Modulated spin waves and robust quasi-solitons in classical Heisenberg rings

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Abstract
We investigate the dynamical behavior of finite rings of classical spin vectors interacting via nearest-neighbor isotropic exchange in an external magnetic field. Our approach is to utilize the solutions of a continuum version of the discrete spin equations of motion (EOM) which we derive by assuming continuous modulations of spin wave solutions of the EOM for discrete spins. This continuum EOM reduces to the Landau–Lifshitz equation in a particular limiting regime. The usefulness of the continuum EOM is demonstrated by the fact that the time-evolved numerical solutions of the discrete spin EOM closely track the corresponding time-evolved solutions of the continuum equation. It is of special interest that our continuum EOM possesses soliton solutions, and we find that these characteristics are also exhibited by the corresponding solutions of the discrete EOM. The robustness of solitons is demonstrated by considering cases where initial states are truncated versions of soliton states and by numerical simulations of the discrete EOM equations when the spins are coupled to a heat bath at finite temperatures.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

There has been remarkable progress in recent years in synthesizing crystalline samples of magnetic molecules of great diversity [1–3]. In parallel there have been notable successes in developing theoretical models that provide a satisfactory description of the thermal equilibrium properties of these magnetic systems [4, 5]. A simplifying feature of magnetic molecules is that the magnetic properties of a sample are due to intra-molecular exchange interactions between the \(N\) magnetic ions (‘spins’) of an individual molecule, while inter-molecular magnetic interactions are negligible. Given the parallel progress in chemical synthesis and theoretical modeling it is timely to focus on the dynamical behavior of finite arrays of interacting spins. In many bulk magnetic systems, magnetic solitons have been detected through their signature in such observables as specific heat, NMR, and neutron scattering [6]. One may thus ask, under what circumstances will magnetic solitons be observable in magnetic molecules? Clearly the quantum character of the individual spins needs to be taken into account, and the number of interacting spins will be a crucial parameter.

In this paper, as a first step toward grappling with the general question that we have posed, we direct our attention to ring structures consisting of \(N\) equally spaced (spacing \(a\)) classical spin vectors (unit vectors) that interact via ferromagnetic nearest-neighbor isotropic exchange and are subject to a uniform external magnetic field \(B = Be\). (The reason that we have excluded antiferromagnetic exchange is discussed at the outset in section 2.) The equations of motion
(EOM) of the spin vectors can be written as
\[
\frac{d}{dt} s_n(t) = s_0(t) \times (s_{n-1}(t) + s_{n+1}(t) + B),
\]
where all variables are dimensionless and the unit vectors \( s_n \) are subject to the cyclic condition \( s_{n+N} \equiv s_n \). For \( N \leq 4 \) the EOM are integrable and this feature has made it possible in the past decade to calculate the equilibrium time correlation functions [7–11] for these ultra-small rings. For \( N > 4 \) the general solution of equation (1) cannot be given in closed form and the spin vectors exhibit chaotic motion except for special initial conditions; see appendix B. The rest of this paper is devoted to these challenging, larger ring systems.

It is well known that the solutions of equation (1) exhibit a wide variety of dynamical characteristics. Among these are: exact analytical solutions, called ‘spin waves’ [12]; numerical solutions that exhibit chaotic behavior [13]; as well as numerical solutions that are discretized versions of the soliton solutions [14–16] of a continuum version of equation (1), specifically the Landau–Lifshitz equation [17] in the case of \( B \neq 0 \):
\[
\frac{\partial S}{\partial t} = S \times \left( \frac{\partial^2 S}{\partial x^2} + B \right).
\]

The key result of this paper is that the EOM of equation (1) admit a wide class of numerical solutions with soliton-like characteristics. They are discretized versions of soliton solutions of a new continuum EOM that includes the soliton solutions of the Landau–Lifshitz equation as a special, limiting case. We will refer to such discretized solutions as ‘quasi-solitons’, using this cautious terminology since we do not know whether they correspond to strict soliton solutions of equation (1). A single-quasi-soliton solution is a localized disturbance that propagates in the ring while for the most part maintaining its initial shape. We also find that it is possible to achieve two-quasi-soliton solutions, where a pair of initially separated single quasi-solitons collide multiple times and emerge from collisions without appreciable modification. Moreover, we identify solutions of equation (1) that exhibit a transition from laminar-like to turbulent-like behavior.

The quasi-solitons investigated in the present paper represent only a certain fraction of solitary phenomena in spin systems known in the literature. Another class of solitons exists for classical chains with a particular form of anisotropy that leads to the sine–Gordon equation [6]. Localized spin modes in finite Heisenberg chains with anisotropy have been found in [18, 19]. Other soliton solutions for continuous EOM describing similar systems have been given in [20–23]. Solitonic solutions of a quantum spin chain have been investigated, for example, in [24]. A very large body of literature (see [6] for a comprehensive review) exists which has shown that these EOM are of direct relevance to a wide class of one-dimensional magnetic materials and provide a variety of theoretical models in quantum field theory.

The layout of this paper is as follows. In section 2, starting from the discrete EOM for the interacting spin system, equation (1), we review the well-known exact spin wave solutions, and then proceed to derive a continuum version of the EOM describing modulated spin waves. Section 3 is devoted to deriving the full set of solutions of the first-order version of the continuum EOM, and in particular to showing that any solution necessarily develops a caustic in the course of time. We include examples of numerical solutions of equation (1) showing such behavior. In section 4 we give a detailed analysis of the soliton solutions of the second-order version of the continuum EOM. We obtain a formula for the dependence of the soliton amplitude \( A \) on the wavenumber \( q \), the soliton velocity \( u \), and the magnetic field \( B \). In the limit \( q \to 0 \) this formula reduces to the well-known result for the Landau–Lifshitz equation. In section 5 we present results of our numerical analysis of the discrete EOM of equation (1). These include single quasi-solitons and multiple quasi-solitons starting from initial profiles obtained from soliton solutions of the second-order continuum EOM. Section 6 is devoted to the effects of starting from initial spin configurations that are truncated versions of soliton states, as well as including the coupling of the discrete spins to a heat bath. In section 7 we summarize our results and discuss open questions. Finally, in two appendices we clarify the distinction between the solitons of our new continuum EOM and those of the Landau–Lifshitz equation (appendix B) as well as the relation of some exact solutions for \( N \leq 4 \) to our approximate solutions for \( N > 4 \) (appendix B).

2. Modulated spin waves

We consider classical spin rings with \( N \) spins interacting via ferromagnetic nearest-neighbor coupling. The EOM are given by equation (1) where \( B = B e \) is the dimensionless magnetic field and \( e \) is chosen as a unit vector in the direction of the 3-axis. Mathematically, the case of antiferromagnetic coupling is included since it can be achieved through the transformation \( s_n \mapsto -s_n \). However, solitons which are excitations of a background of fully aligned spins will be thermodynamically stable only in the ferromagnetic case. In the case of antiferromagnetic coupling, an initially prepared soliton will decay with time, and the decay characteristics will be different for rings with even \( N \) (unfrustrated systems) and odd \( N \) (frustrated systems). An analysis of this subject is worthy of future study.

For \( N > 4 \) the general solution of equation (1) cannot be given in closed form. However, as mentioned above, there exist exact solutions (‘spin waves’) of the form
\[
\begin{pmatrix}
\frac{\sqrt{1 - \frac{1}{2}^2} \cos(qn - Bt - \omega t)}{z} \\
\frac{\sqrt{1 - \frac{1}{2}^2} \sin(qn - Bt - \omega t)}{z}
\end{pmatrix},
\]

appears in the limit

\[
\sum_{a=1}^{N} \frac{\partial}{\partial x_a} \left( s_a \cdot s_{a+1} + g \mu B \frac{\partial}{\partial s_a} s_a \right)
\]

on defining classical spin vectors \( s_n = \frac{B}{\sqrt{\sum s_n^2}} s_n \) and units of time \( t_0 = \frac{h}{\Delta x^2} \) and magnetic field \( B_0 = \frac{\partial \Omega}{\partial B} \) in the limit \( s \to \infty \).

\[5\]

The dimensionless form of the EOM follows from the corresponding quantum (Heisenberg) EOM with Hamilton operator \( H = -\frac{\hbar}{2} \sum_{a=1}^{N} \frac{\partial}{\partial x_a} \left( s_a \cdot s_{a+1} + g \mu B \frac{\partial}{\partial s_a} s_a \right) \)

appears in the limit

\[
\sum_{a=1}^{N} \frac{\partial}{\partial x_a} \left( s_a \cdot s_{a+1} + g \mu B \frac{\partial}{\partial s_a} s_a \right)
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on defining classical spin vectors \( s_n = \frac{B}{\sqrt{\sum s_n^2}} s_n \) and units of time \( t_0 = \frac{h}{\Delta x^2} \) and magnetic field \( B_0 = \frac{\partial \Omega}{\partial B} \) in the limit \( s \to \infty \).

\[5\]
where
\[ q = \frac{2\pi k}{N} \quad (k = 0, \ldots, N - 1), \tag{4} \]
the angular frequency \( \omega \) is given by
\[ \omega = 2(1 - \cos q)z \tag{5} \]
and \( z \) is an arbitrary real number in the interval \(-1 < z < 1\).

Our first goal is to obtain a continuum version of equation (1). This is achieved as follows. In equation (3) we replace \( z \) and \( \omega t \) by two sets of site-dependent functions \( z_n(t) \) and \( \omega_n(t) \), respectively, which are assumed to vary slowly over a distance \( a \). That is, \( s_n(t) \) is given by
\[ s_n(t) = \left( \frac{\sqrt{1 - z_n(t)^2} \cos(qn - \omega_n(t))}{\sqrt{1 - z_n(t)^2} \sin(qn - \omega_n(t))} \right). \tag{6} \]

It is convenient to remove the term \( qn \) by means of the transformation
\[ \tilde{\omega}_n(t) = R_3(-qn)s_n(t), \tag{7} \]
where \( R_3(\alpha) \) denotes the matrix of a rotation about the 3-axis with an angle \( \alpha \).

In the continuum approximation we introduce smooth functions \( z(x, t), \varphi(x, t) \) and \( S(x, t) \) such that \( z(na, t) = z_n(t) \) and \( \varphi(na, t) = \varphi_n(t) \), and
\[ S(x, t) = \tilde{S}_{x/a}(t) = \left( \begin{array}{c} \sqrt{1 - z(x, t)^2} \cos(\varphi(x, t)) \\ -\sqrt{1 - z(x, t)^2} \sin(\varphi(x, t)) \end{array} \right). \tag{8} \]

In this approximation we allow the parameter \( q \) to take on any values in the interval \((-\pi, \pi)\), whereas the Landau–Lifshitz equation is obtained in the limit \( q \to 0 \). After some elementary calculations the continuum version of the equation (1) assumes the form
\[ \frac{\partial}{\partial t} S(x, t) = S(x, t) \times H(x, t), \tag{9} \]
where
\[ H(x, t) = \left[ (S(x + a, t) + S(x - a, t)) \cos q \right. \]
\[ \left. + e \times [S(x + a, t) - S(x - a, t)] \sin q \right. \]
\[ \left. + [B + (z(x + a, t) + z(x - a, t))(1 - \cos q)]e \right]. \tag{10} \]

Equations (9) and (10) are equivalent to a partial differential equation (PDE) of infinite order, as is seen by expanding \( S(x \pm a, t) \) in powers of \( a \), so equation (10) may be written as
\[ H = 2 \left( S + \frac{a^2}{2} S'' + \frac{a^4}{4!} S^{(4)} + \cdots \right) \cos q \]
\[ + 2e \times \left( aS' + \frac{a^3}{3!} S^{(3)} + \cdots \right) \sin q \]
\[ + \left[ B + 2 \left( z + \frac{a^2}{2} z'' + \frac{a^4}{4!} z^{(4)} + \cdots \right)(1 - \cos q) \right] e. \tag{11} \]

Here the arguments \((x, t)\) have been suppressed, and we abbreviate the spatial derivatives of \( S \) and \( z \) as a prime and the time derivatives as a dot in what follows.

In the following we consider truncated versions of equations (9) and (10). In the \( n \)th-order approximation we keep terms containing powers of \( a \) through \( a^n \). In this paper we consider zeroth-, first-, and second-order approximations only. The zeroth-order PDE is given by
\[ \dot{S} = (B + 2z(1 - \cos q))S \times e. \tag{12} \]
This equation is solved by the spin wave solution, equation (3), but it also has more general solutions.

3. First-order equations
In the first-order approximation, equations (9) and (11) reduce to
\[ \dot{S} = [B + 2(1 - \cos q)(e \cdot S)]S \times e - 2a \sin q(e \cdot S)S'. \tag{13} \]

Using the representation of equation (8) we can rewrite this equation as
\[ \dot{\varphi} = B + 2z(x, t)((1 - \cos q) - a \sin q \varphi') \tag{14} \]
\[ \dot{z} = -2a \sin q \varphi''. \tag{15} \]

We will now show that the solutions of equations (14) and (15) necessarily develop caustics after some time \( t_c \). That is, these equations cannot provide a satisfactory approximation to equations (9) and (10) for \( t > t_c \). First we consider equation (15), which is an autonomous equation for \( z(x, t) \). Its solution is well known; see e.g. [25]. Equation (15) essentially describes the velocity field of a system of free particles with a given velocity distribution for \( t = 0 \). To make this more transparent, consider the transformation
\[ v(x, t) \equiv z \left( x - \frac{t}{2a \sin q} \right), \tag{16} \]
which transforms equation (15) into
\[ \dot{v} + vv' = 0, \tag{17} \]
which is known as the inviscid Burgers equation; see [26]. It follows that \( v \) is constant along the lines with slope \( \frac{dv}{dx} = v \) whence the above kinematical interpretation follows. Let \( \xi = x - ut \) be the \( x \)-coordinate of the intersection of the axis \( t = 0 \) and the line through the point \((x, t)\) with slope \( a \). Hence
\[ u = v(\xi, 0), \tag{18} \]
which yields a parametric representation of the graph of the general solution \( x \mapsto v(x, t) \) of equation (17) for fixed \( t \), namely
\[ x = \xi + v(\xi, 0)t, \tag{19} \]
where \( v(\xi, 0) \) is an arbitrary initial condition for the PDE considered. An example of the resulting line field is given in figure 1. We see that there are domains where the
lines in the line field intersect, bounded by curves called ‘caustics’. These domains correspond to points where the parametric representation of equations (18) and (19) defines a multi-valued function. The earliest time when caustics appear is given by

\[ t_c = -\frac{1}{\frac{\partial v(\xi_0, 0)}{\partial \xi}} \],

(20)

where \( \xi_0 \) is the point with the largest negative derivative of \( v(\xi, 0) \). Initial profiles \( v(\xi, 0) \) with only positive slope do not have caustics for \( t > 0 \) but this cannot be realized for a spin ring with periodic boundary conditions.

The same analysis applies to the original form, equation (15), except that the caustic time \( t_c \) in equation (20) has to be divided by \( 2a \sin q \). Hence the first-order PDE predicts that after some time \( t_c \) the profile of the 3-components of the spin ring develops an infinite slope. That is, for later times the first-order analysis is no longer valid and the EOM must be studied by using higher order approximations of equations (9) and (11). Remarkably, there exist examples where the numerical solution of equation (1) is well described by its first-order approximation for times \( t \) with \( 0 \leq t < t_c \). Close to the time \( t = t_c \) the smooth ‘laminar’ time evolution breaks down and a different regime begins to penetrate the spin ring. We will call this regime ‘turbulent’ for the sake of simplicity, but we do not know whether it is genuinely chaotic or still regular on a shorter length scale. From our numerical results the possibility of the latter cannot be excluded. Figure 2 shows the numerical solution \( z_0(t) \) of equation (1) for an \( N = 100 \) spin ring with \( q = 16\pi/100 \), together with the first-order PDE solution \( z(x, t) \) at the time \( t = t_c \). The two sets of results are in close agreement, although at time \( t = t_c \) the continuum approximation is no longer applicable.

We remark that equation (14) can also be solved in closed form. Its general solution utilizes the solution \( z(x, t) \) of equation (15) already obtained and the initial angle distribution \( \varphi_0(x) = \varphi(x, 0) \) and it is given by

\[
\varphi(x, t) = \varphi_0(x) - 2a \sin q z(x, t) + z(x, t) 2(1 - \cos q) t + B t.
\]

(21)

Hence the effects of the caustics will also be manifested in the behavior of the azimuthal angles of the spin vectors.

4. The second-order equations

In section 3 we have seen that the first-order approximation predicts its own breakdown since it will necessarily lead to a caustic or ‘turbulent’ behavior. Hence the question arises of whether higher order approximations give rise to the same or different effects. The second-order equation is given by

\[
\dot{S} = [B + 2(1 - \cos q)(e \cdot S)] S \times e - 2a \sin q (e \cdot S) S' + a^2 S \times [\cos q S'' + (1 - \cos q)(e \cdot S'')] e.
\]

(22)

Substituting equation (8) leads to

\[
\dot{\varphi} = B + 2a(1 - \cos q - a \sin q'') + a^2 \left[ z'' + z \cos q \left( \varphi'' + \frac{z''}{1 - z^2} + \frac{z^2}{(1 - z^2)^2} \right) \right],
\]

(23)

\[
\dot{z} = -2a \sin q z' + a^2 \cos q (2z z' \varphi' - (1 - z^2) \varphi'').
\]

(24)

In solving equation (22) numerically and analytically we have found instances where the onset of turbulence is accelerated as well as instances where it is entirely suppressed. We do not, however, have a clear understanding about the underlying causes for either behavior. As an example of the first case, acceleration of turbulence, in figure 3 we compare results of the numerical solution of the EOM of equation (1) with the numerical solution of equations (23) and (24). The time of the onset of the turbulence is approximately 2.75 times shorter than that predicted by the first-order approximation.

The other case, preservation of laminar behavior, due to second-order effects, can be most impressively demonstrated through the existence of solitons, presented in section 4.1.

4.1. Exact single-soliton solutions

The mathematical derivation of soliton solutions is to a large extent analogous to the Landau–Lifshitz case; see [12, 16]. To simplify the derivation we set \( a = 1 \) in the following.

We seek solutions of equations (23) and (24) of the form

\[
\varphi(x, t) = \Phi(x - ut)
\]

(25)

\[
z(x, t) = Z(x - ut).
\]

(26)

The resulting equation for \( Z(x) \) can be integrated once yielding

\[
\Phi' = \sec q \frac{u(Z - Z_0) - Z^2 \sin q}{1 - Z^2},
\]

(27)

where \( Z_0 \) is some integration constant. Substituting this into the equation resulting from equation (23) yields a second-order equation for \( Z(x) \). Multiplying with \( Z(x) \) and integrating with respect to \( x \) yields an expression for \( Z(x)^2 \) containing an integration constant \( c \). This expression is
analogous to a one-dimensional potential if $Z'(x)^2$ is viewed as the kinetic energy and the total energy is set equal to 0, namely

$$Z^2 = -V(Z) = \frac{1}{2(1 - Z^2(1 - \cos q))}$$

$$× (\sec q - 1 - \frac{2u^2 - 2u^2Z_0^2 + \cos 2q + 4u^2Z_0Z}{2})$$

$$+ 2Z^2 - 8Z^4 \sin^4 \frac{q}{2} - 2(c + 2uZ_0 \tan q)$$

$$+ 2BZ + (2c - \cos q)Z^2 - 2(B + u \tan q)Z^3]. \quad (28)$$

$V(z)$ will be called the pseudopotential. Since $-V(Z)$ is quartic in $Z$ in the numerator and quadratic in the denominator, the integral

$$x - x_0 = \int \frac{dZ}{\sqrt{-V(Z)}} \quad (29)$$

can be expressed in terms of elliptic functions of the first and third kind; see [29]. The inverse function of equation (29), together with the integral of equation (27), gives the inverse function of the soliton solution. However, the analytic expression is very complicated and it is far simpler to calculate the integral of equation (29) numerically. The poles of $V(z)$ lie at $z_p = \frac{\pm 1}{\sqrt{1 - \cos q}}$ and thus are outside the physical domain $Z \in [-1, 1]$ for $0 < |q| < \frac{\pi}{2}$. Hence we will restrict our treatment to the case

$$0 < |q| < \frac{\pi}{2} \quad (30)$$

in the following.

The remaining task is to determine values of the parameters $q, B, u, Z_0,$ and $c$ for which solitary solutions of equations (23) and (24) exist. The inverse function of (29) has the form of a soliton profile if $V(Z)$ has a double root at $Z = Z_1$ and a single root at $Z = Z_2$ such that $-1 < Z_1 < Z_2 < 1$ and $V(Z)$ is negative in the interval $(Z_1, Z_2)$. The spin configuration with $Z = -1$ is not changed by the transformation of equation (7); hence the choice $Z_1 = -1$ yields solitons which are localized excitations of a fully aligned spin background. Thus for the rest of the paper we will only consider the case $Z_1 = -1$.

The condition that $V(Z)$ has a double root at $Z = Z_1 = -1$ gives us two parameters as a function of the remaining two:

$$c = 2(B - 1) + \frac{(2 + Z_0)^2 \cos q + (Z_0^2 - 2) \sec q}{(1 + Z_0)^2} \quad (31)$$

$$u = -\frac{\sin q}{1 + Z_0}. \quad (32)$$

The soliton solutions hence depend on three parameters which we choose to be $B, q$ and $u$. A typical form of $V(Z)$ is shown in figure 4. For the numerical studies in sections 5 and 6 we mostly chose negative wavenumbers $q$ in order to get positive velocities according to equation (32).

The remaining roots $Z_{2,3}$ are

$$Z_{2,3} = \frac{1}{8} \cos^4 \frac{q}{2} [3 + \cos 2q + 2u \sin q]$$

$$- 2 \cos q (2 - B \mp f(B, q, u))] \quad (33)$$
Figure 3. Comparison of a numerical solution for $z_n(t)$ at fixed times $t = 0, 12, \ldots, 60$ of the EOM for an $N = 100$ spin ring (blue dots) with the numerical solution of its second-order continuum approximation equations (23) and (24) (solid red curve) at the times $t = 0, 12, \ldots, 48$. The turbulent regime begins to spread at approximately $t = 48$. By $t = 60$ the numerical solution breaks down and hence cannot be drawn.

Figure 4. The pseudopotential $V(Z)$ according to equation (28) corresponding to the parameters $B = 0$, $q = -\pi/4$ and $u = 1$. Where

$$f(B, q, u) = \sqrt{B^2 - 2u^2 + 2u \sec q (u + B \sin q)}. \quad (34)$$

The condition that $V(Z)$ is negative in the interval $Z \in (-1, Z_2)$ or, equivalently, $V'(-1) < 0$, which is necessary for the existence of solitons, leads to the inequalities

$$-2 \sin q - 2 \cos q \sqrt{(2 - B) \sec q - 2} < u < -2 \sin q + 2 \cos q \sqrt{(2 - B) \sec q - 2}. \quad (35)$$

Figure 5. The soliton velocities $u$ bounded by a function of $q$ and $B$ according to equation (35). The curves shown correspond to $B = -2, -1.5, \ldots, 1.5$. The $\infty$-shaped red curve corresponds to $B = 0$. For $B \to 2$ the curves shrink to two points at $q = \pm \pi/2, u = \mp 2$.

This defines a certain physical domain in the $(B, q, u)$-plane; see figure 5, where solitons exist. It is bounded by $B \leq 2$. The inequalities further imply that only the root $Z_2$ of $V(Z)$ with the minus sign in equation (33) lies inside the physical domain $(-1, 1)$.

Equation (33) yields an explicit relation between the amplitude $A = Z_2 - Z_1 = 1 + Z_2$ and the velocity $u$ of the
Figure 6. Soliton amplitude $A$ as a function of wavenumber $q$ and velocity $U$ for $B = 0$ according to equation (38).

A soliton of the form

$$A = 2 + \frac{u \sin q + (B + f(B, q, u)) \cos q}{4 \sin^2 \frac{q}{2}},$$

with $f(B, q, u)$ defined by equation (34). The two limiting forms are

$$A = 2 + \frac{u^2}{2B} \quad \text{for} \quad q \to 0 \quad \text{and} \quad B < 0,$$

(37)

to be compared to equation (4.7) in [16], and

$$A = 2 + \frac{1}{4} \csc^2 \frac{q}{2} \left( u \sin q - |u|\sqrt{2(\sec q - 1)} \cos q \right)$$

for $B \to 0$.

(38)

The physical part of the surface in $(q, u, A)$-space spanned by the lines defined by equation (38) with $q = \text{const}$ is shown in figure 6. From these equations it follows that the amplitude $A$ diverges for $B, q \to 0$ and hence no solitons exist in this case in accordance with [16].

5. Numerical soliton solutions

In this section we summarize some of our results for numerical solutions of the EOM, equation (1), in the case $B = 0$, for finite spin rings. The initial spin configurations are selected to be soliton profiles as calculated from the second-order continuum PDE using equations (27)–(29). Figure 7 shows the initial profile of a discrete soliton for a spin ring with $N = 100$ and parameters $q = -8\pi/100$ and $u = \sin |q|$. The soliton appears as a localized deviation from an otherwise ferromagnetic alignment of spins. Using this initial profile we solve the EOM, equation (1), numerically to determine the time evolution of the spin vectors. The results are shown in figure 8. In the inset we provide a snapshot of $z_n(t)$ for a particular time $t = 2000$. A comprehensive picture for all calculated times is best displayed as a color contour plot, where the color gives the value of $z_n(t)$ according to the coding defined in the legend. The strict integrity of the solution as a function of time is striking.

Throughout the remainder of this paper we use color contour plots since they provide a very effective tool for visualizing the overall time evolution of the spin profile as measured by $z_n(t)$. In particular, these plots allow one to detect even small changes in the profile, its speed, etc.

Using the initial profile for a single-soliton solution it is easy to prepare the case of two identical solitons moving toward each other. We copy the single-soliton profile of the $N = 100$ spin ring onto one half of an $N = 200$ spin ring and its reversed version onto the second half of the spin ring. As is seen in figure 9, the numerical solution of equation (1) describes two solitons that collide and then move apart while retaining their initial shapes and velocities. This behavior is well known for exact $N$-soliton solutions of other nonlinear wave equations; see e.g. [29]. We have observed repeated collisions of the soliton pairs without noticeable deformation. By using a similar procedure we have created the situation where a faster soliton overtakes a slower one, and the results are shown in figure 10. One can see that the penetration of...
Figure 9. Collision of two solitons of an $N = 200$ spin ring. The initial profile has been calculated from equations (27)–(29) using the parameters $q = \pm \frac{16\pi}{200}$ and $u = -\sin q$. The numerical solutions are displayed for $t = 0, \ldots, 4000$, including the times $t_1 \approx 1000$ and $t_2 \approx 2800$ where collision between the two solitons take place.

Figure 10. Numerical two-soliton solution $z_n(t)$ for an $N = 200$ spin ring and initial data calculated from equations (27)–(29) using the parameters $q = -\frac{16\pi}{200}$ and $u = 0.625 \sin |q|$, respectively. The solution is displayed for $t = 0, \ldots, 2200$. In this case two solitons are created which move in the same direction while one soliton is twice as fast as the other, eventually penetrating the slower one.

Figure 11. Time evolution for an $N = 100$ spin ring and an initial profile, where only $M = 3$ spin vectors are specified as in figure 7 and the remaining 97 spin vectors are initially set parallel to the $z$-axis. Even in this case a rather stable quasi-soliton is created. However, with its generation a small localized perturbation appears which moves in the opposite direction. Its interference with the quasi-soliton can be observed several times (first at time $t \approx 100$).

6. Effects of truncation and finite temperature

The purpose of this section is to explore the extent to which quasi-solitons are robust to various perturbations. We begin by investigating the time evolution of symmetrically truncated versions of initial states that exhibit soliton behavior. In the truncated version, for all but $M$ of the $N$ spins the value of $z_n(0)$ is set equal to $-1$, whereas we retain the original values of $z_n(0)$ for the $M$ spins. The latter are chosen to be centered about the site having the largest value of $z_n(0)$.

On the basis of the initial profile used for the soliton shown in figure 8 ($N = 100$) we have used $M = 10$ as well as $M = 3$ for the corresponding truncated versions. As shown in figure 11, soliton behavior is maintained even for $M = 3$; there is only an increased level of background noise while the major features of the quasi-soliton are retained.

While our quasi-soliton solutions appear to be robust against symmetric truncation we have found that asymmetric off-center truncation leads to far less stable behavior, i.e. the soliton decays after some time which depends on the extent of the asymmetry.

Another way of truncating the initial profile is to reduce the system size while leaving the initial profile intact. Our study is based on the numerical solution of equation (1) with the initial data calculated from equations (27)–(29) using the parameters $q = -\frac{32\pi}{100}$ and $u = \sin |q|$. We find that soliton behavior occurs on using this initial profile when the ring includes 100 or more spins. This initial profile is then symmetrically truncated about the maximum of $z_n(t)$ so as to provide initial values for rings with progressively fewer spins. We continue to find soliton behavior apart from minor background noise and a slight pulsation of the amplitude $z_n(t)$. Even when the number of spins has been reduced to as small as $N = 11$, soliton behavior is still visible; however the pulsation of the amplitude is by now strongly enhanced (see figure A.1).
While in all of the above cases the total energy is a conserved quantity, we now show one specific example of the behavior of the quasi-solitons when the spin system is coupled to a heat bath. The behavior of classical spin systems in contact with a heat bath can be studied very effectively using a constant temperature stochastic spin dynamics approach, such as that used in [13, 28]. Here the spin system is coupled to a heat bath according to a Langevin-type approach by including a Landau–Lifshitz damping term as well as a fluctuating force with white noise characteristics.

Starting from prescribed initial conditions such as those used in figure 8 the temperature is set to a value \( T > 0 \) and the trajectory of the system is calculated numerically by solving a stochastic Landau–Lifshitz equation, thereby allowing the spin system to exchange energy with its environment [13] [28]. Our results are shown in figure A.2. Thermal fluctuations lead to a decay of the quasi-soliton, driving the system toward its (ferromagnetic) equilibrium configuration. However, the soliton persists for a significant length of time before eventually dissipating, as expected.

The cases considered in this section provide a picture of quasi-solitons in classical Heisenberg rings that are remarkably robust even when perturbed by truncations, small system size, and heat bath couplings.

7. Summary

The overriding theme of this paper is that relatively small classical Heisenberg rings exhibit a rich variety of dynamical properties including soliton behavior. We have proposed that an effective strategy for exploring the dynamical behavior of these rings is to solve the system of discrete EOM of equation (1) upon selecting initial spin configurations that are discretized versions of the solutions of a new continuum EOM that we derived by allowing for continuous modulations of the spin wave solutions given by equation (3). In practice, due to the complexity of the analysis, we have limited our analysis to a second-order PDE version, equation (22), of the continuous EOM of equations (9) and (10). This second-order PDE is a generalization of the Landau–Lifshitz equation that has been used extensively in studying one-dimensional magnetic systems, e.g. spin chains. Among the class of solutions of equation (22) we have found soliton solutions. Using discretized versions of the soliton solutions as input data, we have found that the discrete EOM of equation (1) possess quasi-soliton solutions. The robustness of these discrete quasi-solitons has been demonstrated both by considering truncated versions of continuum soliton solutions and by investigating the dynamical behavior when the spins are coupled to a heat bath at finite temperatures. Besides the quasi-soliton behavior there is a vast diversity of other dynamical behavior exhibited by finite spin rings. We have only sparsely investigated this diversity, and at present we have only a limited physical understanding of the behavior that we have observed. We conjecture that the existence of robust quasi-solitons can be explained by the existence of exact solitary solutions of equation (1), i.e. localized solutions satisfying \( \tilde{s}_{n+1}(t + T/N) = \tilde{s}_n(t) \) for all \( n = 1, \ldots, N \) and some fixed \( T \).

As emphasized in section 1, apart from any intrinsic interest in the dynamics of classical Heisenberg spins rings, we were motivated to undertake the present study as a first step of a broad theoretical investigation of the dynamical properties of magnetic molecules. With our findings of robust quasi-solitons in classical spin rings, we suggest that the next step is to deal with the question of what the quantum analogue of solitons in spin rings is, and how these might be detected by experiment. In particular, it would be worth extending some of the results of earlier work on quantum spin chains; see e.g. [30] and [24].

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Appendix A. Relation to solitons of the Landau–Lifshitz equation

The usual way to derive soliton solutions of the classical Heisenberg spin chain is to directly consider the continuum version of equation (1), i.e. replacing \( s_n(t) \) by \( s(x, t) \), where \( x = na \), and deriving the Landau–Lifshitz (LL) equation (2) as the second-order expansion of the EOM. Single and multiple solitons are then found as special exact solutions of this equation.

In this paper we used a different, more general approach, which may be called the modulated spin wave (MSW) ansatz, followed by a second-order expansion of the EOM w.r.t. \( a \). It contains the usual approach as the limit case of the spin wavenumber \( q \to 0 \). In order to elucidate the difference between the two classes of solitons we will present some further related results based on a reversed order of the steps toward the soliton solutions of the EOM. This means that we will first consider the second-order expansion of the EOM and subsequently impose the MSW ansatz, this resulting in different equations.

We will start with the LL equation (2) and prove that, in the case of vanishing field \( B = 0 \), the only traveling wave (TW) solutions are continuous versions of the spin waves described by equation (3). Hence no soliton solutions of equation (2) exist with \( B = 0 \) in contrast to the solitons considered in this paper. This result of course already follows from the analysis of LL solitons given, for example, in [16] but can also be derived in an elementary way as follows.

The TW ansatz

\[
S(x, t) = S(x - ut)
\]
equations (27)–(29) using the parameters $q$ and $\phi$.

Figure A.1. Time evolution for an $N = 11$ spin ring, where the initial data are selected as described in the text. While some features of soliton-like behavior are still visible, because of the small value of $N$ the results are strongly affected by background noise and pulsation of the amplitude $z_n(t)$.

Figure A.2. Finite temperature effects on a quasi-soliton solution $z_n(t)$ for an $N = 100$ spin ring and initial data calculated from equations (27)–(29) using the parameters $q = -\delta \pi /100$ and $u = \sin |q|$. Comparing to the $T = 0$ case shown in figure 8, one observes that thermal fluctuations lead to a decay of the soliton; however, it persists for a significant length of time before eventually dissipating.

is inserted into equation (2) and yields

$$-aS' = S'' \times S = \frac{d}{dx} (S' \times S).$$  

Replacing $z_n$ by $z$ and $z_n'$ by $z'$, this equation becomes

$$S' \times S + uS = S_0 = \text{const.}$$  

Upon forming scalar and vector products of $S$ and equation (43) we obtain

$$S_0 \cdot S = u$$  

and

$$S \times S_0 = S \times (S' \times S)$$  

$$= S'S \cdot S - SS' \cdot S$$  

$$= S'$.$

This means that, for arbitrary fixed $x$, $S$ precesses around the constant vector $-S_0$ with angular velocity $|S_0|$ and $S(x - ut)$ represents a continuous spin wave solution.

Now let us write the LL equation in the form of equations (23), (24) with $q = 0$:

$$\dot{\psi} = B + a^2 \left[ z'''' + z \left( \psi'' + \frac{zz''}{1 - z^2} + \frac{z'^2}{(1 - z^2)^2} \right) \right]$$  

$$\dot{z} = a^2 \left[ 2zz' \psi' - (1 - z^2) \psi'' \right].$$

For the subsequent analysis we employ the MSW ansatz in the form

$$\psi(x, t) = \hat{\psi}(x, t) - \frac{q}{a^2} x.$$  

For the EOM this substitution has the mere effect that $\dot{\psi}'(x, t)$ will be replaced by $\dot{\psi}''(x, t) - \frac{q}{a^2}$ and hence the terms in equations (48), (49) have to be rearranged according to their dependence on $a$. In particular, new terms proportional to $a^0$ and $a^1$ are generated which were absent in the original equations (48), (49). The result reads, skipping the tilde,

$$\dot{\psi} = B + q^2 z - 2aqz'$$

$$+ a^2 \left[ z'' + z \left( \psi'' + \frac{zz''}{1 - z^2} + \frac{z'^2}{(1 - z^2)^2} \right) \right]$$

$$\dot{z} = -2aqzz' + a^2 \left[ 2zz' \psi' - (1 - z^2) \psi'' \right].$$

This is nothing but a truncated version of equations (23) and (24) obtained from the first terms of a Taylor series expansion of $\sin q$ and $\cos q$. It can be shown, in analogy to the approach of section 4.1, that the equations (51) and (52) admit single-soliton solutions, the $z$-component of which is of the form

$$z(x, t) = \frac{2}{B + qu} \frac{u^2}{2} \times \text{sech}^2 \left[ \sqrt{-(B + u(q + u/4))(x - ut)} \right].$$

Interestingly, the $\text{sech}^2$ shape of $z(x, t)$ is similar to that of the solitons of the Korteweg–de Vries equation (see [27] 1.1.16), but the dependences on $u$ of its amplitude and width are different.

The solitons given in equation (53) stand in some intermediate position between the well-known $q = 0$ solitons of the LL equation and the $q \neq 0$ solutions of equations (23), (24) described in section 4.1. Together with the former they are solutions of the LL equations (48) and (49), although not of the TW type, which is destroyed by the back-transformation (50). This also explains why they persist
in the $B = 0$ case in contrast to the $q = 0$ LL solitons. Moreover, the solitons of equation (53) can be used as analytical approximations of certain numerical quasi-soliton solutions of equation (1) in the same way as the soliton solutions of equations (23) and (24). It turns out that, at least for values of $q$ close to $8\pi/100$, they are slightly poorer approximations than the latter ones. For example, if $q = 8\pi/100, B = 0$ and $A = 1.5$, the velocity $u$ calculated by means of (38) exceeds the velocity $u_0 = 0.244$ of the numerical quasi-soliton by 1.9%, whereas $u$ according to equation (53) exceeds $u_0$ by 3.4%.

The latter result can be explained as follows. If one considers higher order approximations of the EOM w.r.t. $a$ together with the MSW ansatz of equation (50) the following replacements occur:

\[ \begin{align*}
(a\tilde{\phi})^m &\rightarrow a^m \left( \tilde{\phi} - \frac{q}{a} \right)^m \\
&= (-q)^m + m a \tilde{\phi} (-q)^{m-1} + \left( \frac{m}{2} \right) a^2 \tilde{\phi}^2 (-q)^{m-2} \\
&\quad + \mathcal{O}(a^3).
\end{align*} \]

They lead to corrections to the equations (51), (52) in second and lower order in $a$. One thus obtains a hierarchy of equations labeled by an even integer $n$, corresponding to the highest power of $a$ to be considered in the EOM, probably possessing soliton solutions for all $n$. They would progressively give better and better approximations to the second-order equations (23) and (24). In fact, summing up all contributions from any power of $a$ would eventually yield an alternative derivation of equations (23) and (24).

To summarize, the $q \neq 0$ soliton solutions of equations (23) and (24), of those of equations (51) and (52) and the corresponding numerical quasi-soliton solutions of (1) are in an approximate correspondence. But all three kinds of solitons are different from and not approximated by the well-known $q = 0$ solitons of the LL equations (48) and (49).

**Appendix B. Exact solutions for small $N$**

As mentioned in section 2 the equation (1) cannot be solved in closed form for $N > 4$. Several studies have focused on the equation of state for small ($N \leq 4$) classical and quantum clusters of spins as well as their spin dynamics; see e.g. [7–11]. In all of the systems considered one can identify at least $N$ commuting constants of motion and hence these systems are integrable in the classical sense and also quantum mechanically; see e.g. [31]. In particular, this applies to spin rings with $N = 2, 3, 4$ spins whereas for $N > 4$ the dynamics of the spin rings will exhibit chaotic motion except for special initial conditions.

One may ask how the exact solutions for $N \leq 4$ are related to the approximate solutions investigated in this paper. It can be easily shown that for rings with $N = 2$ and 3 all spins will uniformly rotate about the total spin vector; hence all solutions of (1) are spin wave solutions corresponding to (3) and there is no possibility of modulated spin waves. However, for $N = 4$ new possibilities arise. Of course, it makes no sense to speak of (quasi-)solitons realized by four spins. But we may look for solutions of (1) which share with the soliton solutions the traveling wave (TW) property expressed in (25) and (26). Note that the TW property applies to motions of spins after the transformation (7) is made; hence its proper formulation for discrete spins will read

\[ \tilde{s}_n \left( t + \frac{T}{N} \right) = \tilde{s}_{n+1}(t), \quad n = 0, 1, \ldots, N - 1, \]

where we have slightly modified the numbering of spins. In particular, the motion satisfying (56) will be periodic in time with period $T$. It is an open question whether solutions of (1) exist for $N > 4$ satisfying the TW property (56), except the well-known spin waves. Hence the positive answer to this question in the case $N = 4$ will be of some interest in this context.

We have found the following two-parameter family of traveling wave solutions for $N = 4$ characterized by

\[ |s_0 + s_2| = |s_1 + s_3|, \]

\[ s \equiv s_0 + s_1 + s_2 + s_4 = -B \quad \text{and} \]

\[ q = \pi, \quad \text{i.e.} \quad k = 2 \quad \text{in} \quad (4). \]

As in section 2 we choose our coordinate system such that $s = -B = -Be_3$. In this case

\[ \tilde{s}_0 = \tilde{s}_0, \quad s_2 = \tilde{s}_2, \quad \text{and} \]

\[ \tilde{s}_1 = Rs_1, \quad \tilde{s}_3 = Rs_3, \]

where

\[ R = R_3(\pi) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \]

The solution can be visualized as four unit vectors $\tilde{s}_0, \tilde{s}_1, \tilde{s}_2, \tilde{s}_3$ pointing to the vertices of a square which is uniformly rotating in spin space; see figure B.1.
Analytically, the solution assumes the form
\[
\mathbf{s}_0(t) = \begin{pmatrix}
\cos \phi \sin \theta & -\sin \phi \cos \theta \sin(2t \cos \phi) \\
\sin \phi \cos(2t \cos \phi) & \cos \phi \cos \theta + \sin \phi \sin \theta \sin(2t \cos \theta) \\
\cos \phi \sin \theta & \sin \phi \cos \theta \sin(2t \cos \phi)
\end{pmatrix},
\] (63)
the other spin vectors being obtained from (56) where
\[T = \frac{2\pi}{\omega} = \frac{\pi}{\cos \phi}.\] (64)
Here \(\phi\) and \(\theta\) are two parameters from the intervals \(\phi \in (0, 2\pi)\) and \(\theta \in (0, \pi)\). There exist other non-trivial TW solutions for the spin ring with \(N = 4\) which are not mentioned here since we are only concerned with the question of whether any exist.

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