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Solitary waves on finite-size antiferromagnetic quantum Heisenberg spin rings

Jürgen Schnack*, Pavlo Shchelokovskyy

Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

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Abstract

Motivated by the successful synthesis of several molecular quantum spin rings we are investigating whether such systems can host magnetic solitary waves. The small size of these spin systems forbids the application of a classical or continuum limit. We therefore investigate whether the time-dependent Schrödinger equation itself permits solitary waves. Example solutions are obtained via complete diagonalization of the underlying Heisenberg Hamiltonian.

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1. Introduction

Magnetic solitons are detected in many magnetic systems due to their special influence on magnetic observables [1–5]. From a theoretical point of view magnetic solitons are solutions of non-linear differential equations, e.g. of the cubic Schrödinger equation [6–8], which result from classical approximations of the respective quantum spin problem. The cubic Schrödinger equation, for instance is obtained if the spins are replaced by a classical spin density [6].

Due to the success of coordination chemistry one can nowadays realize finite size quantum spin rings in the form of magnetic ring molecules. Such wheels—Fe_6, Fe_{10}, and Cr_8 rings as the most prominent examples—are almost perfect Heisenberg spin rings with a single isotropic antiferromagnetic exchange parameter and weak uniaxial anisotropy [9–12].

The aim of the present article is to discuss whether solitary waves can exist on such spin rings and if they do, how they look like. The finite size and the resulting discreteness of the energy spectrum forbid any classical or continuum limit. We therefore investigate, whether the ordinary *linear* time-dependent Schrödinger equation allows for solitary waves. Solitary excitations in quantum spin chains of Ising or sine-Gordon type have already been discussed [7]. Nevertheless, such soliton solutions are approximate in the sense that a kind of Holstein–Primakov series expansion is applied, and the results are accurate only for anisotropies large compared to the spin–spin coupling [7]. This article deals with antiferromagnetic Heisenberg chains without anisotropy, where such derivations cannot be applied. Starting from the time-dependent Schrödinger equation therefore automatically addresses the questions how soliton solutions might be approached starting from a full quantum treatment—a question that to the best of our knowledge is not yet answered [13].

In order to apply the concept of solitons or solitary waves to the linear Schrödinger equation some redefinitions are necessary. The first redefinition concerns the term soliton itself. It is mostly used for domain-wall-like solitons which are of topological character. It is also applied to localized deviations of the magnetization or energy distribution (envelope solitons), here one distinguishes

*Corresponding author. Tel.: +49 541 969 2695; fax: +49 541 960 12695.
E-mail address: jschnack@uos.de (J. Schnack).

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between bright and dark solitons. We will generalize this class of objects and speak only of solitary waves in the following. We call a state $|\Psi_s\rangle$ solitary wave if there exists a time τ for which the time evolution equals (up to a global phase) the shift by one site on the spin ring. This means that solitary waves travel with permanent shape. The property that two solitons scatter into soliton states cannot be used as a definition in the context of the Schrödinger equation since it is trivially fulfilled for a linear differential equation.

A non-trivial question concerns useful observables in order to visualize solitary waves $|\Psi_s\rangle$. The expectation value of the local operator $\underset{\sim}{s}_z(i)$, which reflects a local magnetization is used classically and meaningful also as a quantum mechanical expectation value. Then non-trivial, i.e. non-constant magnetization distributions $\langle \Psi_s | \underset{\sim}{s}_z(i) | \Psi_s \rangle$ arise only for those solitary waves which possess components with a common total magnetic quantum number M, because matrix elements of $\underset{\sim}{s}_z(i)$ between states of different total magnetic quantum number vanish. The energy density which in classical calculations is also used to picture solitons, could quantum mechanically be defined as $\underset{\sim}{\boldsymbol{s}}(i) \cdot \underset{\sim}{\boldsymbol{s}}(i+1)$ starting from a Heisenberg Hamiltonian, compare Eq. (1). It turns out that this observable is not so useful since it is featureless in most cases because the off-diagonal elements for energy eigenstates belonging to different total spin S are zero.

The article is organized as follows. In Section 2 we shortly introduce the Heisenberg model and the used notation, while in Section 3 solitary waves are defined. We will then discuss the construction and stability of (approximate) solitary waves in Section 4. A number of example spin systems will be investigated in Section 5. The article closes with conclusions in Section 6.

2. Heisenberg model

The Hamilton operator of the Heisenberg model with antiferromagnetic, isotropic nearest neighbor interaction between spins of equal spin quantum number s is given by

$$\underset{\sim}{H} \equiv 2 \sum_{i=1}^{N} \underset{\sim}{\boldsymbol{s}}(i) \cdot \underset{\sim}{\boldsymbol{s}}(i+1), \quad N+1 \equiv 1. \tag{1}$$

$\underset{\sim}{H}$ is invariant under cyclic shifts generated by the shift operator $\underset{\sim}{T}$. $\underset{\sim}{T}$ is defined by its action on the product basis $|\boldsymbol{m}\rangle$

$$\underset{\sim}{T} \, |m_1, \ldots, m_N\rangle \equiv |m_N, m_1, \ldots, m_{N-1}\rangle, \tag{2}$$

where the product basis is constructed from single-particle eigenstates of all $\underset{\sim}{s}_z(i)$

$$\underset{\sim}{s}_z(i) \, |m_1, \ldots, m_N\rangle = m_i \, |m_1, \ldots, m_N\rangle. \tag{3}$$

The shift quantum number $k = 0, \ldots, N-1$ modulo N labels the eigenvalues of $\underset{\sim}{T}$ which are the Nth roots of unity

$$z = \exp\left\{-\mathrm{i}\frac{2\pi k}{N}\right\}. \tag{4}$$

k is related to the "crystal momentum" via $p = 2\pi k/N$.

Altogether $\underset{\sim}{H}$, $\underset{\sim}{T}$, the square $\underset{\sim}{\boldsymbol{S}}^2$, and the z-component $\underset{\sim}{S}_z$ of the total spin are four commuting operators.

3. Solitary waves

We call a state $|\Psi_s\rangle$ solitary wave if there exists a time τ for which the time evolution equals (up to a global phase) the shift by one site on the spin ring either to the left or to the right, i.e.

$$\underset{\sim}{U}(\tau) \, |\Psi_s\rangle = \mathrm{e}^{-\mathrm{i}\Phi_0} \underset{\sim}{T}^{\pm 1} \, |\Psi_s\rangle. \tag{5}$$

Decomposing $|\Psi_s\rangle$ into simultaneous eigenstates $|\Psi_\nu\rangle$ of $\underset{\sim}{H}$ and $\underset{\sim}{T}$,

$$|\Psi_s\rangle = \sum_{\nu \in I_s} c_\nu \, |\Psi_\nu\rangle, \tag{6}$$

yields the following relation:

$$\sum_{\nu \in I_s} \mathrm{e}^{-\mathrm{i}(E_\nu \tau/\hbar)} c_\nu \, |\Psi_\nu\rangle = \mathrm{e}^{-\mathrm{i}\Phi_0} \sum_{\mu \in I_s} \mathrm{e}^{\mp \mathrm{i}(2\pi k_\mu/N)} c_\mu \, |\Psi_\mu\rangle. \tag{7}$$

The set I_s contains the indices of those eigenstates which contribute to the solitary wave. Therefore,

$$\frac{E_\mu \tau}{\hbar} = \pm \frac{2\pi k_\mu}{N} + 2\pi m_\mu + \Phi_0 \quad \forall \mu \in I_s$$
$$\text{with } m_\mu \in \mathbb{Z}. \tag{8}$$

Eq. (8) means nothing else than that solitary waves are formed from such simultaneous eigenstates $|\Psi_\nu\rangle$ of $\underset{\sim}{H}$ and $\underset{\sim}{T}$ which fulfill a (generalized) linear dispersion relation.

Since our definition (8) is rather general it comprises several solutions. Some of them are rather trivial waves whereas others indeed do possess soliton character:

- Single eigenstates $|\Psi_\nu\rangle$ of the Hamiltonian fulfill the definition, but they are of course stationary and they possess a constant magnetization distribution. One would not call these states solitary waves or solitons.
- Superpositions of two eigenstates $|\Psi_\mu\rangle$ and $|\Psi_\nu\rangle$ with different shift quantum numbers k_μ and k_ν are also solutions of definition (8) since two points are always on a line in the E–k-plane. It is clear that such a state cannot be well localized because of the very limited number of momentum components. Nevertheless, these states move around the spin ring with permanent shape. An example of such solitary waves are superpositions consisting of ground state and first excited state which have already been investigated under a different focus [14]. The characteristic time τ to move by one site is related to the frequency of the coherent spin quantum dynamics discussed for these special superpositions [14,15].