Semi classical description of isotropic Non-Heisenberg magnets for spin $S = 3/2$ and linear quadrupole excitation dynamics

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Abstract

We discuss system with spin $S = 3/2$ with general isotropic nearest-neighbor exchange within a mean-field approximation possess. We drive equations describing non-Heisenberg isotropic model using coherent states of SU(4) group in real parameters and then obtain dispersion equations of spin wave of dipole and quadrupole branches for a small linear excitation from the ground state.

1 Introduction

Magnetically ordered materials (magnets) are known as essentially nonlinear systems \cite{1,2}. Localized nonlinear excitations with finite energy, or solitons, play an important role in description of nonlinear dynamics, in particular, spin dynamics for low-dimensional magnets, with different kind of magnetic order. To date, solitons in Heisenberg ferromagnets, whose macroscopic dynamics are described by the Landau-Lifshitz equation for the constant-length magnetization vector, have been studied in details\cite{2,3,4,5,6}. In terms of microscopic spin models, this picture corresponds to the exchange Heisenberg Hamiltonian, with the isotropic bilinear spin interaction $J(S_1, S_2)$, where $J$ is exchange constant and $i,j$ are nearest-neighbor in corresponding site. For a spin of $S > 1/2$, specially, for Single-Ion exchange, for more carefully description of magnets, the isotropic interaction is not limited by this term and can include higher invariants such as $J(S_1, S_2)^n$ with $n$ up to $2S$ \cite{7}.

Given that each spin state can be written in the form $|\psi\rangle = \sum_{i=1}^{2S+1} |\psi_i\rangle$, then $2S + 1$ complex parameters are required to describe each spin state and it is equivalent to $4S + 2$ degrees of freedom. However, one degree for normalization condition, $\langle \psi | \psi \rangle = 1$, and another one for arbitrary phase decrease. At the end, $4S$ degrees of freedom are required to describe spin state fully.\cite{8}
In this paper, the general isotropic model with the spin \( S = 3/2 \) and the nearest neighbor interaction is described by the Hamiltonian

\[
\hat{H} = - \sum_i (J(\vec{S}_i \cdot \vec{S}_{i+1}) + K(\vec{S}_i \cdot \vec{S}_{i+1})^2 + L(\vec{S}_i \cdot \vec{S}_{i+1})^3)
\]  

(1)

Where \( \vec{S}_i \) are spin-3/2 operators at the lattice site \( i \); \( J, K, \) and \( L \) are the exchange constants, corresponding to the bilinear, biquadratic, and the bicubic exchange interactions, respectively, and summation over pairs of the nearest neighbors is implied. This Hamiltonian defines a one-dimensional ferromagnetic spin chain and \( J \) is a positive coefficient, also, coefficient \( K \) is exchange integral for quadrapole moment and coefficient \( L \) is exchange integral for octapole moment.

The main purpose here is to develop classical equations for Hamiltonian (1) and then finding solutions of spin wave for small linear excitations above the ground state. We know that coherent states minimize the uncertainty relation, then these states are the nearest states to classical pictures. To this end, in section 2, coherent states for spin \( S = 3/2 \) which are the coherent states in \( SU(4) \) group are introduced. To obtain classical Hamiltonian, average values of spin operator are needed, so in section 3, these values and classical spin relation are derived. In section 4, the resulted Hamiltonian is substituted in classical equation of motion obtained by acting Feynman path integral over coherent states. Finally, obtaining spin wave equations and dispersion equations in case of small linear excitation from the ground state for dipole and quadrapole branches put an end to this research.

2 Coherent states for spin \( S = 3/2 \)

Coherent states are special kind of quantum states that their dynamics are very similar to their corresponding classical system. That which coherent state can be used in problems depends on the operators symmetry in those problems. Due to the operators symmetry in Hamiltonian (1), for full description and considering all multipole excitation, we used from coherent states in \( SU(4) \) group. In this group vacuum state is \((1, 0, 0, 0)^T\) and its coherent state is introduced as:[9]

\[
|\psi\rangle = D^{3/2}(\theta, \phi, \gamma) e^{2i\theta \hat{Q}^{xy}} e^{-i\beta \hat{S}_x} e^{-ik \hat{F}^{xyz}} |0\rangle
\]

(2)

In above relation \( D^{3/2}(\theta, \phi, \gamma) \) is Wigner function for spin \( S = 3/2 \), operator \( Q^{xy} \) is related to quadrapole moment and operator \( F^{xyz} \) is relevant to octapole moment.

This six-parameters state have the properties of \( SU(4) \) coherent state. Two angle, \( \theta \) and \( \phi \), Euler angles, define the orientation of the classical spin vector. The angle \( \gamma \) is the rotation of the quadrapole moment about the spin vector. The parameter, \( g \), defines change of the spin vector magnitude and that of the
quadruple moment, the angle $\beta$ is the rotation of the octuple moment about the spin vector and parameter $k$, defines change of the spin vector magnitude and that of the octuple moment. It should be noted that, range of angles, $\phi, \gamma$ and $\beta$ are between zero to $2\pi$ and angle $\theta$ change between $-\pi$ to $\pi$. Using the state (2), one can construct the coherent state path integral and find the lagrangian $L$: [9]

$$L = \cos 2k \cos^2 g(3\cos^2 g \beta t + \cos \theta \phi t + \gamma t) - H(\theta, \phi, g, \beta, k)$$  \hspace{1cm} (3)$$

Where $x_t = \partial / \partial t$ and $H$ is the classical (mean-field) energy of the system, which equals to the quantum mean value of the Hamiltonian with the state (2). Note that in deriving Lagrangian of spin system using path integral, two more terms appeared. First term is dynamic term that has Berry phase characteristics and takes many attentions in phenomena like spin tunneling and the other term is boundary term depends on boundary values of path. Both of these terms are not interested here and hence omitted.

3 Average spin operators and their products in SU(4) group

Here we consider classical counterparts of the spin operators and their products contained in the Hamiltonian (1). The vector

$$\vec{S} = \langle \psi | \hat{\vec{S}} | \psi \rangle$$ \hspace{1cm} (4)$$

Can be regarded as a classical spin vector, and

$$\hat{Q}^{ij} = \frac{1}{2}(\hat{S}_i \hat{S}_j + \hat{S}_j \hat{S}_i - \frac{4}{3} \delta_{ij} I)$$ \hspace{1cm} (5)$$

components of quadrupole moment. Because we can write any coherent state as multiple of single site coherent states, namely:

$$|\psi\rangle = \prod_i |\psi_i\rangle$$ \hspace{1cm} (6)$$

Then Spin operators in ground state of non-single ions Hamiltonian can be commute in different lattices [10]; so

$$\langle \psi | \hat{S}_n^i \hat{S}_n^{j+1} | \psi \rangle = \langle \psi | \hat{S}_n^i | \psi \rangle \langle \psi | \hat{S}_n^{j+1} | \psi \rangle$$ \hspace{1cm} (7)$$

where $|\psi\rangle = |\psi_n\rangle |\psi\rangle_{n+1}$.

Then average values expressions in SU(4) group for coherent state (2) are:
\[ \langle S^+ \rangle = \frac{3}{2} e^{i\phi} (1 - 4\cos^2 g) \cos 2k \sin \theta \]
\[ \langle S^- \rangle = \frac{3}{2} e^{-i\phi} (1 - 4\cos^2 g) \cos 2k \sin \theta \]
\[ \langle S^z \rangle = \frac{3}{2} (1 - 4\cos^2 g) \cos 2k \cos \theta \]  \hspace{1cm} (8)

and also

\[ S^2 = \frac{9}{4} (1 - 4\cos^2 g)^2 \cos^2 2k \]
\[ q^2 = \frac{9}{4} (1 - 4\cos^2 g)^2 \sin^2 2k \]
\[ S^2 + q^2 = \frac{9}{4} (1 - 4\cos^2 g)^2 \]  \hspace{1cm} (9)

In the above relation \( S^2 \) related to dipole moment and \( q^2 \) is related to quadrupole moment. If we only consider quadruple moment, must be set \( g = 0 \), then

\[ S^2 + q^2 = cte \]  \hspace{1cm} (10)

In classical limit, if we used from above relations for Hamiltonian (1), the classical Hamiltonian in continuous limit obtained in the following form:

\[
H = -\int \frac{dx}{a_0} \left( \frac{9}{4} JA^2 \cos^2 2k + \frac{81}{16} KA^4 \cos^4 2k + \frac{729}{64} LA^6 \cos^6 2k \right. \\
- \frac{a_0^2}{2} \left( J + \frac{9}{2} KA^2 \cos^2 2k + \frac{243}{16} LA^4 \cos^4 2k \right) \times \\
\left. \times (36g_x^2 \cos^2 2k \sin^2 2g + \frac{9}{4} A^2 \cos^2 2k (\theta_x^2 + \sin^2 \theta \phi_x^2) \right) \\
+ 9k_x^2 A^2 \sin^2 2k \right)
\]  \hspace{1cm} (11)

where \( a_0 \) is a lattice crystal length and

\[ A = (1 - 4\cos^2 g) \]  \hspace{1cm} (12)

4 Classical Equations

To obtain the dynamic equation, we vary the Lagrangian (3), obtaining the set of equations, but because we only consider quadruple moment we set \( g = 0 \). These equations completely describe nonlinear dynamics of Hamiltonian of problem
under study up to quadrupole branch. Solution of these equations are magnetic solitons. Then classical equation is:

\[ \frac{1}{\omega_0} \phi_t = \frac{81}{512} (\cos^2 k (128 J + 81(32 K + 729 L)) + 324(8 K + 243 L) \cos 4k) \times 19683 L \cos 8k) (\theta_{xx} \csc \theta + \phi_x^2 \cos \theta) a_0^2 \]

\[ \frac{1}{\omega_0} \theta_t = -\frac{81}{64} \phi_{xx} \cos 2k (16 J + 648 K \cos^2 2k + 19683 L \cos^4 2k) \times \sin \theta a_0^2 \]

\[ \frac{1}{\omega_0} \beta_t = \frac{27}{32} (16 J \cos 2k + 648 K \cos^3 2k + 19683 L \cos^5 2k) \]

\[ + 27 \left( 39366 k_{xx} \cos^4 2k \sin 2k + 8 k_{xx} \sin 2k (4 J + 81 K + 81 K \cos 4k) + 19683 L \cos^5 2k (4 k_x^2 - 3 \theta_x^2 + 3 \phi_x^2 \sin^2 \theta) + 648 \cos^3 2k \times (4 k_x^2 - 2 K \theta_x^2 - 243 L k_x^2 \sin^2 2k - 2 K \phi_x^2 \sin^2 \theta - 16 \cos 2k) \times (162 K k_x^2 \sin^2 2k + J (-4 k_x^2 + \theta_x^2 + \phi_x^2 \sin^2 \theta)) a_0^2 \right) \]

\[ \frac{1}{\omega_0} \gamma_t = -\frac{81}{16} (16 J \cos 2k + 648 K \cos^3 2k + 19683 L \cos^5 2k) \]

\[ - \frac{81}{64} (19683 L \cos^5 2k (8 k_x^2 - 6 \theta_x^2 + 1/2 (-5 + 7 \cos 2 \theta + \theta_{xx} \csc \theta) \phi_x) + 64 J k_{xx} \sin 2k + 78732 L k_{xx} \sin 2k \cos^5 2k + 8 \cos 2k (J (16 k_x^2 - 4 \theta_x^2 - \phi_x^2 + 3 \phi_x^2 \cos 2 \theta + 2 \theta_{xx}) - 648 K k_x^2 \sin^2 2k) + 648 \cos^3 2k \]

\[ (8 k_x^2 - 4 K \theta_x^2 + K (\frac{1}{2} \phi_x^2 (-3 + 5 \cos 2 \theta) + \theta_{xx} \csc \theta) - 486 L k_x^2 \sin^2 2k) \]

\[ + 648 K k_{xx} (\sin 2k + \sin 6k)) a_0^2 \]

\[ \frac{1}{\omega_0} \kappa_t = 0 \]

\[ \frac{1}{\omega_0} g_t = 0 \] (13)

Where \( \omega_0 = \hbar a_0 \). In the above equations, if quadrapole and octapole excitations are ignored, \( (g = 0, k = 0) \), these equations are reduced to Landau-Lifshitz equation. As a result, these equations compared to Landau-Lifshitz equation are more complete and also they enjoy higher degrees of freedom.

In order to investigate the ferromagnets with anisotropy, it is necessary to find the classical ground states of these magnets. In this order, we consider in Hamiltonian (11) only part of without derivative:

\[ H_0 = - \int \frac{dx}{a_0} \left( \frac{9}{2} J \cos^2 2k + \frac{9}{2} \phi_x^4 K \cos^4 2k + \frac{9}{2} \theta_x^6 L \cos^6 2k \right) \] (14)

In order to this terms is minimum must be \( k = 0 \) or \( k = \frac{\pi}{2} \). The minimum value of classical Hamiltonian (14) is
Let us examine the classical equations near the ground state. in this order we change the following relation for the parameter k

\[ 2k \rightarrow \pi + k \]  

in the point \( \theta = \frac{\pi}{2} \), in linear small excitation the classical equations change in the following form

\[
\begin{align*}
\frac{1}{\omega_0} \phi_t &= \Lambda \theta_{xx} a_0^2 \\
\frac{1}{\omega_0} \theta_t &= -\Lambda \phi_{xx} a_0^2 \\
\frac{1}{\omega_0} \beta_t &= \frac{2\Lambda}{3} \\
\frac{1}{\omega_0} \gamma_t &= -4\Lambda \\
\frac{1}{\omega_0} k_t &= 0 \\
\frac{1}{\omega_0} g_t &= 0
\end{align*}
\]  

(17)

where

\[
\Lambda = \frac{81}{64} (16J + 648K + 19683L)
\]  

(18)

and \( x_t = \frac{\partial}{\partial t} \). Although exchange integrals K and L are small, numerical values which are multiplied by them in the above relation demonstrate that quadrupole and octapole excitations in this problem are noticeable. Also, it is shown that for isotropic ferromagnets, the magnitude of average quadrupole moment is constant and its dynamics, is rotational dynamics around the classical spin vector.

We consider now the dispersion of spin wave propagating near the ground state. To this end we considering two functions \( \theta, \phi \) in the form of plane waves, \( \phi = \phi_0 e^{i(\omega t - kx)} + \bar{\phi}_0 e^{-i(\omega t - kx)} \)

\[ \theta = \theta_0 e^{i(\omega t - kx)} + \bar{\theta}_0 e^{-i(\omega t - kx)} \]  

(19)

we obtain the following equation for the spin wave propagating near the ground state for this isotropic Hamiltonian
\[
\begin{align*}
\omega_1^2 &= (J + 2K + 3L)^2 a_0^2 \omega_0^2 k^4 \\
\omega_2 &= \frac{2}{3} \Lambda \omega_0 \\
\omega_3 &= -4 \Lambda \omega_0 
\end{align*}
\]

It is evident from equation (20) that in addition to the dispersion acoustic branch, there exist two non-dispersion optical branches which are related to the dipole and quadrupole excitations.

5 Discussion

In terms of spin coherent states we have investigate $S = 3/2$ spin quantum system with the bilinear, biquadratic and bicubic isotropic exchange in the continuum limit. the proper Hamiltonian of the model can be written as bilinear on the generator SU(4) group[11]. Knowledge of such group structure enables us to obtain some new exact analytical results. The analysis of the proper classical model allows us to get different soliton solutions with finite energy and the spatial distribution of spin-dipole, spin-quadrupole and/or spin-octapole moments termed as dipole, quadrupole, octapole and dipole-quadrupole, dipole-octapole and quadrupole-octapole soliton, respectively.

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