[6] A. E. Borovik, V. N. Robuk, *Linear pseudopotentials and conservation laws for the Landau–Liftshitz equation describing the nonlinear dynamics of a ferromagnet with uniaxial anisotropy*, Theor. Math. Phys. **46**(1981), 242–248.

[7] M. P. Calvo, A. Iserles, A. Zanna, *Numerical Solution of Isospectral Flows*, Math. Comp. **66**(1997), 1461–1486.

[8] A. L. Carey, K. C. Hannabus, L. J. Mason, M. A. Singer, *The Landau–Lifshitz Equation, Elliptic Curves and the Ward Transform*, Commun. Math. Phys. **154**(1993), 25–47.

[9] L. D. Fadeev, L. A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons*, Springer–Verlag, New York, 1987.

[10] Y. I. Granovskii, A. S. Zhedanov, *Solutions of Domain Type in Anisotropic Magnetic Chains*, Theor. and Math. Phys. **71**(1987), 438–446.

[11] E. Haier, Ch. Lubich, G. Wanner, *Geometric Numerical Integration: Structure–Preserving Algorithms for Ordinary Differential Equations*, Springer–Verlag, 2002.

[12] S. Krešić–Jurić, *A loop group approach to the C. Neumann problem and Moser–Veselov factorization*, J. Math. Phys. **40**(1999), 5014–5025.

[13] S. Krešić–Jurić, *On the Birkhoff factorization problem for the Heisenberg magnet and nonlinear Schrödinger equations*, J. Math. Phys. **47**(2006), 063501.

[14] L. D. Landau, E. N. Lifshitz, *On the Theory of the Dispersion of Magnetic Permeability in Ferromagnetic Bodies*, Phys. Z. Sowjetunion **8**(1935), 153–169.

[15] M. Lakshmanan, *Continuum spin system as an exactly solvable dynamical system*, Phys. Lett. A **61**(1977), 53–54.

[16] S. V. Manakov, *Note on the integration of Euler's equations of the dynamics of an n–dimensional ridig body*, Funct. Anal. Appl. **11**(1976), 328–329.

[17] A. V. Mikhailov, *The Landau–Lifshitz Equation and the Riemann Boundary Problem on a Torus*, Phys. Lett. **92A**(1982), 51–55.

[18] J. Moser, *Three Integrable Hamiltonian Systems Connected with Isospectral Deformations*, Adv. Math. **16**(1975), 197–220.

[19] J. Moser, *Integrable Hamiltonian systems and spectral theory*, Scuola Normale Superiore, Pisa, 1981.

[20] C. Neumann, *De problemate quodam mechanico, quod ad primam integrallium ultraellipticorum classem revocatur*, J. Reine Angew. Math. **56**(1859), 46–63.

[21] T. Ratiu, *The C. Neumann problem as a completely integrable system on an adjoint orbit*, Trans. Am. Math. Soc. **246**(1981), 321–329.

[22] S. Reich, *Symplectic Integration of Constrained Hamiltonian Systems by Composition Methods*, SIAM J. Numer. Anal. **33**(1996), 475–491.

[23] L. Yu. Rodin, *The Riemann boundary problem on Riemann surfaces and the inverse scattering problem for the Landau–Lifshitz equation*, Physica D **11**(1984), 90–108.

[24] E. K. Sklyanin, *On complete integrability of the Landau–Lifshitz equation*, Preprint LOMI E–3–79, Leningrad, 1979.

[25] A. P. Veselov, *The Landau–Lifshitz equation and integrable systems of classical mechanics*, Sov. Phys. Dokl. **28**(1983), 458–459.

[26] V. E. Zakharov, L. A. Takhtajan, *Equivalence of the nonlinear Schrödinger equation and the equation of a Heisenberg ferromagnet*, Theor. Math. Phys. **57**(1979), 17–23.