Solitary objects
on quantum spin rings

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Dipl.-Phys. Pavlo Shchelokovskyy
aus Charkiw / Ukraine

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Betreuer : apl. Prof. Dr. Jürgen Schnack
            apl. Prof. Dr. Heinz-Jürgen Schmidt
            Prof. Dr. Klaus Bärwinkel
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1. Introduction

The central aim of this work is to investigate whether soliton like localized states exist in magnetic ring molecules. It is also of interest to determine their properties, i.e. whether they have characteristic quantum numbers or other regularities.

Magnetic molecules are quantum spin systems which cannot be described neither by a continuous spin density nor by classical spins. Therefore, ring molecules provide good candidates to accommodate quantum magnetic solitons. In addition solitons may turn out to be a valuable tool to investigate magnetic molecules experimentally. If the characteristics of magnetic solitons can unambiguously be connected to the structure of the spin Hamiltonian, the measurement of the soliton properties may result in a more accurate determination of the Hamiltonian than given by other methods.

Since magnetic molecules are essentially quantum systems, one cannot employ definitions used in connection with classical solitons, but needs to redefine what solitary objects on a quantum spin system with translational symmetry ought to be. Thus, we will start our contribution by defining which quantum states possess solitary character. In addition we will discuss useful observables in order to visualize solitary quantum states.

Then using complete diagonalization techniques and thus avoiding any classical or continuum approximations we demonstrate for various quantum spin rings that solitary quantum states indeed exist, and that they are moving around the spin ring without changing their shape in the course of time.

This thesis is organized as follows. In the Chapter 1 a short introduction to the basics and history of the magnetic spin ideas along with ones for solitons is given. After that Chapters 2 and 3 provide an overview of the main achievements in classical and quantum theory of one-dimensional magnetic spin systems and solitary excitations.

Chapter 4 contains a description of the system under our investigation. Different operators are introduced and discussed with their corresponding eigenvectors and various basis sets of the Hilbert space of the system are built on them. Also important commutation relations between operators of the system are established and
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their consequences are pointed out.

In the Chapter 5 the new definition of the solitary object for a quantum magnetic spin system is introduced. Based on it, the dispersion relation of a linear type is obtained, allowing to choose particular basis states of the system which can contribute to a solitary object. Useful observables of the system are discussed, and the third component of the local spin (related to the local magnetization) is calculated. The question of stability of the solitary objects is also taken under consideration in this chapter.

Chapter 6 presents results of numerical calculations made for systems of different size with different Hamiltonians. It is shown, that some systems can host solitary objects introduced in the previous chapters, and examples of such objects are provided.

Finally, results of this work are summarized in the Chapter 7, and an outlook to the possible development of the approach is given.

1.1. Magnetic spin systems

1.1.1. The concept of spin in quantum mechanics

In the beginning of the XX century a certain number of experiments (such as Stern-Gerlach experiment) was accumulated, which state of physical theory, in particular quantum mechanics, of those days failed to describe adequately. This problem was solved in 1925, when Ralph Kronig (unpublished) and independently George Uhlenbeck and Samuel Goudsmit [1, 2] introduced the concept of spin in quantum physics.

In modern physics, spin is an intrinsic angular momentum associated with microscopic particles. It is a purely quantum mechanical phenomenon without any analogy in classical mechanics. Whereas classical angular momentum arises from the rotation of an extended object, spin is not associated with any rotating internal masses, but is intrinsic to the particle itself. Elementary particles such as the electron can have non-zero spin, even though they are point particles possessing no internal structure.

As a quantum mechanical property, spin possesses a number of qualities that distinguish it from classical angular momentum. It is quantized, and can only take on discrete values. For instance, the spin angular momentum of an electron, measured along any particular direction, can only take on the values $+\hbar/2$ or $-\hbar/2$. Fur-
furthermore, the magnitude of the spin (a direction-independent quantity) is uniquely
determined by the type of particle. Electrons are said to be "spin-half" particles,
because the magnitude of every electron’s spin is one half times $\hbar$. Other spin-half
particles include neutrinos, protons, and neutrons. Photons are spin-one particles,
and the hypothetical graviton is a spin-two particle. Certain exotic particles, such
as pions, possess spin zero. The principles of quantum mechanics indicate that spin
is restricted to integer or half-integer values.

Mathematically, spin is not described by a vector, unlike classical angular mo-
momentum. It is described by objects known as spinors, which act differently from
vectors under coordinate rotations.

It turns out that the spin of a particle is closely related to its properties in sta-
tistical mechanics. Particles with half-integer spin obey Fermi-Dirac statistics, and
are known as fermions. They are subject to the Pauli exclusion principle, which
forbids them from sharing quantum states, and are described in quantum theory by
"antisymmetric states". Particles with integer spin, on the other hand, obey Bose-
Einstein statistics, and are known as bosons. These particles can share quantum
states, and are described using "symmetric states". This relation between spin of
the particle and type of statistic it obeys is known as the spin-statistics theorem,
which was proved by Wolfgang Pauli in 1940 [3]. This theorem relies on both quan-
tum mechanics and the theory of special relativity. In fact, the connection between
spin and statistics is one of the most important and remarkable consequences of
special relativity.

Particles with spin possess a magnetic moment, just like a rotating electrically
charged body in classical physics. However, this magnetic moment exists even for
point particles like the electron, and for electrically neutral particles like the neutron.
This magnetic moment can be experimentally observed, by the deflection of particles
by inhomogeneous magnetic fields (as in the Stern-Gerlach experiment) or by the
magnetic fields generated by the particles themselves. In particular, ferromagnetism
arises from the alignment of the spins of the atoms in a solid.

Spin was first discovered in the context of the emission spectrum of alkali metals.
To explain it Wolfgang Pauli in 1924 introduced what he called a "two-valued quan-
tum degree of freedom" associated with the electron in the outermost shell [4]. This
allowed him to formulate the Pauli exclusion principle, stating that no two electrons
can share the same quantum numbers. In 1927 Pauli formalized the theory of spin
using the theory of quantum mechanics discovered by Schrödinger and Heisenberg,
creating the non-relativistic spin theory [5]. Starting point of the relativistic theory
of spin was the paper of Paul Dirac, published in 1928, where he introduced his Dirac equations for relativistic electron [6, 7].

1.1.2. Models of the spin systems

Magnetic materials may be modeled by a system of spins located at certain positions in a lattice, where the interaction of neighboring spins contributes to the total energy of the system.

The general form of the Hamiltonian for a one-dimensional spin system looks as follows [8]:

\[
\hat{H} = -\sum_{i,j} \tilde{S}_i J_{ij} \tilde{S}_j - \sum_i \tilde{S}_i \tilde{F}_i ,
\]

with indices denoting a particular spin site. Here \( J_{ij} \) is spin-spin coupling and is generally a tensor, and \( \tilde{F}_i \) is some external field and is generally a vector.

The simplest model of the magnetic system, called Ising model, results from the (1.1) under following approximations: the dimensionality of the spin \( S_i \) is taken to be one, interspin interaction has nearest-neighbors type (\( J_{ij} = J \) only if \( j = i \pm 1 \)), and the external field \( F \) is constant for all spin sites.

More generally, the term "Ising model" used to name every model where spin is one-dimensional. An opposite case, where dimension of the spin is larger than one, is called Potts model. In particular, the Potts model with 3-dimensional spin is called the Heisenberg model.

In general, the spin-spin interaction may be anisotropic or isotropic, both in the space and the spin dimensions. The spin-spin coupling can be nearest neighbor, farther than nearest neighbor, etc. One can also consider either a zero or a nonzero external field, \( F \), which may be coupled either isotropically or anisotropically in the space and spin dimensions. Another detail that arises is whether or not the spins have a fixed size. There are so-called soft spin models [9], where the spins are allowed to have any size, but the Hamiltonian for these soft-spin models is generally taken to be different from that of equation (1.1).

1.2. The rise of solitons

The beginning of soliton physics in often dated back to the month of August 1834 when John Scott Russell observed the "great wave of translation". He describes what he saw in Ref. [10]:

"I believe I shall best introduce this phenomenon by describing the circumstances of my own first acquaintance with it. I was observing the motion of a boat which was pulled rapidly along a narrow channel by a pair of horses, when the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation; then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well defined heap of water, which continued its course along the channel apparently without change of form or dimension of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to foot and half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such, in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon which I have called the Wave of Translation, a name which it now very generally bears."

Complete theoretical explanation of the phenomena observed by Russell was done only 60 years later, in 1895, by Korteweg and de Vries, who derived and solved a nonlinear partial differential equation for surface waves in shallow water, named soon after them (shortly referred as KdV-equation). The explicit word "soliton" was first mentioned in the talk of Martin Kruskal in 1965 Ref. [11], which was devoted to solitary solutions of KdV-equation.

The most simple form of the KdV-equation can be written as:

$$\frac{\partial u}{\partial t} + 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0.$$  (1.2)

One of the solutions of this PDE is the following:

$$u(x, t) = \frac{1}{2}c \text{sech}^2 \left( \frac{1}{2}\sqrt{c}(x - ct + \delta) \right),$$  (1.3)

and one immediately sees (Fig. 1.1), that the object, described by (1.3) moves along the $x$-axis with constant speed $c$ without any change of the envelope function, i.e. with constant shape. Also the size of the soliton is directly connected with its speed, so the bigger the soliton, the faster it moves.
Figure 1.1: Plot of the solution 1.3 of the KdV equation for initial time. All parameters set to 1.
2. Classical models of magnetic solitons

2.1. Simplest classical model

One of the most simple classical models which possess some soliton-like solutions is the magnetic chain with an easy-axis symmetry and nearest-neighbor interaction:

\[ H = -J \sum_n \vec{S}_n \cdot \vec{S}_{n+1} - A \sum_n (S^z_n)^2. \] (2.1)

Using the continuum approximation (with \( x \) being the continuous coordinate of a spin cite instead of the discrete coordinate \( n \)), switching to polar coordinates for the spin direction and rewriting the Hamiltonian as a classical energy depending on two angles \( E(\Theta(x), \Phi(x)) \)

\[ E(\Theta(x), \Phi(x)) = JS^2 \int dx \left\{ \frac{1}{2} \left( \frac{d\Theta}{dx} \right)^2 + \frac{1}{2} \sin^2 \Theta \left( \frac{d\Phi}{dx} \right)^2 - \frac{A}{J} \sin^2 \Theta \right\}, \] (2.2)

one ends up with the following expression for those angles:

\[
\begin{cases}
\Phi(x) = \text{constant}; \\
\frac{d^2\Theta}{dx^2} = \frac{A}{J} \sin(2\Theta).
\end{cases}
\] (2.3)

Thus one obtains a static sine-Gorgon equation as a basic equation for static solutions of this simple model. Its fundamental solution is the basic kink solution ((Fig. 2.1):

\[ \Theta(x) = 2 \arctan \left\{ \exp \left[ \pm \left( \frac{2A}{J} (x - x_0) \right)^{1/2} \right] \right\}. \] (2.4)

This is the expression for ferromagnetic domain walls introduced by Bloch in Ref. [12], first written in such form in Ref. [13].
2. Classical models of magnetic solitons

Figure 2.1: Plot of $\Theta(x)$ for the static soliton solution (2.4). $A/J$ is set to 1.

2.2. Classical sine-Gordon chain

In a continuum limit the classical sine-Gordon chain is defined by the following Hamiltonian:

$$H = E_0 a \int_{-\infty}^{\infty} dx \left\{ \frac{1}{2} \left( \frac{\partial \Phi}{\partial x} \right)^2 + \left( \frac{1}{2c^2} \frac{\partial \Phi}{\partial t} \right)^2 + m^2 (1 - \cos \Phi) \right\} \, . \quad (2.5)$$

The sine-Gordon system is characterized by an energy scale $E_0$, a limiting velocity $c$ (somewhat analogous to the speed of light), a mass parameter $m$, which determines the strength of nonlinear potential and an underlying lattice constant $a$, needed for dimensional reasons. The variable of this model is $\Phi(x,t)$ - the angle of the spin direction in the plane perpendicular to the $x$-axis.

This Hamiltonian results in an equation of motion of sine-Gordon type:

$$\frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} - \frac{\partial^2 \Phi}{\partial x^2} + m^2 \sin \Phi = 0 \, . \quad (2.6)$$

This system was extensively discussed in the literature (see Refs. [14, 15, 16]), a first application to solid-state physics was given in Ref. [17]. It arises there from description of the lattice with lattice constant $a$. For that case a discrete analog of (2.6) looks like
2. Classical models of magnetic solitons

\[
a^2 \frac{\partial^2 \Phi_n}{\partial t^2} = \Phi_{n+1} + \Phi_{n-1} - 2\Phi_n - (ma)^2 \sin \Phi_n .
\]  

(2.7)

This equation was investigated by Peyrard and Kruskal in Ref. [18]; it was found that solutions are well described by a continuous approximation for \( ma \ll 1 \). But when the width of soliton approaches the lattice constant (i.e. \( ma > 1 \)) strong discreteness effects and instabilities are observed.

Ablowitz et al. (Ref. [19]) and Takhtajan and Fadeev (Ref. [20]) have shown that the system described by Hamiltonian (2.5) is completely integrable for appropriate boundary conditions. The Hamiltonian can be represented in action and angle variables of three different types. Thus the time evolution of the field \( \Phi(z,t) \) can be decomposed into contributions of three different solution modes:

- Small oscillations in the form of plane-wave solutions, also referred to as magnons:

\[
\Phi(x,t) = A_k \exp[i(kx - \omega_k t)] ;
\]  

(2.8)

- Finite amplitude localized solutions travelling without changing their shape with arbitrary velocity \( u \) (\( |u| < c \)), called solitons and antisolitons (Fig. 2.2):

\[
\Phi(x,t) = 4 \arctan \left( \exp[\pm \gamma m(x - ut - x_0)] \right) ;
\]  

(2.9)

- Localized solutions, travelling with constant shape, characterized by an additional internal degree of freedom, denoted as breathers. A breather at rest is given by

\[
\Phi(x,t) = 4 \arctan \left( \frac{1}{(l^2 m^2 - 1)^{1/2}} \frac{\sin(\Omega_l t)}{\cosh(x/l)} \right)
\]  

(2.10)

(see Fig. 2.3), and a moving breather can be obtained from (2.10) by applying the Lorentz transformation. Breathers can be considered as bound soliton-antisoliton pairs where the length \( l \) is the internal degree of freedom and determines in particular the breather energy and internal frequency.
2. Classical models of magnetic solitons

Figure 2.2: Classical sine-Gordon kink soliton and antisoliton (2.9) for $t = 0$. Parameters $\gamma, m, u$ are set to 1, $x_0 = 1$.

Figure 2.3: Classical sine-Gordon breather at rest (2.10). Parameters are set as follows:

$l = 1, \Omega_l = 1, m^2 = 2$. 

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2.3. Heisenberg chains

While the model described in section 2.2 and some of its limiting cases are rather well applicable to a quite large amount of substances (Ref. [21]), generally spin dynamics has to be described by a vector field $\vec{S}(x, t)$ rather than by a scalar field $\Phi(x, t)$. Of course this would complicate all calculations, but there are some models which allow a full solution of this problem. One of the simplest is an isotropic ferromagnetic Heisenberg chain with nearest neighbor interaction exposed to a uniform magnetic field. The Hamiltonian of this system reads as

$$H = -J \sum_n \vec{S}_n \cdot \vec{S}_{n+1} - \mu B \sum_n S_n^z,$$

where $J > 0$, \hspace{1cm} (2.11)

and Poisson brackets

$$\{ S^a_m, S^b_n \} = i \epsilon^{abc} S^c_m \delta_{mn}.$$ \hspace{1cm} (2.12)

Representing spin in polar coordinates $\vec{S} = S \{ \sin \Theta \cos \Phi, \sin \Theta \sin \Phi, \cos \Theta \}$ and using the continuum approximation, the above equations are transformed to

$$H = JS^2 a \int dx \left\{ \frac{1}{2} \left( \frac{\partial \Theta}{\partial x} \right)^2 + \frac{1}{2} \sin^2 \Theta \left( \frac{\partial \Phi}{\partial x} \right)^2 - b \cos \Theta \right\},$$

$$\{ \cos \Theta(x, t), \Phi(x', t) \} = \frac{a}{S} \delta(x - x'),$$ \hspace{1cm} (2.13)

$$\frac{\partial S}{\partial t} = \vec{S} \times \frac{\partial^2 \vec{S}}{\partial x^2},$$

$$\frac{\partial \Theta}{\partial t} = -\frac{1}{\sin \Theta} \frac{\partial}{\partial x} \left( \sin^2 \Theta \frac{\partial \Phi}{\partial x} \right),$$ \hspace{1cm} (2.15)

where $b = \frac{\mu B}{JS}$.

The equation of motion in this continuum case is the Landau-Lifshitz equation (using rescaling of time by a factor $(JS)^{-1}$ and length by a factor $a$):

$$\frac{\partial \vec{S}}{\partial t} = \vec{S} \times \frac{\partial^2 \vec{S}}{\partial x^2},$$

$$\frac{\partial \Theta}{\partial t} = -\frac{1}{\sin \Theta} \frac{\partial}{\partial x} \left( \sin^2 \Theta \frac{\partial \Phi}{\partial x} \right),$$ \hspace{1cm} (2.16a)

$$\frac{\partial \Phi}{\partial t} = \frac{1}{\sin \Theta} \frac{\partial^2 \Theta}{\partial x^2} - \cos \Theta \left( \frac{\partial \Phi}{\partial x} \right)^2 - b.$$ \hspace{1cm} (2.16b)

Now one searches for solutions with constant profile (solitary waves) or soliton trains. An analytical solution of this problem was first made by Nakamura and Sasada [22] and by Tjon and Wright [23]. They searched for such soliton solutions of equations (2.16), that depend on $x$ and $t$ only via the variable

$$s = x - ut.$$ \hspace{1cm} (2.17)
In this case one has to integrate the following system of equations
\[
\begin{align*}
\frac{\partial^2 \Theta}{\partial s^2} &= \sin \Theta \left[ \cos \Theta \left( \frac{I_1 - u \cos \Theta}{\sin^2 \Theta} \right)^2 - u \left( \frac{I_1 - u \cos \Theta}{\sin^2 \Theta} \right) + b \right], \\
\frac{\partial \Phi}{\partial s} &= \frac{I_1 - u \cos \Theta \sin \Theta}{\sin^2 \Theta},
\end{align*}
\] (2.18)
which leads to
\[
\left( \frac{dx}{ds} \right)^2 = F(x),
\] (2.19)
with
\[
x = \cos \Theta F(x) = -(I_1 - ux)^2 - 2bx(1 - x^2) + I_2(1 - x^2),
\] (2.20)
$I_1$ and $I_2$ being integration constants. As discussed in Ref. [24], the general solution of this equation (with arbitrary $I_1$ and $I_2$) corresponds to a soliton wave train, while with varying constants of integration one can continuously come to such limit cases as solitary waves (one soliton) or small-amplitude magnons.

Since a soliton is a localized solution it requires $\Theta = \Theta' = 0$ at infinity, which corresponds to $I_1 = u$. On the assumption that all zeroes of $F(x)$ are known, the solution can be expressed in terms of elliptic functions. So, for example, for the particular parameters $I_1 = u, I_2 = 2b$ and $v = \frac{u}{2\sqrt{b}} < 1$ one has the following soliton solution (Refs. [22, 23]):
\[
\cos \Theta = 1 - A \text{sech}^2[\mu(s - s_0)],
\] (2.21)
\[
\Phi = \sqrt{b}(s - s_0) + \arctan \left( \frac{-\sqrt{1 - v^2}}{v} \tanh[\mu(s - s_0)] \right),
\] (2.22)
where
\[
A = 2(1 - v^2), \quad \mu = \sqrt{b(1 - v^2)}.
\] (2.23)

2.4. Modern state of research

A very extensive and quite modern review of the field of one-dimensional magnetic systems can be found in Ref. [21]. As a summary of this seminal work for classical methods one can say that modern variants of the classical approach are capable to describe real one-dimensional magnets rather well. Mainly models with Heisenberg, planar Heisenberg or Ising Hamiltonians are used, and the classical sine-Gordon approximation is the favorite one to give results which are in good agreement with experimental works. However, this agreement bears a qualitative character, while quantitative reasonable agreement is achieved by including corrections, which somehow take into account discreteness effects, out-of-plane interactions and the quantum nature of spin dynamics.
2. Classical models of magnetic solitons

For example, in Ref. [25] the classical Heisenberg chain with a Hamiltonian in form of

\[ H = - \sum_n \left\{ \vec{S}_n \cdot \vec{S}_{n+1} + h S^z_n + \frac{\alpha}{2} (S^z_n)^2 \right\} \]

(2.24)

and generalized boundary conditions is investigated. It is shown, that for the case of easy-plane anisotropy and for the isotropic case soliton solutions of this model are in fact unstable. Numerical simulations made for the case \( \alpha < 0 \) show that solitons are rather stable, but collisions and interactions with magnons reveal a small instability (see Figure 2.4), which is understood to appear as a manifestation of discreteness effects.
2. Classical models of magnetic solitons

Figure 2.4: Interaction of two classical solitons (plot taken from Ref. [25]). Inserts are enlarged with respect to $S_z$.
First graph - two solitons are approaching each other.
Second graph - interaction of two solitons.
Third graph - two solitons after interaction moving apart from each other.
Generally one sees that the interaction process looks very "soliton-like" - both solitons have kept their envelope unchanged. But the enlarged insert on the third graph shows emission of small magnon packets after interaction. This points out an instability of this soliton solution in the classical continuous model.
3. Quantum models of magnetic solitons

Despite the success of classical models to adequately describe a lot of existing materials, it is only an approximation to the real nature of spin dynamics. Furthermore, there exist materials that really should be described taking into account quantum aspects of spin interactions. First of all these are compounds where items forming a spin structure have small spin quantum number, while the classical approximation by default assumes large $S$. Among these materials are tetramethylaminomanganese chloride, shortly TMMC, ($S = \frac{5}{2}$), CsNiF$_3$ ($S = 1$), CsCoCl$_3$ ($S = \frac{5}{2}$).

The general case of a quantum spin chain can be described with the following Hamiltonian:

$$\hat{H}_{xyz} = -2 \sum_n \{ J(1 + \gamma)S^x_n S^x_{n+1} + J(1 - \gamma)S^y_n S^y_{n+1} + J_z S^z_n S^z_{n+1} \} .$$

(3.1)

3.1. Bethe-ansatz

The Hamiltonian in the form of (3.1) was studied in the famous work of Bethe [26], where he introduced his Bethe-ansatz to calculate ground-state wavefunctions in the isotropic limit of the Hamiltonian (3.1), i.e. $\gamma = 0, J_z = J$. The ground-state energy was obtained by Hulthén [27]. In the following a short description of their ideas is given (for details see Ref. [28]): One starts with the Heisenberg antiferromagnet chain Hamiltonian:

$$H = \sum_{i=1}^{N} \left\{ \frac{1}{2} \left( S^+_i S^-_{i+1} + \text{h.c.} \right) + g S^z_i S^z_{i+1} \right\} \quad \text{for} \quad g = 1, s = \frac{1}{2}, N \text{is even} .$$

(3.2)

The ground state of such a system belongs to the subspace with $M = 0$, i.e. contains $N$ “particles”. Starting with 2 “particles”, and using a procedure valid only for $s = \frac{1}{2}$ we assign to unphysical amplitudes $f_{i,i}$ the value defined by

$$f_{i,i} + f_{i+1,i+1} = f_{i,i+1} + f_{i+1,i} = 2f_{i,i} \, ,$$

(3.3)

whereas physical amplitudes $f_{i,j} = f_{j,i}$ (for $i \neq j$) are defined by

$$(E - E_f + 2)f_{i,j} - \frac{1}{2}(f_{i,j+1} + f_{i,j-1} + f_{i+1,j} + f_{i-1,j}) = 0 .$$

(3.4)
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The physical amplitudes (3.3) play the role of a boundary condition. This homogeneous equation is solved by plane waves via the Bethe ansatz:

\[ f_{i,j} = e^{i(k_i+k'_j+1/2\psi)} + e^{i(k_j+k'_i-1/2\psi)} \quad \text{for } j \geq i, \]

(3.5)

where \( f_{i,j} \) for \( j < i \) is given by symmetry \( f_{i,j} = f_{j,i} \). The phase factor \( \psi \) is in the range \([-\pi, \pi]\).

Inserting (3.5) into (3.3) and doing some algebra one ends up with

\[ 2 \cot \frac{1}{2} \psi = \cot \frac{1}{2} k - \cot \frac{1}{2} k', \]

(3.6)

determining \( k \) and \( k' \):

\[ k = \frac{\pi(2p) + \psi}{N} \quad \text{and} \quad k' = \frac{\pi(2p') - \psi}{N}, \]

(3.7)

where \( p \) and \( p' \) are integers.

Thus the energy, measured from the ferromagnetic level \( E_f = \frac{1}{4}N \) (magnon vacuum energy) is given by

\[ E - E_f = -(1 - \cos k) - (1 - \cos k'), \]

(3.8)

and is just the energy of 2 noninteracting magnons; interaction is included implicitly through the phase shifts in \( k \), Eqs. (3.6) and (3.7).

Now turning to many-particles states, Bethe’s ansatz implies that amplitudes are subjects to phase shifts that are simply given by the sum of all possible two-particles phase shifts. So, for a given ordering \( i \leq j \leq n \), one has

\[ f_{i,j,...,m,n} = \left\{ \exp \left[ i \left( k_1 i + k_2 j + k_n n + \frac{1}{2} \sum_{r=1}^{n} \sum_{t>r}^{n} \psi_{k_r k_t} \right) \right] \right\} \]

(3.9)

If one needs elements of another ordering, they can be obtained from the symmetry \( f_{i,j,...,m,...} = f_{i,m,...,j,...} \), so it is necessary to know \( f_{i,j,...} \) only in some region. Analogous to the 2-particle case one can derive

\[ 2 \cot \frac{1}{2} \psi_{kk'} = \cot \frac{1}{2} k - \cot \frac{1}{2} k', \]

(3.10)

and
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\[ k = \frac{\pi(2p) + \sum_{k' \in \text{present in (3.9)}}^n \psi_{kk'}}{N} \quad p = 0, \pm 1, \ldots \] \hspace{1cm} (3.11)

The sum here involves only those \(k'\), which are present in (3.9). The energy can be expressed similarly to (3.8) as

\[ E - E_f = -\sum_{t=1}^n (1 - \cos k_t) \] \hspace{1cm} (3.12)

Going to the continuum limit \(N \to \infty\), which is possible due to regular spacing between spin sites, one gets

\[ E - E_f = -N \int_0^1 \frac{\sin^2 \frac{k(x)}{2}}{dx} \] \hspace{1cm} (3.13)

where

\[ 2 \cot \frac{\psi(x, y)}{2} = \cot \frac{k(x)}{2} - \cot \frac{k(y)}{2} \] \hspace{1cm} (3.14)

and

\[ k(x) = 2\pi x + \frac{1}{2} \int_0^1 \psi(x, y) dy \] \hspace{1cm} (3.15)

After some calculations including Fourier transformation the famous result, being the first exact result for a non-trivial quantum many-body problem, can be obtained (see Ref. [27]):

\[ E - E_f = -2N \int_0^\infty \frac{dk}{1 + e^{-2|k|}} = -N \ln 2 \] \hspace{1cm} (3.16)

Studies that followed were concerning generalization to some anisotropic cases [29, 30], calculation of the one-magnon spectrum [31], and magnetic susceptibility [32]. Baxter in Refs. [33, 34] succeeded to apply Bethe’s method to the fully anisotropic case of a linear chain with Hamiltonian (3.1).

3.2. Lieb-Mattis theorem

Another important result in the field of the quantum description of spin systems was obtained in 1962 by Lieb and Mattis. In Ref. [35] they formulated and proved what is now called Lieb-Mattis theorem. Its short description is given in what follows.
3. Quantum models of magnetic solitons

For any finite set $\Lambda$ and $J = \{J_{uv} \in \mathbb{R} : u \neq v \in \Lambda; J_{uu} = 0\}$, one defines a Heisenberg model by the Hamiltonian

$$H_{\Lambda} = \sum_{u \neq v \in \Lambda} J_{uv} S_u \cdot S_v.$$  \hspace{1cm} (3.17)

The Hamiltonian is termed as reducible if there exist $\Lambda_1$ and $\Lambda_2$ such that

$$\Lambda = \Lambda_1 \cup \Lambda_2$$

and

$$J_{uv} = 0 \ \forall \ u \in \Lambda_1, \ v \in \Lambda_2.$$  \hspace{1cm} (3.18)

Otherwise the model is irreducible.

A special class of Heisenberg models is obtained when $\Lambda = A \cup B$, and $J$ satisfies

$$\begin{cases} J_{uv} \geq 0 & \text{for } u \in A, v \in B; \\ J_{uv} \leq 0 & \text{for } u, v \in A, \text{ or } u, v \in B. \end{cases}$$  \hspace{1cm} (3.19)

A particular example is when $-J$ is the adjacency matrix of a bipartite graph. Therefore, we will call these Heisenberg models $(A,B)$-bipartite. One can allow different spins at different sites: $s_u \in \frac{1}{2}\mathbb{N}$. For an $(A,B)$-bipartite model, one defines

$$S_A = \sum_{u \in A} s_u, \quad S_B = \sum_{u \in B} s_u.$$  \hspace{1cm} (3.20)

Let $E(\Lambda, S)$ be the minimum energy among all vectors with total spin $S$.

The theorem states that if one supposes that $H_{\Lambda,J}$ is an irreducible, $(A,B)$-bipartite Heisenberg Hamiltonian and denotes $S = |S_A - S_B|$, then one has

$$E(\Lambda, S + 1) > E(\Lambda, S) \quad \text{for all } S \geq S,$$  \hspace{1cm} (3.21)

and

$$E(\Lambda, S) > E(\Lambda, S) \quad \text{for all } S < S.$$  \hspace{1cm} (3.22)

A particular solvable model is

$$\begin{cases} J_{uv} = +1 & \text{for } u \in A, v \in B; \\ J_{uv} = -1 & \text{for } u, v \in A, \text{ or } u, v \in B. \end{cases}$$  \hspace{1cm} (3.23)

One can calculate the spin for the ground state in the $S^3$-eigenspace with eigenvalue $M$:

$$\begin{cases} |M| & \text{for } |M| > S; \\ S & \text{for } |M| > S. \end{cases}$$  \hspace{1cm} (3.24)

This theorem leads to a couple of important conclusions. First of all, it allows one to estimate or even calculate the ground state energy just by itself, without having
3. Quantum models of magnetic solitons

calculated the whole spectrum, which might be too tough for analytical or numerical calculations. And second, it introduces an ordering in minimal energy levels as a function of total spin.

3.3. Current state of the field

A big part of methods used to-date to describe one-dimensional magnetic systems can be denoted as "semiclassical" ones. Their main feature is that the formulation of the problem is given in the quantum way, commutation relations for proper to the task operators are established, and quantum equations of motion are obtained. After that some assumptions are made, which lead to simplification of the problem towards the classical case.

One example of such approach is the "quasidiscreteness" method of Ref. [36]. The core of this approach is that after having written spin dynamics equations and only after that treating spin as classical ones, one expands \( s_n^+(t) \) as a series in some small parameter \( \varepsilon \):

\[
s_n^+(t) = \varepsilon s_n^{(1)} + \varepsilon^2 s_n^{(2)} + \varepsilon^3 s_n^{(3)} + \cdots .
\]  

(3.25)

The main advantage of this method is that solutions obtained are adequate in the whole Brillouin zone. Based on this approximation, all possible types of nonlinear localized small-amplitude solutions (bright solitons, dark and antidark solitons) are found analytically and the validity of these results is checked with the help of numerical simulations (for example see Figure 3.1).

Intrinsic localized spin modes (ILSM) were studied in Refs. [37] and [38]. The authors found that a finite chain of appropriate spins possesses a rich spectrum of intrinsic nonlinear spin excitations and presented a numerical method to simulate moving modes. They found that under certain conditions objects obtained exhibit soliton-like properties, preserving their shape, speed and identity in collisions (Figure 3.2). However, interactions are rather complex, especially when taking into account possible defects in spin chains. In this case it is possible to achieve a trapping of ILSM on the impurity or a reflection from it (Figure 3.3).

Bloch oscillations of magnetic solitons were studied in Refs. [39] and [40]. This effect can be characterized as oscillatory behavior of the system in response to a constant external force, thus being one of the interesting manifestations of the quantum nature of spin systems. This effect was theoretically shown to appear in biaxial and
3. Quantum models of magnetic solitons

Figure 3.1: Example of the soliton solution based on the quasidiscreteness approach (3.25). Plot taken from Ref. [36].

Figure 3.2: Collision of two ISLM solitons in the chain of 500 spins. Solitons are reflected from the borders of the chain (due to boundary conditions of the system) and pass through each other with no change of their speed or envelope. Plot taken from Ref. [38].
3. Quantum models of magnetic solitons

Figure 3.3: Propagation of ILSM soliton in the chain of 500 spins with a defect (absent spin) on site number 251. The soliton is reflected both from the border and from the defect. Plot taken from Ref. [38].

uniaxial Ising-like ferromagnets, and also in Ising-like antiferromagnets, and materials which are likely to possess such effect are singled out.

The role of dynamical magneto-elastic coupling in spin-Peierls chains is investigated by numerical and analytical techniques in Ref. [41]. It is shown that a Heisenberg spin chain coupled to dynamical optical phonons exhibits a transition towards a spontaneously dimerized state in a wide range of parameter space and the low energy excitations are characterized as solitons.
4. Spin ring systems

4.1. Magnetic molecules

Magnetic molecules are a recently discovered class of materials, and they have been of great interest in the last decade. These molecules consist of several metal ions, surrounded by organic or anorganic ligands. They exist in many structures and with various spin Hamiltonians. Ring molecules are a large subgroup, where the most prominent are "ferric wheels", rings with paramagnetic iron atoms of spin \( s = 5/2 \) [42] and "chromic wheels", rings with chromium ions of spin \( s = 3/2 \) [43] (for example of both chromic and ferric wheels see Figure 4.1).

Due to their small size and small magnitude of the spin of each ion, magnetic molecules are genuine quantum spin systems. Thus they cannot be described neither by a continuous spin density nor by classical spins. Therefore, ring molecules provide good candidates to accommodate quantum magnetic solitons. In addition solitons may provide a valuable tool to investigate magnetic molecules experimentally. If the characteristics of magnetic solitons can unambiguously be connected to the structure of the spin Hamiltonian, the measurement of the soliton properties may result in a more accurate determination of the Hamiltonian than given by other methods.

Because of their simple geometry, their related symmetry and their experimental availability we focus our investigations on spin ring-systems.

4.2. Hamiltonian and product basis

We investigate rings of equal spins with antiferromagnetic nearest-neighbors interaction. The Hamilton operator of our system is of Ising type

\[
\tilde{H} = J \sum_{i=1}^{N} \tilde{s}_z(i) \cdot \tilde{s}_z(i + 1), \tag{4.1}
\]

or Heisenberg type

\[
\tilde{H} = J \sum_{i=1}^{N} \tilde{s}(i) \cdot \tilde{s}(i + 1), \tag{4.2}
\]
4. Spin ring systems

Figure 4.1: Examples of magnetic molecules. Left hand side - molecule Fe6. Right hand side - molecule Cr8.

with $J = 1$ without losing generality. These Hamiltonians have eigenstates $|\psi_n\rangle$ with a corresponding set of eigenvalues $E_n$:

$$\tilde{H} |\psi_n\rangle = E_n |\psi_n\rangle . \quad (4.3)$$

These eigenstates form a basis of the Hilbert space of our system. We can also construct another basis, the so called ”product basis”:

$$|m\rangle = |m_1, m_2, \ldots, m_N\rangle , \quad (4.4)$$

were $m_i$ are eigenvalues of the operator of the third spin component on the $i$-th spin site,

$$\tilde{s}_z(i) |m\rangle = m_i |m\rangle . \quad (4.5)$$

4.3. Shift operator

Now following Ref. [44] we introduce a shift operator $\tilde{T}$, which acts on a vector of product basis in the following way:

$$\tilde{T} |m_1, m_2, \ldots, m_N\rangle = |m_N, m_1, m_2, \ldots, m_{N-1}\rangle , \quad (4.6)$$

i.e., it just shifts all spins by one position. The shift operator also has its own eigenstates and eigenvalues:

$$\tilde{T} |\chi_n\rangle = \exp\left(-\frac{2\pi i}{N} k_n\right) |\chi_n\rangle , \quad (4.7)$$

where $k_n$ is called translational (shift) quantum number (it has something in common with wave quantum number or momentum).
4. Spin ring systems

4.4. Commutation relations

The first thing one faces when trying to solve such a problem numerically is the huge amount of RAM needed by a computer. For example, let’s take a small system of 14 spins with spin=1/2. In this case, the Hamiltonian matrix has the dimension $2^{14} \times 2^{14}$. Each element of the matrix is a complex number, which is stored in double precision, that means 16 bytes per element. Thus to operate with this matrix in RAM we need at least $2^{14} \times 2^{14} \times 16$ bytes = 4 Gigabytes. And with increasing the number of spins this number grows exponentially. Moving to higher spin quantum numbers (3/2, 5/2,...), which is the point in magnetic molecules, also increases the RAM demand.

So the problem looks like to be solved only on some big mainframes. But we can reduce this big problem to a set of small ones, thus being able to solve problems of such kind on a PC.

All the operators mentioned above mutually commute [44], which leads to an important property of the Hilbert space of our quantum system:

$$\left[\hat{H}, \hat{S}_z\right] = 0 \implies \mathcal{H} = \bigoplus_{M=-S_{\text{max}}}^{S_{\text{max}}} \mathcal{H}(M). \quad (4.8)$$

That means that the whole Hilbert space $\mathcal{H}$ can be divided into a set of orthogonal subspaces with respect to different values of the total magnetic quantum number $M$. Moreover,

$$\begin{cases} 
\left[\hat{H}, \hat{T}\right] = 0 \\
\left[\hat{S}_z, \hat{T}\right] = 0 
\end{cases} \implies \mathcal{H} = \bigoplus_{M,k} \mathcal{H}(M, k), \quad (4.9)$$

which makes it possible to divide the mentioned subspaces $\mathcal{H}(M)$ once again with respect to different shift quantum numbers $k$.

Thus we can divide our (very) big Hilbert space into (comparatively) small subspaces and solve our problem in these subspaces one-by-one. This drastically reduces the necessary calculation power.
5. Solitary objects

When describing magnetic systems with classical (Chapter 2) or semiclassical (Chapter 3, section 3.3) approaches solitons appear naturally as solutions of nonlinear differential equations, which are obtained as a consequence of classical approximation to the underlying quantum problem. For instance, replacing quantum spins by classical spin density results in the cubic Schrödinger equation [28].

But we want to investigate the quantum case without any classical approximation. Our system obeys the ordinary linear time-dependent Schrödinger equation. And in order to apply ideas of solitons or solitary waves to such a case the redefinition of the term ”soliton” is needed. The well known property that two solitons scatter into soliton states can not be used, because for a differential equation, which obeys the linear superposition principle, this is trivially fulfilled. Thus another definition is necessary.

We call a state $|\psi_s\rangle$ solitary wave (or solitary state) if there exists a time $\tau$ for which the time evolution, described by the linear time-dependent Schrödinger equation, is equal (up to global phase) to shifting by one site on the spin ring.

If some system indeed allows existence of such state $|\psi_s\rangle$, than, by definition, the profile of any observable, related to $|\psi_s\rangle$ would move around the ring without changing its envelope, producing an object with solitary properties.

5.1. Linear dependence

We demand, that the time evolution of the system in a ”soliton” state is equivalent to shifting the system (movement without ”changing shape”). This brings us to equation

$$\tilde{T} |\psi_s\rangle = \exp \left( -\frac{i}{\hbar} \tilde{H} \tau - i\phi \right) |\psi_s\rangle .$$  \hspace{1cm} (5.1)

Now we can expand the ”soliton” wave function in the basis of eigenstates $\{|\psi_n\rangle\}$

$$|\psi_s\rangle = \sum_{n \in \{D_s\}} c_n |\psi_n\rangle ,$$  \hspace{1cm} (5.2)
where \( D_\psi \in \mathbb{N} \) corresponds to some set of states taken for the expansion and \( \{ | \psi_n \rangle \} \) eigenstates being simultaneously eigenstates of the shift operator and the Hamilton operator of the system

\[
\tilde{T} | \psi_n \rangle = \exp \left( -i \frac{2\pi k_n}{N} \right) | \psi_n \rangle ,
\]

\[
\tilde{H} | \psi_n \rangle = E_n | \psi_n \rangle .
\]

Thus inserting (5.2) into (5.1) we obtain

\[
\sum_{n \in \{ D_\psi \}} c_n \exp \left( -i \frac{2\pi k_n}{N} \right) | \psi_n \rangle = \sum_{n \in \{ D_\psi \}} c_n \exp \left( -i \frac{\hbar}{\hbar} E_n \tau - i \phi \right) | \psi_n \rangle .
\]

Now it can be easily seen, that this equation fulfills only if

\[
\frac{2\pi}{N} (k_n + Nl) = \frac{\tau}{\hbar} E_n + \phi \quad \forall n \in \{ D_\psi \}, l \in \{ \mathbb{Z} \} .
\]

So we see, that for a "soliton" we need to have Hamiltonian eigenvalues and wave quantum numbers in some sense linear dependent on each other. Because of the rotational invariance we can prolong our energy spectrum in \( k \) in both directions. And since \( k \) and \( k \pm nN \) are the same we can search for linear dependant states not only in the first Brillouin zone but in all of them (see sketch in Fig. 5.1).

Note, that in fact the energy through all of our calculations is scaled by factor \( J \) from (4.1) or (4.2). Thus for the first Brillouin zone the equation (5.6) can be rewritten as

\[
E_n = \frac{2\pi \hbar J}{N \tau} k_n - \frac{\hbar J}{\tau} \phi .
\]

It is clear that the tangent angle of the dispersion relation (5.7) is directly connected to the speed of the object, since by our definition \( \tau \) is a time needed to shift to one position between spin sites. Thus knowledge of tangent coefficient in the linear dispersion relation (5.7), interspin distance and speed of the solitary object allows to determine interaction parameter \( J \) in the Hamiltonian of our system very easily.

### 5.2. \( s_z \) as an observable

The next question arising is what observable of the given quantum system one better uses to investigate that system. The first natural choice is the energy density, which
5. Solitary objects

Figure 5.1: Illustration of the condition (5.6). The sketch shows a sample piece of the $E$ vs $k$ dependence.

a) States represented by points $A_0$ and $B_0$ are on the straight line, but state $C_0$ is definitely out of line.

b) But if there exist some Brillouin zone, where corresponding to the $C_0$ point $C_n$ lies on the same straight line with points $A_0$ and $B_0$, then state $C_0$ can be taken together with states $A_0$ and $B_0$ to construct a solitary state (5.2).

in case of quantum mechanics can be defined as estimation value of $\hat{s}(i) \cdot \hat{s}(i + 1)$ starting from Hamiltonian (4.1) or (4.2). But it turns out, that in most cases this observable is practically useless, while off-diagonal elements for energy eigenvalues belonging to the different total $S$ subspaces are zero [45].

Another choice is the expectation value of the local operator $\hat{s}_z(i)$. Let’s calculate the expectation value of the third spin component $s_z$ on the spin site number $i$:

$$\langle \psi | \hat{s}_z(i) | \psi \rangle = \sum_{\nu,j} \langle \psi | m_{\nu} \rangle \langle m_{\nu} | \hat{s}_z(i) | m_{j} \rangle \langle m_{j} | \psi \rangle = \sum_{\nu,j} m_{\nu}(i) \langle \psi | m_{\nu} \rangle \langle m_{\nu} | m_{j} \rangle \langle m_{j} | \psi \rangle. \quad (5.8)$$

But $\langle m_{\nu} | m_{j} \rangle = \delta_{\nu,j}$. Thus we have

$$\langle \psi | \hat{s}_z(i) | \psi \rangle = \sum_\nu m_{\nu}(i) \left| \langle m_{\nu} | \psi \rangle \right|^2. \quad (5.9)$$

In our calculations we shall use a parameter $a_{\nu}(i)$ rather than $m_{\nu}(i)$, so that

$$a_{\nu}(i) = s - m_{\nu}(i). \quad (5.10)$$

Thus we can say, that the set of states $|a_{\nu}\rangle$ is equivalent to set of states $|m_{\nu}\rangle$, and
5.2.1. $|\psi\rangle = |\psi_n\rangle$

$$\langle a_\nu|\psi_n\rangle = \sum_j \langle a_\nu|\chi_j\rangle \langle \chi_j|\psi_n\rangle ,$$  \hspace{1cm} (5.12)

where $|\chi_j\rangle$ are eigenstates of shift operator $\tilde{T}$. In this case $\langle \chi_j|\psi_n\rangle$ is the result of the diagonalization procedure of our numerical program (see Appendix B) and $\langle a_\nu|\chi_j\rangle$ can be rewritten as

$$\langle a_\nu|\chi_j\rangle = \frac{1}{\sqrt{Z_{Dim}j}} \exp \left( \frac{2\pi i}{N} k_j (\nu - MBSt_j) \right) ,$$  \hspace{1cm} (5.13)

if $0 \leq \nu - MBSt_j \leq Z_{Dim}j - 1$, and $\langle a_\nu|\chi_j\rangle = 0$ in all other cases (for details see Appendix A).

So finally we have the following expression for $\langle \psi|\tilde{s}_z(i)|\psi\rangle$:

$$\langle \psi|\tilde{s}_z(i)|\psi\rangle = s_z(i) = \sum_\nu (s - a_\nu(i)) \left| \sum_j \frac{1}{\sqrt{Z_{Dim}j}} \exp \left( \frac{2\pi i}{N} k_j (\nu - MBSt_j) \right) \langle \chi_j|\psi_n\rangle \right|^2 ,$$  \hspace{1cm} (5.14)

$0 \leq \nu - MBSt_j \leq Z_{Dim}j - 1$.

5.2.2. $|\psi\rangle = |\psi_s\rangle$

In this case we can expand $|\psi_s\rangle$ on $|\psi_n\rangle$:

$$|\psi_s\rangle = \sum_{n \in D_\psi} c_n |\psi_n\rangle ,$$  \hspace{1cm} (5.15)

where $D_\psi$ is a set of Hamiltonian eigenstates, which have linear dependence between energy and shift quantum number (5.6). Thus we can represent our result in the following way:

$$\langle \psi_s|\tilde{s}_z(i)|\psi_s\rangle = s_z(i) = \sum_\nu (s - a_\nu(i)) \times \left| \sum_{n \in D_\psi} c_n \sum_j \frac{1}{\sqrt{Z_{Dim}j}} \exp \left( \frac{2\pi i}{N} k_j (\nu - MBSt_j) \right) \langle \chi_j|\psi_n\rangle \right|^2$$  \hspace{1cm} (5.16)
5. Solitary objects

5.3. Stability

Now what is going to happen if, for example, one of the states one takes to construct the solitary wave function $|\psi_s\rangle$ (5.2) does not fulfill the linear dispersion relation (5.6) exactly? This situation could be the case in our calculations because of two reasons. First, our numerical estimations are always done with some finite precision, thus resulting in not mathematically exact fulfilling the equation (5.6). And second, because not all systems could have necessary sets of states to fulfil condition (5.6), it might be interesting to try to construct an object on the basis of the dispersion relation which is close to the linear one.

In any case, not exactly linear dispersion will result in an instability of the soliton. For that matter we should introduce some value to represent this instability. Let’s choose for this purpose the overlap between our soliton wave function after shifting and after evolving for time $\tau$ (see previous section), namely, one minus modulus of such overlap.

So, if we have soliton wave function $|\psi_s\rangle$, then

$$|\psi^T_s\rangle = \tilde{T} |\psi_s\rangle$$

is the soliton wave function after the shift, and

$$|\psi^{evol}_s\rangle = \tilde{U} |\psi_s\rangle = \exp \left( -\frac{i}{\hbar} \tilde{H} \tau - i\phi \right) |\psi_s\rangle$$

is the same wave function after evolution of time $\tau$.

Our measure of the instability is the following:

$$\Delta = 1 - |\langle \psi^T_s |\psi^{evol}_s\rangle|.$$ (5.19)

Now let us calculate $\Delta$ for the case, that $N-1$ energy levels fulfill linear dispersion relation (5.6), and the $N$th level does not.

$$\tilde{U} = \exp \left( -\frac{i}{\hbar} \tilde{H} \tau - i\phi \right),$$ (5.20)

$$|\psi_s\rangle = \sum_{j=1}^{N} a_j |\psi_j\rangle,$$ (5.21)

where

$$\tilde{H} |\psi_j\rangle = E^0_j |\psi_j\rangle \quad \forall j < N,$$ (5.22)
5. Solitary objects

\[ \hat{H} |\psi_N\rangle = (E_N^0 + \varepsilon) |\psi_N\rangle, \quad (5.23) \]

and \( \forall j E_j^0 \) fulfil the dispersion relation (5.6).

\[ \hat{T} |\psi_s\rangle = \sum_{j=1}^{N} a_j \exp\left(\frac{2\pi i N k_j}{N} \right) |\psi_j\rangle. \quad (5.24) \]

\[ \hat{U} |\psi_s\rangle = \sum_{j=1}^{N-1} a_j \exp\left(-\frac{i}{\hbar} E_j^0 \tau - i\phi \right) |\psi_j\rangle + a_N \exp\left(-\frac{i}{\hbar} E_N^0 \tau - i\varepsilon \tau - i\phi \right) |\psi_N\rangle. \quad (5.25) \]

So

\[ \langle \psi_s | \hat{T}^+ \hat{U} |\psi_s\rangle = \sum_{j=1}^{N-1} |a_j|^2 + |a_N|^2 \exp\left(-\frac{i}{\hbar} \varepsilon \tau \right). \quad (5.26) \]

Using the normalization condition

\[ \sum_{j=1}^{N} |a_j|^2 = 1 \quad (5.27) \]

now we can write following:

\[ \Delta = 1 - \left| 1 - |a_N|^2 \left(1 - \exp\left(-\frac{i}{\hbar} \varepsilon \tau \right) \right) \right|. \quad (5.28) \]

As one can see on the Figure 5.2 \( \Delta \) is a periodic function, which of course starts at zero for small arguments \( \varepsilon \tau \). Thus we can make a conclusion, that if \( \varepsilon \) is small enough, our object would not be destroyed in the course of its evolution, but rather will periodically disperse and pulled back together, displaying a recurrent time evolution.
Figure 5.2: Plot of the stability parameter $\Delta$ vs time for different values of $|a_N|$ (see expression (5.28)).
6. Results obtained for various ring systems

In this section we mainly stick to the system of 8 spin sites, because the real system we aim at is Cr8 with 8 chromium ions (Fig. 4.1). Some interesting results for systems of other sizes will also be provided.

Before starting presenting results of our investigation, certain features of our procedure for searching solitary states in quantum spin rings must be explained.

First of all, we are looking for well localized objects, because they could be easier found in scattering experiments, which are the most used ones for studying solitons in magnetic systems. In order to do this, we are looking for a state, combined from as much basis states with different values of the shift quantum number $k$ as possible. The reason is clear - the more different $k$ values contribute to the state (the broader the spectrum of the state in the space of wave vector) the narrower will this state be in physical coordinate space. Thus we are looking mostly for nontrivial sets of states consisting of 3 or more states, while 2 states always build up a combination which fulfills condition (5.6).

The second observation made while making calculations for different systems is that in order to obtain a well localized solitary object and not a series of several of such objects one needs $k$-values of contributing states to form a continuous sequence, without any gaps (see Fig.6.1). That is why we restricted our procedure for searching of suitable sets of basis states only to such cases.

The third point to be mentioned is that we use only real coefficients in the expansion series (5.2). This significantly simplifies the search of well localized states, since the number of variable parameters in the expansion becomes two times smaller.

6.1. Ising Hamiltonian

First we consider systems with Ising Hamiltonian. The beauty of the Ising model is that the energy eigenvalues are known exactly and form a regular pattern. Thus it is very easy to point out groups of states which fulfill the condition (5.6).

The energy spectrum calculated for the system of 8 spins is represented on Fig. 6.2
6. Results obtained for various ring systems

Figure 6.1: Example of a not localized and a localized object on a spin ring of 6 spins-1/2 with Heisenberg Hamiltonian. States taken to form the expansion (5.2) fulfill the condition (5.6).

Left hand side - the best result achieved for states with \( k = 0, 1, 5 \)
Right hand side - the best result achieved for states with \( k = 1, 2, 3 \)
One can see, that the object on the right hand side is much better localized as the other one.

and Fig. 6.3.

Figure 6.2: Energy spectrum for the Ising Hamiltonian (4.1) for system of \( N = 8 \) spin sites with \( s = \frac{1}{2} \)
6. Results obtained for various ring systems

Figure 6.3: Energy spectrum for the Ising Hamiltonian (4.1) for system of $N = 8$ spin sites with $s = \frac{1}{2}$

Having calculated the energy spectrum one can try to build up a combination of ground state and first exited one. But it brings out nothing but a trivial distribution of magnetization in form of a flat line (Fig. 6.4).

The explanation lies in the fact, that since

$$\langle m_1, m_2, \ldots | \tilde{s}_z(i) | m'_1, m'_2, \ldots \rangle = m_i \delta_{m_1 m'_1} \delta_{m_2 m'_2} \cdots,$$

(6.1)

to have a non-zero overlap between functions $|\psi_n\rangle$ in the linear combination (5.2) at least two of them must belong to the same $M$-subspace. But states taken have no common value of $M$, thus resulting in the trivial flat local magnetization profile. This feature was found to be general for all sets of states where states have different energies in the Ising model.

But nevertheless one can build states with a nontrivial profile of magnetization. However these states are no more "moving" objects, because they are built only from states, whose energies are equal, making the speed of such objects equal to zero (Fig. 6.5).

Summarizing, the objects of the type discussed in the system with Ising interactions could be divided into 2 groups. Objects of the first type move around the
6. Results obtained for various ring systems

Figure 6.4: Distribution of the local magnetization in the ring of 8 spins-1/2 with Ising Hamiltonian. The states taken to form an expansion series (5.2) are the ground state \( E = -4, k = 0 \) and a first excited state \( E = -2, k = 1 \). This produces a trivial profile of magnetization.

ring, but have trivial constant magnetization profile (so it is indeed hard to speak about any "movement"). Objects of the second type have nontrivial magnetization profile, but are "frozen" and therefore don’t move around the ring.

Thus, we need to consider another type of Hamiltonian in order to find objects which simultaneously move around the ring and have a localized magnetization profile.

6.2. Heisenberg Hamiltonian

In this section we will consider systems with a Hamiltonian of Heisenberg type. This type of Hamiltonian is more appropriate for real magnetic molecules, thus it’s investigations can give us more information about realistic systems.

As for the first try let us consider a trivial case - a state, combined only from ground state and first exited one.
6. Results obtained for various ring systems

Figure 6.5: Nontrivial local magnetization profile for system of 8 spin-1/2 with Ising Hamiltonian. The expansion is made from following states: 
\[ |\psi_s\rangle = c_1 |\psi_7\rangle + c_2 |\psi_8\rangle + c_3 |\psi_9\rangle, \]
where \( E_7 = 2, k_7 = 5, c_1 = 0.577350269 \), \( E_8 = 2, k_8 = 6, c_2 = 0.8 \), \( E_9 = 2, k_9 = 7, c_3 = 0.163299316 \). Note that these states lie on a horizontal line (Figure 6.2). Thus this object does not move around the ring (see section 5.1).

By default, such a combination fulfills the condition (5.6), thus the resulting periodic structure moves around the ring as it is, without changing its shape. This effect is known as quantum rotation of the Néel vector and was predicted quite long ago. However this effect was only recently observed in experiments on chromic wheels [46], and our results can be considered as another explanation for the nature of this effect.

As one can see in Fig. 6.6 the spectrum has no such regular pattern as for the Ising model. Thus in this case if we want to find really localized configurations (combined from more than 2 basis states), we really have to imply an algorithm for searching states suitable for our purpose. Further possible sets of states are singled out. One must note, that naturally, when decreasing the accuracy of the searching procedure more suitable sets could be found. But in this case the instability which arises from finite numerical calculations precision (see Section 5.3) gradually increases, so the
behavior of the objects obtained will be far from solitary one.

In Fig. 6.9 straight lines connect different sets of states, which fulfill condition (5.6). Calculations are done with the same precision, as calculation of the energy spectra in general ($10^{-6}$). We find only two possible sets of states. As one can see, these sets are symmetric ones, and at identical conditions they will produce identical objects that are moving around the ring in opposite directions. Further on the one connected with a bold line is considered.

Every of the states represented in the energy spectrum is indeed a multiplet of states, belonging to different $M$ subspaces (Fig. 6.10).

First for the construction of the solitary state (5.2) we take all the states from the same $M$ subspace, namely $M = 3$. By varying coefficients in the linear composition of the basis state considered we have found the following combination, which produces a rather well localized object.

Further we vary signs of coefficients in the linear composition, keeping the absolute values of coefficients the same.

Figure 6.6: Energy spectrum for the Heisenberg Hamiltonian (4.2) for system of $N = 8$ spin sites with $s = \frac{1}{2}$.
6. Results obtained for various ring systems

![Graph showing energy spectrum for the Heisenberg Hamiltonian (4.2) for system of N=8 spin sites with s=1/2.](image)

Figure 6.7: Energy spectrum for the Heisenberg Hamiltonian (4.2) for system of $N = 8$ spin sites with $s = \frac{1}{2}$

One can note, that similar results could be obtained, if for the linear combination one takes states of the same multiplets, but with opposite sign of $M$. In the following graph the result of the calculations with the same coefficients, as in Fig. 6.12, but this time all the states belong to $M = -3$ subspace.

Also one can take different states from corresponding multiplets. Results of such variations are presented in the Figures 6.15-6.19.

### 6.2.1. Larger systems

As one could see from the previous figures, the objects we get in the system of 8 spins are not so well localized as one would like it to be. They span around larger part of the system. And it is clear, that this is an unavoidable consequence of the small size of our system. Thus, it is natural to suppose that enlarging the system will produce better localized states (compare Fig. 6.20 and Fig. 6.21).
6. Results obtained for various ring systems

Figure 6.8: Profile of magnetization for the state formed by the ground state \((E = -7.30218682, k = 0, M = 0)\) and first excited state \((E = -6.25683813, k = 4, M = 0)\). Coefficient for the ground state in the linear combination (5.2) is taken to be \(\frac{1}{\sqrt{2}}\), 0.3 or 0.9, coefficient of the first excited state calculated from the normalization rule (5.27). Since these states lie not on the horizontal line in the spectrum of the system (see Figure 6.6), the whole configuration moves around the ring as it is, without any change of the shape. This effect corresponds to quantum rotation of the Néel vector.

However, as it was discussed before, in the Heisenberg model it is impossible to predict the existence of sets with more than 2 states with linear dispersion relation between them. Thus first we need to examine different systems to find out whether these systems can in principle host objects of the type discussed. Further results of this examination are given.

- \(N = 10\)

This system has no linear dispersion sets of states within accuracy of the spectrum itself.

- \(N = 12\)
6. Results obtained for various ring systems

Figure 6.9: Energy spectrum for the Heisenberg Hamiltonian (4.2) for system of $N = 8$ spin sites with $s = \frac{1}{2}$. Two lines connect two different sets of states which fulfill condition (5.6). This two sets are the only ones existing in this system if one searches for suitable sets with same precision as the energy spectrum itself.

This system has 10 suitable sets of states within accuracy of the spectrum itself, but none of them has more than 3 states with successive $k$ quantum numbers. Based on the these sets, the following object can be constructed (see Figure 6.22):

State No. 1345, $k = 8$, $E = -1.2991302$, $M = 1$, coefficient = 0.1 State No. 1422, $k = 9$, $E = -0.0946973354$, $M = 1$, coefficient = 0.9 State No. 1489, $k = 10$, $E = -0.0946627023$, $M = 1$, coefficient = 0.424264119

• $N = 14$

This system is already too large for our numerical procedure to diagonalize it completely, find all suitable sets of states and calculate the local third spin component at once. But nevertheless our calculations show that this system has at least one set of states fulfilling the condition (5.6), and it has 5 states with successive $k$ quantum numbers. This is rather promising while this could allow to construct a solitary object that is better localized on our system. And
6. Results obtained for various ring systems

Figure 6.10: The same plot as in Figure 6.6, but every point represented as corresponding multiplet of states.

indeed, based on this set of basis states the object with the local magnetization profile pictured in the Figure 6.23 was created.

State shown on the Figure 6.23 is combined from the following basis states:

State No. 672, k= 4, E= 1.79196226, M= 2, coefficient = 0.1
State No. 732, k= 5, E= -3.82950945, M= 2, coefficient = 0.9
State No. 877, k= 6, E= -3.82946959, M= 2, coefficient = 0.4
State No. 1023, k= 7, E= -3.27135162, M= 2, coefficient = 0.1
State No. 1266, k= 8, E= 3.51434969, M= 2, coefficient = 0.1
6. Results obtained for various ring systems

Figure 6.11: Nontrivial local magnetization profile for system of 8 spin-1/2 with Heisenberg Hamiltonian. The expansion is made from following states: $|\psi_s\rangle = c_1 |\psi_7\rangle + c_2 |\psi_8\rangle + c_3 |\psi_9\rangle$, where \{\(E_7 = 2, k_7 = 5, c_1 = 0.577350269\}\}, \{\(E_8 = 2, k_8 = 6, c_2 = 0.8\)\}, \{\(E_9 = 2, k_9 = 7, c_3 = 0.163299316\)\}. All the states in this combination belong to the subspace with \(M = 3\).
Figure 6.12: States based on the state, presented in the Figure 6.11, but with different signs of the coefficients. Note, that total inversion of the sign of all coefficients simultaneously has no effect.
6. Results obtained for various ring systems

Figure 6.13: The same as in Figures 6.11 and 6.12, but states taken for linear combination (5.2) belong to another $M$-subspace of corresponding multiplets. In this case all the states belong to $M = -3$ subspace. The object obtained are just a mirror of the ones in the Figure 6.12.
Figure 6.14: The $M$-subspace of the first state in the linear combination for the object in the Figure 6.11 is varied.
Figure 6.15: The $M$-subspace of the second state in the linear combination for the object in the Figure 6.11 is varied. Since this state has a highest weight in the linear combination (see caption to Figure 6.11), the effect of varying of this state is most drastic.
Figure 6.16: The $M$-subspace of the third state in the linear combination for the object in the Figure 6.11 is varied. Since this state has a lowest weight in the linear combination (see caption to Figure 6.11), the effect of varying of this state is much less pronounced in comparison to other cases.
Figure 6.17: The $M$-subspace of all the states in the linear combination for the object in the Figure 6.11 is varied simultaneously.
Figure 6.18: One of the states in the linear combination is taken from $M = 0$ subspace. Once again, the most pronounced effect is obtained when manipulating the state with highest weight in the linear combination.
6. Results obtained for various ring systems

Figure 6.19: Two states in the linear expansion are taken from $M = 0$ subspace, and the one with the highest weight is taken from $M = 1$ subspace. The structure similar to domain walls is obtained.

Figure 6.20: Sketch of the small system with a solitary object on it. The object is rather small and spans over just a couple of spin sites. But since the system is also small, the object is not well localized.

Figure 6.21: Sketch of the system, which is considerably bigger as one in the Figure 6.20. The object has nearly the same size, but now it is much better localized on the ring.
Figure 6.22: Solitary object on the ring of 12 spins-1/2. Just like objects on Figures 6.11 - 6.18 this object is composed from 3 states, but it is better localized due to the larger size of the system.
Figure 6.23: Solitary object on the ring of 14 spins-1/2. This object is composed from 5 different basis states, and much better localized on the ring as ones in Figures 6.11 etc.
7. Summary and outlook

One-dimensional magnetic systems have been of great interest in the last decades. Different systems were realized and described during this time. All these substances are systems of rather long chains of ions with small interchain interaction, thus being a suitable experimental model for large one-dimensional linear systems. Continuous classical approximation in the form of the sine-Gordon model proved itself as a very good approximation for a qualitative understanding of the processes and even for some quantitatively comparison with experimental results in these systems.

But recent achievements in chemistry allowed to construct a class of substances, where the size of the corresponding magnetic systems and smallness of the spin prohibit the implementation of both classical and continuum approximations. These systems are metal-organic compounds with metal ions whose intrinsic spins are located on nearly ideal rings. Quantum methods are the proper ones to deal with these substances. However results in this field of theoretical description of quantum spin systems are much less detailed then ones in the field of classical approximation.

From the results of both classical and quantum methods it is clear, that solitary excitations in one-dimensional magnetic systems carry important role in their properties [47]. In this work an attempt to realize what is a solitary excitation in a purely quantum case of a small magnetic system is made.

In this work a simple and intuitive definition of a solitary object for a quantum case is proposed. It is shown, that such a basic property of these objects as their velocity is directly connected to the spin-spin coupling coefficient, which is a fundamental parameter of the system. This could provide a possibility to measure the coupling constant with higher precision as other methods. Based on the introduced definition of the solitary object different systems are examined whether they host such objects. It is found, that indeed some, but not all, systems can host rather well localized objects, which are moving around the ring without changing their envelope of magnetization. In particular, the model proposed describes a rotation of the quantum Néel vector in the ring, governed by interspin interactions of Heisenberg type.

The future development of this approach must first of all include consideration of
ion spin values higher than \( \frac{1}{2} \), since this will bring the results of the calculations closer to real materials, which are built from spins \( \frac{3}{2} \) or \( \frac{5}{2} \). But due to exponential growth of the calculation power needed (see section 4.4) the considerable enhancement of the numerical algorithm is required. Also a contribution of the objects found to the thermodynamical properties of the spin wheels should be explored.

A separate question concerns the possibility of exciting and detecting such states. While it seems that the detection is quite possible with, for example, inelastic neutron scattering experiments, the problem of excitation is more tricky, since most states found so far lie in the high-energy part of the spectrum of the system.

Another direction of investigations could be switching to higher spatial dimensions. Recently molecular magnets such as Fe\(_{30}\) were synthesized [48]. There one has spin items (ions of iron) located on planar rings intersecting in three dimensions (Figure 7.1). And since these iron atoms have spin value of \( \frac{5}{2} \) the extension to the approach proposed even with some approximations would be a challenging task for future investigations.

---

Figure 7.1: Molecule of Fe\(_{30}\).

a) The structure of the molecule.

b) The same but only iron atoms are shown. Spins are arranged in 3 dimensions on intersecting rings.
A. Derivation of expression for $s_z(i)$

To any state $|a_i\rangle$ we put in accordance 3 numbers:

- $k_i$ - shift quantum number for this state;
- $MBSt_i$ - number of the $|a_i\rangle$-state, from which one has to start building a corresponding $|\chi_i\rangle$;
- $ZDim_i$ - number of consequent states needed to build a corresponding $|\chi_i\rangle$-state (starting with state number $MBSt_i$).

Then we produce $|\chi_i\rangle$-states in the following way (see Ref. [44]):

$$|\chi_j\rangle = \frac{1}{\sqrt{ZDim_j}} \sum_{\mu=MBSt_j}^{MBSt_j+ZDim_j-1} |a_\mu\rangle \exp\left\{ \frac{2\pi i}{N} k_j(\mu - MBSt_j) \right\}.$$  \hfill (A.1)

It is easy to check that states constructed in such a way are indeed eigenstates of shift operator with corresponding shift quantum number $k_j$, i.e.

$$\tilde{T} |\chi_j\rangle = e^{-\frac{2\pi i}{N} k_j} |\chi_j\rangle.$$  \hfill (A.2)

Thus we have

$$\langle a_\nu|\chi_j\rangle = \frac{1}{\sqrt{ZDim_j}} \sum_{\mu=MBSt_j}^{MBSt_j+ZDim_j-1} \langle a_\nu|a_\mu\rangle \exp\left\{ \frac{2\pi i}{N} k_j(\mu - MBSt_j) \right\}.$$  \hfill (A.3)

Since $\langle a_\nu|a_\mu\rangle = \delta_{\nu\mu}$ we can simply drop out the sum, but only in case if $\nu$ is in range of $\mu$. Thus we end up with the following expression for $\langle a_\nu|\chi_j\rangle$:

$$\langle a_\nu|\chi_j\rangle = \begin{cases} \frac{1}{\sqrt{ZDim_j}} \exp\left\{ \frac{2\pi i}{N} k_j(\mu - MBSt_j) \right\} & \text{if } 0 \leq \nu - MBSt_j \leq ZDim_j - 1; \\ 0 & \text{in all other cases.} \end{cases}$$  \hfill (A.4)
B. Numerical algorithm

The FORTRAN77 [49] programming language was used to write a program for numerical calculations. g77, a part of GNU Compiler Collection [50], was used to compile executables from the source code under Debian Linux [51]. jEdit, an open source Java text editor [52], was used to write the program and manipulate the whole project.

B.1. Structure of algorithm

The numerical procedure works as follows:

- Matrix $J$ of interspin interactions is calculated
- Magnon vacuum ($M = 0$ subspace) is calculated separately.
- Decomposition of the whole Hilbert space to $M$-subspaces is made; cycles are found and basis vectors are sorted on them; Hamiltonian matrix for every $M$-subspace is calculated.
- Decomposition of $M$-subspaces to ($M,k$)-subspaces is made; Hamiltonian matrix for every such subspace is calculated; ”cycle”-related properties of every basis state ($ZDim, MBSt,k$), are defined.
- Hamiltonian matrices for ($M,k$)-subspaces are diagonalized using subroutine ZHEEV from LAPACK numerical library [53]. Results (diagonalized Hamiltonian matrix and eigenvectors) are stored.
- The whole ($E,k$) array is searched for sets of states which satisfy ”linearity” condition (5.6). Found results are stored.
- One particular set of states is taken, and values of $\langle \tilde{s}_z \rangle$ on each spin site are calculated according to expression (5.16). Results are stored.
B. Numerical algorithm

B.2. Source code

Table B.1: Variables used in analytical calculations vs variables used in FORTRAN code of the numerical procedure

<table>
<thead>
<tr>
<th>Variable used in analytical calculations</th>
<th>Variable used in numerical procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>n or StateNumber(n) – a number of the state</td>
</tr>
<tr>
<td>$2s$</td>
<td>sMal2</td>
</tr>
<tr>
<td>$S_z(i)$</td>
<td>SZ(i)</td>
</tr>
<tr>
<td>$E_n$</td>
<td>HEigenwerte(n)</td>
</tr>
<tr>
<td>$k_n$</td>
<td>AllEigenwerte(3,n)</td>
</tr>
<tr>
<td>$2M_n$</td>
<td>AllEigenWerte(2,n)</td>
</tr>
<tr>
<td>$2S_n$</td>
<td>AllEigenwerte(1,n)</td>
</tr>
<tr>
<td>$a_\nu(i)$</td>
<td>BasisElement(i,\mu)</td>
</tr>
<tr>
<td>$c_n$</td>
<td>Coeff(n)</td>
</tr>
<tr>
<td>$Z Dim_\mu$</td>
<td>Kbasis(\mu,2)</td>
</tr>
<tr>
<td>$k_\mu$</td>
<td>Kbasis(\mu,1) – shift quantum number</td>
</tr>
<tr>
<td>$MBSt_\mu$</td>
<td>Kbasis(\mu,3)</td>
</tr>
</tbody>
</table>
B. Numerical algorithm

B.2.1. Listing of the source code

program soliton

* Diagonalization of small spin systems
* Ring geometry
* Search for soliton-like states
* JMAT - Coupling matrix
* SymmetryDim - Number of symmetry operations ZSHIFT, which lead to the initial state

implicit none

integer N, sMal2, AbrDim
integer DIM, EVNumber, LastEVNumber, FirstMIndex

system and spin size are defined
parameter (N=8,sMal2=1,DIM=300000,AbrDim=5700)

integer SymmetryDim
parameter (SymmetryDim=N)

integer BasisElement (N,DIM), MBasisElement (N, AbrDIM)
integer TestElement (N), Element1 (N), Element2 (N)
integer Absenker, AbsenkTabelle (N*sMal2)
integer k, l, m, i, j, L1, ml, Lk, mk, im, iL
integer AbGes, Feldplatz
integer AbGesListe (N*sMal2)
integer ZList (DIM), ZListLen, ZListPlatz, ZListSum
integer HDim
integer Error

real E, Hamilton, MGes
real HEigenWertL (AbrDim), rk (3*AbrDim+1)
real Overlap, Difference, Dif
real Pi, C, HQuerC, GMuK

real AllEigenWerteI (1, )=2 S, AllEigenWerteI (2, )=2 M,
AllEigenWerteI (3, )=k, AllEigenWerteI (4, )=1 or 0

real AllEigenWerteH (DIM)
integer AllEigenWerteI (4, DIM)

real JMAT

complex H (AbrDim, AbrDim), HElement
save H
complex HEigenvector
complex wk (3*AbrDim+1)
complex ui

for truncating procedure to M-subspaces
integer AbGesMax, AbGesMin
B. Numerical algorithm

for sorting states on k-values before searching for lines

integer StatesK(0:SymmetryDim−1), MaxStatesK

variables for searching lines

integer NLines, MaxStatesCount, Temp(DIM)
integer*4 MaxLines
real*8 lineaccur
parameter (MaxLines=100000, lineaccur=1.0d−6)
parameter (MaxStatesCount=100)
integer*4 StatesNumbers(MaxStatesCount, MaxLines)
integer*4 StatesCount(MaxLines)
real*8 ALines(MaxLines), BLines(MaxLines)

variables for creating array of eigenvectors

integer*4 HDimBack
integer EigVecDim
parameter (EigVecDim=2**N) /* complete case, can be truncated */
complex*16 EigVec(EigVecDim, EigVecDim)
save EigVec

variables for calculating the Sz spin component

real*8 SZ(N), SumTemp, Coef
integer*4 NofStates, nu, mu
parameter (NofStates=3) /* number of states to form a soliton */
integer*4 StateN(NofStates)
complex*16 sum1, sum2, Coeff(NofStates)

*******************************************************************************

Bases transformation

KBasis represents EV and T as superposition of Isingbasis
KBasis(i,1)=k,
KBasis(i,2)=Dim. of cycles,
KBasis(i,3)=No of the first vector in a cycle

integer*4 KBasis(Dim,3)
save KBasis

character Version*150

real time1
integer*4 Count1, Count2, Rate, Max

common/JMatrix/JMAT(N,N)
common/const/Pi, C, HQuerC, GMuK

Pi = 3.1415926535d0
HQuerC = 197.327053d0
C = 2.99792458d23
GMuK = 2.0*0.6717d0
ui = DCMPLX(0.0d0, 1.0d0)

Version= 'soliton 02 Juergen Schnack & Pavlo Shchelokovskyy 1.10.04'

output of N and s
B. Numerical algorithm

\[ \text{write}(6,*)'\'' \]
\[ \text{write}(6,'(a')'\text{Version} \]
\[ \text{write}(6,'(a,i4,a,f15.6)')'N = ',N,', s = ','0.5d0*\text{Mal2} \]

* JMatrix is defined
* call MakeJMatrix(N,JMAT)
* other initializations
* do i=1,Dim
    do j=1,3
        KBasis(i,j)=0
    enddo
* enddo

************
* define in which M-subspaces calculations are done
* for the complete case AbGesMin=1, AbGesMax=N*Mal2/2
* AbGesMin=1
* AbGesMax=4
* initialization of eigenvectors array
* do i=1,EigVecDim
    do j=1,EigVecDim
        EigVec(i,j)=DCMPLX(0.0d0,0.d0)
    enddo
* enddo

HDimBack=1
* definition of basis states and coefficient to form a soliton
* Initializing StateN
* StateN(1)=552
* StateN(2)=629
* StateN(3)=696
* Coef=sqrt(1/real(NofStates))
* Creating coefficients of superposition
* Coeff(1)=cmplx(Coef,0.d0)
* Coeff(2)=cmplx(Coef,0.d0)
* SumTemp=0.0d0
* do i=1,NofStates-1
    SumTemp=SumTemp+abs(Coeff(i))**2
* enddo
* Coeff(NofStates)=sqrt((1.0d0,0.d0)-SumTemp)

************
* first loop goes over downsteps (Absenkungen)
B. Numerical algorithm

Magnonvacuum, i.e. downstep (Absenkung) = 0 in the beginning

\[
\begin{align*}
\text{do } & j=1,N \\
\text{Element1}(j) &= 0 \\
\text{Element2}(j) &= 0
\end{align*}
\]

\[
E=\text{Hamilton}(N, sMal2, \text{Element1}, \text{Element2}, JMAT)
\]

\[
\begin{align*}
\text{EVNumber} &= 1 \\
\text{AllEigenWerteH}(\text{EVNumber}) &= E \\
\text{AllEigenWerteI}(1, \text{EVNumber}) &= N \ast sMal2 \\
\text{AllEigenWerteI}(2, \text{EVNumber}) &= N \ast sMal2 \\
\text{AllEigenWerteI}(3, \text{EVNumber}) &= 0 \\
\text{AllEigenWerteI}(4, \text{EVNumber}) &= 1 \\
\text{LastEVNumber} &= \text{EVNumber}
\end{align*}
\]

\[
\begin{align*}
\text{do } & j=1,N \\
\text{BasisElement}(j, \text{EVNumber}) &= 0 \\
\text{Element1}(j) &= 0 \\
\text{Element2}(j) &= 0
\end{align*}
\]

\[
\begin{align*}
\text{KBasis}(\text{EVNumber}, 1) &= 0 \\
\text{KBasis}(\text{EVNumber}, 2) &= 1 \\
\text{KBasis}(\text{EVNumber}, 3) &= \text{EVNumber}
\end{align*}
\]

\[
\begin{align*}
\text{do } & \text{AbGes} = \text{AbGesMin, AbGesMax} \ \text{partial or complete case} \\
\text{MGes} &= 0.5 \ast N \ast sMal2 \ast \text{AbGes} \\
\text{FirstMIndex} &= \text{EVNumber}+1
\end{align*}
\]

\[
\begin{align*}
\text{do } & j=1,\text{Abges} \\
\text{AbsenkTabelle}(j) &= 1 \ \text{all downsteps (Absenker) on site 1}
\end{align*}
\]

\[
\begin{align*}
\text{do } & j=\text{Abges+1},N\ast sMal2 \\
\text{AbsenkTabelle}(j) &= 0
\end{align*}
\]

FeldPlatz = 0

1000 continue

\[
\begin{align*}
\text{do } & j=1,N \\
\text{TestElement}(j) &= 0
\end{align*}
\]

\[
\begin{align*}
\text{do } & j=1,\text{Abges} \\
\text{TestElement}(\text{AbsenkTabelle}(j)) &= \\
\text{TestElement}(\text{AbsenkTabelle}(j)) + 1
\end{align*}
\]

\[
\begin{align*}
\text{do } & j=1,N \\
\text{if } & (\text{TestElement}(j) \gt sMal2) \text{ goto 1100 } \text{ not a valid state}
\end{align*}
\]

\[
\begin{align*}
\text{if}(\text{FeldPlatz}.\ge.\text{DIM}) \text{ goto 9999} \\
\text{FeldPlatz} &= \text{FeldPlatz} + 1 \\
\text{do } & j=1,N \\
\text{MBasisElement}(j, \text{FeldPlatz}) &= \text{TestElement}(j)
\end{align*}
\]
B. Numerical algorithm

1100 continue

Absenker = 1
AbsenkTabelle(Absenker) = AbsenkTabelle(Absenker) + 1
if(AbsenkTabelle(Absenker) .le. N) goto 1000 ! new downstep (Absenker) a.k.

1200 continue
Absenker = Absenker + 1
if(Absenker .gt. Abges) goto 1300
AbsenkTabelle(Absenker) = AbsenkTabelle(Absenker) + 1
if(AbsenkTabelle(Absenker) .le. N) then
    do j=1,Absenker-1
        AbsenkTabelle(j) = AbsenkTabelle(Absenker)
    enddo
    goto 1000
else
    goto 1200
endif

1300 continue ! no further downsteps(Absenkungen)
AbGesListe(AbGes) = FeldPlatz

sort basis on cycles

if(SymmetryDim .gt. 1) then
    do L=1,AbGesListe(AbGes)
        call ZSHIFT(N, MBasisElement(1,L) , TestElement)
        do k=L+1,AbGesListe(AbGes)
            if (Overlap(N, TestElement , MBasisElement(1,k)) .gt. 0.999d0) then
                do j=1,N
                    MBasisElement(j,k) = MBasisElement(j,L+1)
                    MBasisElement(j,L+1) = TestElement(j)
                enddo
            endif
        enddo
    enddo
enddo
do L=1,AbGesListe(AbGes)
    do j=1,N
        BasisElement(j,EVNumber+L) = MBasisElement(j,L)
    enddo
enddo
endif

calculate Hamiltonmatrix for subspace with constant downstep (Absenkung)
MGes = 0.5d0 * N * sMal2 - AbGes

Generate list of cycles

dim J=1,DIM
ZList(j) = 0
enddo
ZListLen = 0
ZListPlatz = 0
ZListSum = 0
B. Numerical algorithm

L = 1

\textbf{do while} (L > \text{AbGesListe}(\text{AbGes}))

\hspace{1cm} L1 = L
\hspace{1cm} ZListPlatz = ZListPlatz + 1

\hspace{1cm} ZList(ZListPlatz) = ZList(ZListPlatz) + 1
\hspace{1cm} ZListLen = ZListLen + 1
\hspace{1cm} ZListSum = ZListSum + 1

\hspace{1cm} \textbf{do} j=1,N
\hspace{2cm} Element1(j) = MBasisElement(j,L1)
\hspace{2cm} Element2(j) = MBasisElement(j,L1)
\hspace{1cm} \textbf{enddo}

\hspace{1cm} \textbf{do} i=1,SymmetryDim-1
\hspace{2cm} \textbf{do} j=1,N
\hspace{3cm} TestElement(j) = Element2(j)
\hspace{2cm} \textbf{enddo}
\hspace{1cm} \textbf{call} ZSHIFT(N,TestElement,Element2)
\hspace{1cm} \textbf{if} (Overlap(N,Element2,MBasisElement(1,L1+i)).lt.1.d-6)
\hspace{2cm} \textbf{goto} 200 ! Cycle finished
\hspace{1cm} \textbf{then}
\hspace{2cm} \textbf{ZList}(ZListPlatz) = ZList(ZListPlatz) + 1
\hspace{2cm} \textbf{ZListSum} = ZListSum + 1
\hspace{1cm} \textbf{enddo}
\hspace{1cm} \textbf{continue}
\hspace{1cm} L = L + ZList(ZListPlatz)
\hspace{1cm} \textbf{enddo}

\hspace{1cm} \textbf{continue}
\hspace{1cm} now subspace can be divided to orthogonal subspaces in respect to
\hspace{1cm} shift quantum number k=0,..
\hspace{1cm} Matrixelements H(Lk,mk)
\hspace{1cm} do k=0,SymmetryDim-1
\hspace{2cm} HDim = 0
\hspace{2cm} do L=1,ZListLen
\hspace{3cm} \textbf{if} (MOD(k,SymmetryDim/ZList(L)).eq.0) HDim = HDim + 1
\hspace{2cm} \textbf{enddo}
\hspace{2cm} KBasis
\hspace{2cm} Lk = 0
\hspace{2cm} L1 = FirstMIndex-1
\hspace{2cm} do L=1,ZListLen
\hspace{3cm} \textbf{if} (MOD(k,SymmetryDim/ZList(L)).eq.0) then ! shift QN. divides k
\hspace{4cm} Lk = Lk + 1
\hspace{4cm} KBasis(EVNumber+Lk,1) = k
\hspace{4cm} KBasis(EVNumber+Lk,2) = ZList(L)
\hspace{4cm} KBasis(EVNumber+Lk,3) = L1+1
\hspace{3cm} \textbf{endif}
\hspace{3cm} L1 = L1 + ZList(L)
\hspace{2cm} \textbf{enddo}
\hspace{2cm} \textbf{continue}
\hspace{2cm} Lk = 0

500
B. Numerical algorithm

```plaintext
L1 = 0  ! Feld Platz

do L=1,ZListLen
  if (MOD(k,SymmetryDim/ZList(L)).eq.0) then ! shift QN. divides k
    Lk = Lk + 1
    mk = 0
    m1 = 0  ! Feld Platz
    do m=1,ZListLen
      if (MOD(k,SymmetryDim/ZList(m)).eq.0) then ! shift QN. divides k
        mk = mk + 1
        H(Lk,mk) = DCMPLX(0.d0,0.d0)
      endif
      do j=1,N
        Element1(j) = MBasisElement(j,L1+iL)
      enddo
      do j=1,N
        Element2(j) = MBasisElement(j,m1+im)
      enddo
      Dif = Difference(N,Element1,Element2)
      if ( (Dif.lt.1.d-6).or.(DABS(Dif-2.d0).lt.1.d-6))then
        H(Lk,mk) = H(Lk,mk)
        + Hamilton(N,sMal2,Element1,Element2,JMAT)
        * CEXP(-ui*2.d0*Pi*k*iL/SymmetryDim)
        * CEXP( ui*2.d0*Pi*k*im/SymmetryDim)
        / DSQRT(1.d0*ZList(L)*ZList(m))
      endif
    enddo
  endif
  m1 = m1 + ZList(m)
enddo

if (HDim.le.AbrDim) then
  call ZHEEV('V', 'U', HDim,H,AbrDim,HEigenWertL, wk, &
             3*AbrDim+1,rk, Error)
  do i=1,HDim
    EVNumber = EVNumber + 1
    AllEigenWerteH(EVNumber) = HEigenWertL(i)
    AllEigenWerteI(1, EVNumber) = -1
    AllEigenWerteI(2, EVNumber) = N * sMal2 - 2*AbGes
    AllEigenWerteI(3, EVNumber) = k
    AllEigenWerteI(4, EVNumber) = 1
  enddo
endif
```

Diagonalizing

```plaintext
```
B. Numerical algorithm

```plaintext
391 * storing array of eigenvectors
392 *
393   do i=1,HDim
394   do j=1,HDim
395       EigVec( HDimBack+i, HDimBack+j ) = H( i, j )
396     enddo
397   enddo
398   HDimBack=HDimBack+HDim
399 *
400 ******************************************************************************
401 *
402   else
403   write( 6, '(a)' ) 'Dimension zu gross!'
404   endif
405 *
406   9998 continue
407   enddo
408 *
409   arranging S
410 *
411 * Eigenvalue L
412   do j=1,AbGesListe( AbGes )
413       L = j + LastEVNumber
414   * compare with eigenvalue on site i
415   do i=1,LastEVNumber
416       if ((DABS( AllEigenWerteH( i )− AllEigenWerteH( L ) )< 1.d−8)
417         & ( AllEigenWerteI(3,L) .eq. AllEigenWerteI(3,i) )
418         & ( AllEigenWerteI(4,i) .gt. 0 )
419   then ! not yet occupied
420       AllEigenWerteI(1,L)=AllEigenWerteI(1,i)
421       AllEigenWerteI(4,i)=0
422     goto 300
423   endif
424   enddo
425   if( AllEigenWerteI(1,L) .lt. 0 ) then
426     AllEigenWerteI(1,L)=IABS( N * sMal2 − 2 * AbGes)
427   endif
428   300 continue
429   enddo
430 *
431 * LastEVNumber = EVNumber
432 *
433 * 8888 continue
434   enddo
435 *
436 *
437 *
438 ******************************************************************************
439 * Main Output
440 *
441 *
442   write( 6, '(a)' ) '*****************************************************************************'
443   write( 6, '(214, i9 , 14 , f8.3 )' ) N, sMal2, (sMal2+1)*N, 0 , 1. d0
444   write( 6, '(a,a,a)' ) ' E S
445 & ' M k S (S+1)
446 & ' No'
```
B. Numerical algorithm

```plaintext

k = 0

do j=1,LastEVNumber
    k = k + 1
    write(6,'(5f19.10,i12.1)')
    & AllEigenWerteH(j)
    & ,0.5d0*AllEigenWerteI(1,j)
    & ,0.5d0*AllEigenWerteI(2,j)
    & ,1.0d0*AllEigenWerteI(3,j)
    & ,0.5d0*AllEigenWerteI(1,j)*(0.5d0*AllEigenWerteI(1,j)+1.d0)
    & ,k
endo

write(6,'(a)') '******************************************************************************'
write(6,'(2i4,i9,i4,f8.3)') N, sMal2, k, 0, 1.d0

```

Determine, how many states are in particular k-number subspace and calculate maximal of these values

```plaintext

do i=0,SymmetryDim-1
    StatesK(i)=0
endo

do i=1,LastEVNumber
    StatesK(AllEigenWerteI(3,i))=StatesK(AllEigenWerteI(3,i))+1
endo

MaxStatesK=StatesK(0)
do i=1,SymmetryDim-1
    if (MaxStatesK.lt.StatesK(i)) then
        MaxStatesK=StatesK(i)
    endif
endo

```

Call the line-extraction procedure and output its results

```plaintext

do i=1,LastEVNumber
    Temp(i)=AllEigenWerteI(3,i)
endo

call Extrlines(Temp, AllEigenWerteH, LastEVNumber, lineaccur , & MaxLines, StatesNumbers, StatesCount , & MaxStatesCount, NLines , & ALines, BLines, SymmetryDim , & StatesK, MaxStatesK )

```

Output of lines with corresponding states and coefficients

```plaintext

write (6,*) '***********'
write (6,*) 'Accuracy=', lineaccur
write (6,*) 'AbGesMin=', AbGesMin
write (6,*) 'AbGesMax=', AbGesMax
write (6,*) '***********'
if (NLines.eq.0) then
```

---

68
B. Numerical algorithm

\begin{verbatim}
write (6,*) '********************'
write (6,*) 'NO LINES!
write (6,*) '********************'
else
   do i=1,NLines
      write (6,*) '********************'
      write (6,*) 'Line No.', i
      write (6,*) 'a=', ALines(i), ' b=', BLines(i)
      write (6,*) StatesCount(i), ' states:
      do j=1,StatesCount(i)
         write (6,*) 'k=', AllEigenWerteI(3, StatesNumbers(j, i)),
         & ' E=', AllEigenWerteH(StatesNumbers(j, i)),
         & ' M=', 0.5d0*AllEigenWerteI(2, StatesNumbers(j, i)),
         & ' State No.', StatesNumbers(j, i)
      enddo
   enddo
endif

# calculate the Sz spin component on every spin site

SZ(i) = Sz on site i
State Number = state from results of diagonalizing procedure.
EigVec(1,1)=(1.0d0, 0.0d0)

write (6,*) ''
do i=1,NofStates
   write (6,*) ''
   write (6,*) 'Point', i
   write (6,*) 'State Number=', StateN(i)
   write (6,*) 'E=', AllEigenWerteH(StateN(i))
   write (6,*) 'k=', AllEigenWerteI(3, StateN(i))
   write (6,*) 'M=', AllEigenWerteI(2, StateN(i))/2
   write (6,*) 'S=', AllEigenWerteI(1, StateN(i))/2
   write (6,*) 'Coefficient=', Coeff(i)
enddo
write (6,*) '********************'
write (6,*) 'SZ(i)'
write (6,*) ''
do i=1,N
   SZ(i)=0! initialize SZ(i)
   do nu=1, LastEVNumber
      sum2=0! initialize sum
      do k=1, NofStates! by subset of states
         sum1=0
         do mu=1, LastEVNumber
            if (((nu-KBasis(mu, 3)).ge.0)
   ...
B. Numerical algorithm

& . and .
& \((\text{nu–KBasis(mu, 3)}) \text{, i.e. (KBasis(mu, 2)–1)})\)
&
then
&
sum1=sum1+
& \((1/(\text{sqrt(real(KBasis(mu, 2))))*\exp((2*Pi*ui/N)*
& \text{KBasis(mu, 1)}*(\text{nu–KBasis(mu, 3)}))))\)*
&
EigVec(StateN(k),mu) ! "StateN" corresponds to superposition of states
&
else
&
sum1=sum1+DCMPLX(0.d0, 0.d0)
&
endif
&
sum2=sum2+Coeff(k)*sum1
&
enddo
&
SZ(i)=SZ(i)+(0.5d0*sMal2–BasisElement(i, nu))(*(ABS(sum2)**2)
&
enddo
&
write (6,*) SZ(i)
&
enddo
&

---

Subroutines

---

real+8 function Overlap(N,Element1,Element2)
&
implicit none
&
integer*4 N, j
&
integer*1 Element1(N),Element2(N)
&
real*8 Test
&
Test=0.0d0
&
do j=1,N
&
   Test=Test+DABS(1.d0*(Element1(j)–Element2(j)))
&
endo
&
if(Test.lt.1.d-6) then
&
   Overlap=1.0d0
&
else
&
   Overlap=0.d0
&
endif
&
return
B. Numerical algorithm

```
615    end
616
617    real*8 function Difference(N, Element1, Element2)
618    implicit none
619    integer*4 N, j
620    integer*1 Element1(N), Element2(N)
621    real*8 Test
622    do j = 1, N
623        Test = Test + DABS(1.0d0 * (Element1(j) - Element2(j)))
624    enddo
625    Difference = Test
626    return
627    end

633    real*8 function Hamilton(N, sMal2, Element1, Element2, JMAT)
634    implicit none
635    integer*4 N, sMal2, i, j, k
636    integer*1 TestElement(N), Element1(N), Element2(N)
637    real*8 s, Overlap
638    real*8 GammaXY, GammaZ
639    real*8 E
640    real*8 JMAT(N,N)
641    
642    ! here different type of the Hamiltonian can be choosed
643    ! Ising: GammaZ=1, GammaXY=0
644    ! Heisenberg: GammaZ=1, GammaXY=1
645    
646    GammaZ = 1.0d0  ! Anisotropy: I = isotrop
647    GammaXY = 1.0d0  ! Anisotropy: I = isotrop
648    s = 0.5d0 * sMal2
649    E = 0.0d0
650    
651    ! Loop over spin cites
652    do i = 1, N
653        do j = 1, N
654            if (DABS(JMAT(i, j)).gt.1.0d-6) then
655                
656                if (Overlap(N, Element1, Element2).gt.0.999d0) then
657                    E = E + JMAT(i, j)
658                    & GammaZ*(s-Element1(i))*(s-Element2(j))
659                end if
660            end if
661        enddo
662    enddo
```
B. Numerical algorithm

```fortran
endif

B. Numerical algorithm

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enddo

do k=1,N

testElement(k)=Element2(k)
enddo

testElement(j)=testElement(j)+1

testElement(i)=testElement(i)-1

e = e + jmat(i,j)
&
* gammaXY*0.5d0*overlap(N,element1,testElement)
&
* DSQRT((s-s+TestElement(j))*(s+s-TestElement(j)+1))
&
* DSQRT((s+s-TestElement(i))*(s-s+TestElement(i)+1))

do k=1,N

testElement(k)=Element2(k)
enddo

testElement(j)=testElement(j)-1

testElement(i)=testElement(i)+1

e = e + jmat(i,j)
&
* gammaXY*0.5d0*overlap(N,element1,testElement)
&
* DSQRT((s-s+TestElement(j))*(s+s-TestElement(j)+1))
&
* DSQRT((s+s-TestElement(i))*(s-s+TestElement(i)+1))

enddo

enddo

enddo

enddo

hamilton = -e

return

end

---

subroutine MakeJMatrix(N,JMat)

---

implicit none

integer*4 N,i,j

real*8 JMat(N,N)

real*8 J1

write(6,'(a)') 'Structure: Ring'

Loop over spincites

do i=1,N
    do j=1,N
        JMat(i,j) = 0.0d0
    enddo
endo
B. Numerical algorithm

\[
J1 = -1.0d0
\]
\[
\text{do } j = 1, N-1
\]
\[
\text{JMAT}(j, j+1) = J1
\]
\[
\text{JMAT}(j+1, j) = J1
\]
\[
\text{enddo}
\]
\[
\text{JMAT}(1, N) = J1
\]
\[
\text{JMAT}(N, 1) = J1
\]
\[
\text{return}
\]
\[
\text{end}
\]

\[
\text{subroutine ZSHIFT}(N, \text{Element1}, \text{Element2})
\]
\[
\text{do } j = 1, N-1
\]
\[
\text{Element2}(j+1) = \text{Element1}(j)
\]
\[
\text{Element2}(1) = \text{Element1}(N)
\]
\[
\text{return}
\]
\[
\text{end}
\]

\[
\text{subroutine Extrlines}(X,Y,N, \text{accur}, \text{MaxLines}, \text{PointsNumbers}, \text{PointsCount}, \text{MaxPointsCount}, \text{ALines}, \text{BLines}, \text{CycleLenth}, \text{StatesX}, \text{MaxStatesX})
\]
\[
\text{copyright by Pavlo Shchelokovskyy, 10 Nov 2003.}
\]
\[
\text{version 3.0 - only lines with no gaps in x are taken;}
\]
\[
\text{condition of cycling in x is kept in mind, so that}
\]
\[
\text{now subroutine corresponds to specific task:}
\]
\[
\text{x} \leftrightarrow \text{shift quantum number in the RING.}
\]

\[
\text{implicit none}
\]
\[
\text{integer } i, j, k, l, m, N, \text{MaxPointsCount}
\]
\[
\text{integer } \text{CycleLenth}
\]
B. Numerical algorithm

```plaintext
integer StatesX (0:(CycleLenth − 1)), MaxStatesX
integer XY(0:(CycleLenth − 1),MaxStatesX)
real*8 Y(N), accur
integer MaxLines, X(N)
integer Nlines, Nl, T1
integer PointsCount (MaxPointsCount)
integer PointsNumbers (MaxPointsCount, MaxLines)
integer Counter (0:(CycleLenth − 1))
real*8 MaxY, MinY, DY, Q
real*8 ALines(Maxlines), BLines(MaxLines), a, b
real*8 bL(Maxlines), aL(MaxLines)
logical thresh1

Finding max & min Y

MaxY=Y(1)
MinY=Y(1)
do i=2,N
    if (Y(i) . gt .MaxY) then
        MaxY=Y(i)
    endif
    if (Y(i) . lt .MinY) then
        MinY=Y(i)
    endif
enddo
DY=(MaxY−MinY)/CycleLenth

Sorting 2 1-dim arrays to 1 2-dim array

do i=0,CycleLenth−1
    Counter(i)=0
enddo

do i=1,N
    Counter(X(i))=Counter(X(i))+1
    XY(X(i),Counter(X(i)))=i
enddo

write (6,*), 'Done finding DY'

Building 3-points segments

write (6,*), 'Done storing 2-dim array'

all 3 points are on the line

do i=0,CycleLenth−3
```

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B. Numerical algorithm

do j=1,StatesX(i)
do k=1,StatesX(i+1)
a=(Y(XY(i+1,k))−Y(XY(i,j)))/(X(XY(i+1,k))−X(XY(i,j)))
b=Y(XY(i,j))−a*X(XY(i,j))
Q=abs(int(DY/a))+1
do l=1,StatesX(i+2)
if (abs(Y(XY(i+2,l))−a*X(XY(i+2,l))−b).le.accur)then
  Nl=Nl+1
  aL(Nl)=a
  bL(Nl)=b
endif
endo
dendo
endo
dendo

do i=0,CycleLenth−3
do j=1,StatesX(i)
do k=1,StatesX(i−1)
a=(Y(XY(i−1,k))−Y(XY(i,j)))/(X(XY(i−1,k))−X(XY(i,j)))
if (abs(a).gt.(10∗accur)) then
  b=Y(XY(i,j))−a*X(XY(i,j))
  Q=abs(int(DY/a))+1
  do l=1,StatesX(i+2)
    if (abs(Y(XY(i+2,l))−a*X(XY(i+2,l))−b−m*a∗CycleLenth) & .le.accur)then
      Nl=Nl+1
      aL(Nl)=a
      bL(Nl)=b
    endif
  enddo
endo
dendo
dendo
endo
dendo
dendo
dendo
dendo

write (6,*)'Done 3–d point out of line'

* 1–st point out of line

* 839     do j=1,StatesX(i)
 840     * 841     do k=1,StatesX(i+1)
 842     a=(Y(XY(i+1,k))−Y(XY(i,j)))/(X(XY(i+1,k))−X(XY(i,j)))
 843     b=Y(XY(i,j))−a*X(XY(i,j))
 844     Q=abs(int(DY/a))+1
 845     do l=1,StatesX(i+2)
 846     if (abs(Y(XY(i+2,l))−a*X(XY(i+2,l))−b).le.accur)then
 847     Nl=Nl+1
 848     aL(Nl)=a
 849     bL(Nl)=b
 850     endif
 851     enddo
 852     enddo
 853     enddo
 854     enddo
 855     *
 856     ***********
 857     * 3–d point out of line
 858     ***********
 859     *
 860     do i=0,CycleLenth−3
 861     do j=1,StatesX(i)
 862     do k=1,StatesX(i−1)
 863     a=(Y(XY(i−1,k))−Y(XY(i,j)))/(X(XY(i−1,k))−X(XY(i,j)))
 864     if (abs(a).gt.(10∗accur)) then
 865     b=Y(XY(i,j))−a*X(XY(i,j))
 866     Q=abs(int(DY/a))+1
 867     do l=1,StatesX(i+2)
 868     if (abs(Y(XY(i+2,l))−a*X(XY(i+2,l))−b−m*a∗CycleLenth) & .le.accur)then
 869     Nl=Nl+1
 870     aL(Nl)=a
 871     bL(Nl)=b
 872     endif
 873     enddo
 874     enddo
 875     enddo
 876     enddo
 877     endif
 878     enddo
 879     enddo
 880     enddo
 881     enddo
 882     *
 883     write (6,*) 'Done 3–d point out of line'
 884     *
 885     ***********
 886     * 1–st point out of line
 887     ***********
 888     *
 889     do i=CycleLenth−1,2,−1
 890     do j=1,StatesX(i)
 891     do k=1,StatesX(i−1)
 892     a=(Y(XY(i−1,k))−Y(XY(i,j)))/(X(XY(i−1,k))−X(XY(i,j)))
 893     if (abs(a).gt.(10∗accur)) then
 894     enddo
 895     enddo
 896     enddo
 897     enddo
 898     enddo
 899     enddo
 900     enddo
 901     enddo
 902     enddo
 903     enddo
 904     enddo
 905     enddo
 906     enddo
 907     enddo
 908     enddo
 909     enddo
 910     enddo
 911     enddo
\[ b = Y(XY(i, j)) - a \times X(XY(i, j)) \]

\[ Q = \text{abs}(\text{int}(DY/a)) + 1 \]

\[ \text{do } l = 1, \text{StatesX}(i - 2) \]

\[ \text{do } m = -Q, Q \]

\[ \text{if } (\text{abs}(Y(XY(i - 2, l)) - a \times X(XY(i - 2, l)) - b - m \times a \times \text{CycleLenth})) \& \text{. i.e. accur} \text{ then} \]

\[ N_l = N_l + 1 \]

\[ a_L(N_l) = a \]

\[ b_L(N_l) = b \]

\[ \text{endif} \]

\[ \text{enddo} \]

\[ \text{endif} \]

\[ \text{enddo} \]

\[ \text{endif} \]

\[ \text{enddo} \]

\[ \text{endif} \]

\[ \text{write}(6, \ast) \ '\text{Done 1-st point out of line}' \]

\[ \text{*************} \]

\[ \text{*************} \]

\[ \text{do } i = 0, \text{CycleLenth} - 3 \]

\[ \text{do } j = 1, \text{StatesX}(i) \]

\[ \text{do } k = 1, \text{StatesX}(i + 2) \]

\[ a = (Y(XY(i + 2, k)) - Y(XY(i, j))) / (X(XY(i + 2, k)) - X(XY(i, j))) \]

\[ \text{if } (\text{abs}(a).gt.(10 \times \text{accur})) \text{ then} \]

\[ b = Y(XY(i, j)) - a \times X(XY(i, j)) \]

\[ Q = \text{abs}(\text{int}(DY/a)) + 1 \]

\[ \text{do } l = 1, \text{StatesX}(i + 1) \]

\[ \text{do } m = -Q, Q \]

\[ \text{if } (\text{abs}(Y(XY(i + 1, l)) - a \times X(XY(i + 1, l)) - b - m \times a \times \text{CycleLenth})) \& \text{. i.e. accur} \text{ then} \]

\[ N_l = N_l + 1 \]

\[ a_L(N_l) = a \]

\[ b_L(N_l) = b \]

\[ \text{endif} \]

\[ \text{enddo} \]

\[ \text{endif} \]

\[ \text{enddo} \]

\[ \text{enddo} \]

\[ \text{enddo} \]

\[ \text{write}(6, \ast) \ '\text{Done 1nd point out of line}' \]

\[ \text{*************} \]

\[ \text{*************} \]

\[ \text{*************} \]

\[ \text{*************} \]

\[ \text{limit cases in X} \]

\[ \text{*************} \]

\[ \text{*************} \]

\[ \text{building segment on 2 last X's, cheking 1st} \]

\[ \text{*************} \]

\[ \text{*************} \]
B. Numerical algorithm

\[ i = \text{CycleLenth} - 2 \]
\[ \text{do } \ j = 1, \text{StatesX}(i) \]
\[ \text{do } \ k = 1, \text{StatesX}(i+1) \]
\[ a = (Y(XY(i+1,k)) - Y(XY(i,j)))/(X(XY(i+1,k)) - X(XY(i,j))) \]
\[ \text{if } (\text{abs}(a) > 10 \times \text{accur}) \text{ then} \]
\[ b = Y(XY(i,j)) - a \times X(XY(i,j)) \]
\[ Q = \text{abs}(\text{int}(DY/a)) + 1 \]
\[ \text{do } l = 1, \text{StatesX}(0) \]
\[ \text{if } (\text{abs}(Y(XY(0,l)) - a \times X(XY(0,l)) - b + a \times \text{CycleLenth}) \]
\[ \text{&} \text{.i.e. accure) then} \]
\[ Nl = Nl + 1 \]
\[ aL(Nl) = a \]
\[ bL(Nl) = b \]
\[ \text{endif} \]
\[ \text{enddo} \]
\[ \text{endif} \]
\[ \text{enddo} \]
\[ \text{endif} \]
\[ \text{enddo} \]
\[ \text{*} \]
\[ \text{write} (6,*) 'Done 2 last X’’s, cheking 1st' \]
\[ \text{*} \]
\[ \text{***********} \]
\[ \text{building segment on last and 1st X’s, cheking 2nd} \]
\[ \text{***********} \]
\[ \text{*} \]
\[ i = \text{CycleLenth} - 1 \]
\[ \text{do } \ j = 1, \text{StatesX}(i) \]
\[ \text{do } \ k = 1, \text{StatesX}(0) \]
\[ a = (Y(XY(0,k)) - Y(XY(i,j)))/(X(XY(0,k)) - X(XY(i,j)) + \text{CycleLenth}) \]
\[ \text{if } (\text{abs}(a) > 10 \times \text{accur}) \text{ then} \]
\[ b = Y(XY(0,k)) - a \times X(XY(0,k)) \]
\[ Q = \text{abs}(\text{int}(DY/a)) + 1 \]
\[ \text{do } l = 1, \text{StatesX}(1) \]
\[ \text{do } m = Q, Q \]
\[ \text{if } (\text{abs}(Y(XY(1,l)) - a \times X(XY(1,l)) - b + a \times \text{CycleLenth}) \]
\[ \text{&} \text{.i.e. accure) then} \]
\[ Nl = Nl + 1 \]
\[ aL(Nl) = a \]
\[ bL(Nl) = b \]
\[ \text{endif} \]
\[ \text{enddo} \]
\[ \text{enddo} \]
\[ \text{endif} \]
\[ \text{enddo} \]
\[ \text{enddo} \]
\[ \text{*} \]
\[ \text{write} (6,*) 'Done last and 1st X’’s, cheking 2nd' \]
\[ \text{*} \]
\[ \text{***********} \]
\[ \text{building segment on 2 first X’’s, cheking last} \]
\[ \text{***********} \]
\[ \text{*} \]
\[ \text{i} = 1 \]
\[ \text{do } \ j = 1, \text{StatesX}(i) \]
B. Numerical algorithm

do k=1,StatesX(i−1)
a=(Y(XY(0,k))−Y(XY(i,j)))/(X(XY(0,k))−X(XY(i,j)))
if (abs(a).gt.(10*accur)) then
b=Y(XY(i,j))−a*X(XY(i,j))
Q=abs(int(DY/a))+1
do l=1,StatesX(CycleLenth−1)
   m=Q
   if (abs(Y(XY(1,l))−b&m∗a∗CycleLenth).le.accur) then
   Nl=Nl+1
endif
enddo
endif
doin=−Q,Q
if (abs(Y(XY(i,l))−a∗X(XY(i,l))−b−m∗a∗CycleLenth).le.accur) then
Nl=Nl+1
endif
enddo
endif
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B. Numerical algorithm

if (abs(a).gt.(10*accur)) then
  b=Y(XY(i,j))-a*X(XY(i,j))
  Q=abs(int(DY/a))+1
  do l=1,StatesX(i+1)
    do m=-Q,Q
      if (abs(Y(XY(i+1,l))-a*X(XY(i+1,l)))-b-m*a*CycleLenth) & .le. accur then
        Nl=Nl+1
        aL(Nl)=a
        bL(Nl)=b
      endif
    enddo
  enddo
endif
enddo

write (6,*) 'Done prelast and 1st X's, checking last'

****

building segment on last and 2nd X's, checking 1st

****

i=CycleLenth-1
do j=1,StatesX(i)
  do k=1,StatesX(1)
    a=(Y(XY(1,k))-Y(XY(i,j)))/(X(XY(1,k))-X(XY(i,j))+CycleLenth)
    if (abs(a).gt.(10*accur)) then
      b=Y(XY(1,k))-a*X(XY(1,k))
      Q=abs(int(DY/a))+1
      do l=1,StatesX(0)
        do m=-Q,Q
          if (abs(Y(XY(0,l))-a*X(XY(0,l))-b-m*a*CycleLenth) & .le. accur then
            Nl=Nl+1
            aL(Nl)=a
            bL(Nl)=b
          endif
        enddo
      enddo
    endif
  enddo
enddo

write (6,*) 'Done last and 2nd X's, checking 1st'

C=*C  write (6,*) 'Nl=',Nl

if (Nl.ne.0) then
  combine and delete duplicates
endif

Nlines=1
B. Numerical algorithm

```
ALines(NLines)=aL(1)
BLines(NLines)=bL(1)

do i=2,Nl
   T1=NLines
   thresh1=.true.
   do j=1,T1
      if ((abs(aL(i)-ALines(j)).le.accur).and.
         & (abs(bL(i)-BLines(j)).le.accur)) then
         thresh1=.false.
      endif
   enddo
   if (thresh1.eqv.true.) then
      NLines=NLines+1
      ALines(NLines)=aL(i)
      BLines(NLines)=bL(i)
   endif
endo

write (6,'Done combine and delete duplicates ')

```

```
do i=1,Nlines
   PointsCount(i)=0
   Q=abs(int(DY/ALines(i)))+1
   do j=1,N
      do m=-Q,Q
      if (abs(Y(j)-ALines(i)*X(j)-BLines(i)*m*CycleLenth*ALines(i)
         & ).le.accur) then
         PointsCount(i)=PointsCount(i)+1
         PointsNumbers(PointsCount(i),i)=j
      endif
endo
endo
else
   NLines=0
endif

write (6,'Done building lines ')
return
```

```
```
Bibliography


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Eidesstattliche Erklärung

Hiermit erkläre ich an Eides Statt, die vorliegende Abhandlung selbständig und ohne unerlaubte Hilfe verfaßt, die benutzten Hilfsmittel vollständig angegeben und noch keinen Promotionsversuch unternommen zu haben.


(P. Shchelokovskyy)

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Tag der mündlichen Prüfung: 10. Dezember 2004