NUMERICAL INVESTIGATION OF AN EXTERNALLY DRIVEN SPIN DYNAMICS IN SEARCH OF A CLASSICAL CONDENSATION OF WAVES

by

Nikolay Yegovtsev

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As members of the Thesis Committee, we certify that we have read the thesis prepared by Nikolay Yegovtsev entitled

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and recommend that it be accepted as fulfilling the thesis requirement for the Degree of Bachelor of Science.

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Dmitriy Beznosko

Vassilios Kovanis V.I.K. Date: May 6, 2017

Vassilios Kovanis

Final approval and acceptance of this thesis is contingent upon the candidate's submission of the final copies of the thesis to the Department of Physics.

I hereby certify that I have read this thesis prepared under my direction and recommend that it be accepted as fulfilling the thesis requirement.

Vassilios Kovanis V.I.K. Date: May 6, 2017

Thesis Director: Vassilios Kovanis

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Abstract

The following work is a numerical study of a recently discovered Bose-Einstein condensation of magnons at room temperature by purely classical means. The classical Hamiltonian of the system includes exchange and dipolar interaction as well as interaction with external magnetic field. The system under consideration is a 2-dimentional lattice of classical spins with fixed positions. Classical equations of motions are derived from this Hamiltonian by applying the Poisson-bracket formalism. Equations of motions were solved numerically by the 4^{th} order Runge-Kutta algorithm and obtained spin dynamics is transformed to the frequency space by the means of Fourier transform. This spectral decomposition of the dynamics allows monitoring the occupation of the energy states and observing condensation into the lowest energy state. In this work, we were able to reproduce the dispersion curve with characteristic minimum at non-zero value of the wave-vector by varying parameters of the system. We discuss models for pumping and dissipation, and hope to implement them in the future work.

1. Introduction

The development of experimental condensed matter physics in the last two decades made it possible to investigate exotic phases of matter such as Bose-Einstein condensates and quantum spin liquids. The quantum nature of the majority of those systems makes it difficult to numerically investigate their properties due to exponentially increasing number of eigenstates that scales with the size of the system. Classical or semi-classical picture requires fewer variables to describe the system of interest and therefore it allows one to perform simulations of considerably larger systems. This becomes a great advantage for spin systems, where classical picture provides results close to quantum simulations. One can study the corresponding properties of quantum systems using their classical analogs to address several classes of problems. First example is the investigation of the properties that are also present in classical picture, such as phase transitions and glassy dynamics. The second class consists of 1/Z expansion, where Z is the coordination number [1], and other 'beyond mean field' models that can be used to test various sample Hamiltonians for the emergence of properties of interest. For instance, studying the coherence and correlations, one can hope to find a suitable system for the quantum computer.

In 2006, Demokritov et al. claimed the first observation of the Bose-Einstein condensation (BEC) of magnons at room temperature in yttrium-iron-garnet (YIG) thin films under pumping [2]. Magnon BEC became an attractive topic after recent proposals to employ magnon BEC as qubits for quantum computing [3]. This provides grounds for testing of classical simulation applicability to quantum systems in the following ways. First, knowing that the low energy excitations of the spin system are wave-like, it is interesting, whether it is possible to produce condensation of the classical waves in this system. Second, it is interesting to test the 1/Z method on how robust it is in describing the critical phenomena and try to apply it the BEC. The current work deals only with the simulation of classical dynamics under external drive. It is expected to generalize 1/Z so that it could account for long-range interactions and apply it to the BEC of magnons in future works.

2. Theoretical description

A. BEC of particles and quasi-particles

Bose-Einstein condensation is the one of the most fascinating predictions of quantum theory. This phenomenon leads to the formation of collective quantum state of the integer

spin particles and thus can be characterized by a single wave-function. This happens when at a finite temperature a macroscopic fraction of particles occupies a single particle state. Here we give a brief discussion of the BEC.

Typically, if the size of the system is large, we expect that the spacing between the energy levels approaches zero, so we can change all summations with integrations, and can express the number of particles in the system by the following formula in terms of volume V, one-particle density of states D(E) and Bose distribution function:

$$\mathbf{N = V \int_0^\infty \frac{D(E)dE}{e^{(E-\mu)/kT} - 1}} \tag{1}$$

Since the Bose-distribution function is nonnegative, the value of chemical potential μ cannot exceed the minimal value of energy E. For further analysis, let us consider BEC of an ideal gas in 3-D, then expression (1) reads [4]:

$$\mathbf{\frac{N}{V} = \frac{g(mT)^{3/2}}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty \frac{\sqrt{z}dz}{e^{z-\mu/T} - 1}} \tag{2}$$

The expression under the integral contains parameterized energy distribution function for bosons and one-particle density of states. If we fix the N/V in the equation (2) and keep lowering the temperature, then the value of chemical potential will gradually increase, reaching its maximum value $\mu = 0$ at some temperature T_0. At temperatures $T<T_0$ the value of the N/V is smaller than the expression on the right side of the equation. The occurring contradiction is due to the fact that it is not allowed to replace the sum with the integral under such conditions, and when we do so, we multiply the first term in the sum by $\sqrt{E} = 0$, and it falls out of the sum. It turns out that the above formula will describe only particles in the excited states, while the rest of the particles will condense to the ground state. From this line of thought, it is natural to assume that, when the chemical potential is equal to the minimum value of energy in the system, the macroscopic fraction of the particles occupies the lowest energy state and this leads to the condensation in the momentum space. It is important to realize that the density of states plays an important role in the discussion above. In the case of 1-D or 2-D, the density of states is proportional to $\frac{1}{\sqrt{E}}$ and const. respectively. In both of those cases, the expression (2) diverges on the lower limit, so it does not have a maximum. This means that we can always choose $\mu<0$ and BEC will not occur. This story is different for finite samples, because in finite geometry, ground state is greater than zero, as clearly seen

from the expression for the ground state for the particle in the box: $\frac{\hbar^2\pi^2}{2mL^2}$. Interaction of the system with external potential may also change the density of states; therefore, it is possible to investigate BEC of dilute atomic gases in the traps.

From the expression (2) one can observe that there are two ways, in which condensation can occur: either to decrease the absolute temperature of the sample keeping the density of the gas constant, or to increase the density under the constant temperature. In both of these cases the chemical potential will increase (remaining negative) and will reach its maximum at μ = 0.

The Bose-Einstein condensation of quasi-particles representing collective excitations of the medium is somewhat specific, because for some systems the number of collective excitations is not equal to the total number of particles. When the number of quasi-particles is not fixed, it is determined by the equilibrium condition and the value of chemical potential in this equilibrium. Chemical potential can be defined as a partial derivative of a free energy with respect to number of particles with the fixed temperature and volume:

$$\mu = \left(\frac{\partial \mathbf{F}}{\partial \mathbf{N}}\right)_{\mathbf{T,V}} \tag{3}$$

In the thermodynamic equilibrium, free energy has a minimum; therefore, chemical potential is identically zero. This means that in equilibrium, system chooses how to occupy eigenstate and there is no any constrain that would make macroscopic number of particle fall into the ground state, so that condensation may not occur. This difficulty can be formally overcome by driving the system externally, so that the system will be in some partial equilibrium state. In such a state, chemical potential may differ from zero, so by pumping quasi-particles into the system, one can increase their density keeping the temperature constant, by incorporating a heat sink that would not allow the system to absorb all the energy, and reaching infinite temperature. By this technique, one can attain the correct parameters for the BEC condition, and observe condensation on the timescales of the lifetime of such non-equilibrium state.

B. Condensation of classical nonlinear waves.

Although the BEC condensation is a purely quantum effect, that relies on the corresponding statistics, recent studies of the wave turbulence have indicated that a classical ensemble of waves with random phases can manifest condensation in momentum space

similar to the BEC. The role of collisions in such systems plays four-wave (2 in-2 out) mixing, and maximum entropy principle drives the system towards equipartition of energy, because the classical waves have quadratic dispersion relation. In order to consider the system statistically, one need random ensemble of waves and an interaction between various modes. The evolution of the spectral distribution of modes is governed by Boltzmann-like kinetic equation [5]:

$$\frac{\partial n_{k_1}}{\partial t} = g^2 \int d\mathbf{k}_2 d\mathbf{k}_3 d\mathbf{k}_4 \, W_{k_1 k_2; k_3 k_4} (n_{\mathbf{k}_3} n_{\mathbf{k}_4} n_{\mathbf{k}_1} + n_{\mathbf{k}_3} n_{\mathbf{k}_4} n_{\mathbf{k}_2} - n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} - n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_4}) \tag{4}$$

The kinetic term on the right describes four-wave interaction, g is the strength of the nonlinear interaction, $W_{k_1 k_2; k_3 k_4} = \sigma\delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\delta({k_1}^2 + {k_2}^2 - {k_3}^2 - {k_4}^2)$ is the collision term, and σ is the scattering matrix, which is a constant factor for the case of homogeneous system. The presence of the δ-function is present for purpose of the momentum and energy conservation during the collisions. As in the kinetic theory, where Boltzmann H-theorem states, that evolution of the system is subject to the constraint $\frac{dS}{dt} \geq 0$, where S is the entropy of the system. The equilibrium distribution function is obtained from the condition $\frac{dS}{dt} = 0$, and the constraint on conservation of total energy and power (proportional to the number of particles), so the results reads:

$$n_{\mathbf{k}}^{eq} = \frac{T}{k^2 - \mu} \tag{5}$$

This is Rayleigh-Jeans distribution. Note that as in case of Bose gas, $\mu < E_{min}$. If we substitute this result into expression for total energy and number of particles, we see that they both diverge at the ultraviolet limit $k \to \infty$. Therefore, one need to introduce the ultraviolet cutoff k_c, the physical justification for it is that for numerical simulations it is avoided by spatial discretization of the equation, while in real systems it is absent due to viscosity and diffusion [6]. In this work, we consider the system defined on a lattice with periodic boundary conditions, and therefore all physical wave-vectors are within the first Brillouin zone.

Let us do the similar analysis of the condensation of classical waves in 3D [6]:

$$\frac{N}{V} = 4\pi T k_c \left[1 - \frac{\sqrt{-\mu}}{k_c} \arctan\left(\frac{k_c}{\sqrt{-\mu}}\right)\right] \tag{6}$$

If we fix N/V, and start decreasing the temperature, $\mu = 0$ at T_c and below we can use distribution with $\mu = 0$. The remaining particles will be in the ground state. The cases for other dimensions are also qualitatively similar to BEC results. It is important that in bounded systems condensation in 2D at finite temperature is still possible [5].

Experimental investigation of the condensation of classical light in self-focusing photorefractive crystal showed that the effects of nonlinearity are essential for condensation to occur [5]. By increasing the strength of nonlinearity g, the distribution becomes more narrowly peaked about the minimum value of energy. This result is important for our further analysis, because the resulting classical equation of motion will be nonlinear and by appropriate choice of coupling parameters one can control strength of nonlinearity and potentially the thermalization rate.

C. Magnons.

One interesting property of physical problems is that when one is considering the Hamiltonian, which is a quadratic form in its dynamics variables, the result is analogous to the solution to harmonic oscillator. The recipe is as follows: one solves the classical analog of the system in terms of eigen-frequencies, and then substitutes them to the energy levels of quantum harmonic oscillator. This is applicable to the oscillations of magnetic moment. Quantized version of the spin wave is called magnon and here we will give simplified and a bit unrealistic description of spin waves in the theory of ferromagnetism of 1D-spin chains, because the following results in 1D can be generalized to higher dimensions, where this theory works properly. Since the energy of spin system is written as sum of energies of non-interacting harmonic oscillators $E_i = \omega_i(n_i + \frac{1}{2})$ (where$\hbar = 1$), we see that multiple magnons can occupy single particle state and therefore they are bosons. Consider the following Hamiltonian with periodic boundary conditions [7]:

$$\boldsymbol{H} = -2\boldsymbol{J}\sum_{\boldsymbol{i=1}}^{\boldsymbol{N}} \boldsymbol{S_i}\,\boldsymbol{S_{i+1}} \tag{7}$$

Here J>0 is a nearest neighbor exchange coupling, and **S** is a spin at site i. In this model, spins can be treated as vectors in 3D. This Hamiltonian corresponds to the ferromagnetic state: at zero temperature all spins are aligned in the same direction. Note that at zero temperature there are no magnons, thus their number is generally temperature-dependent. This suggests that they are quasi-particles. The elementary excitations of such a

spin system have wave-like form, where each consecutive spin is slightly misaligned from the previous one. The energy of such configuration is smaller than of the configuration, where only one spin is flipped. The equations of motion for a spin can be obtained by using Poisson-bracket formalism that replaces commutators in quantum mechanics, so that time derivative of the spin variable reads [8]:

$$\frac{\boldsymbol{dS_{i,\alpha}}}{\boldsymbol{dt}} = \left\{\widehat{\boldsymbol{H}}, \boldsymbol{S_{i,\alpha}}\right\} \tag{8}$$

Where index α corresponds to the x, y, z components of the magnetization vector. In order to expand right hand side of (8), we use the commutation relations for the angular momenta variables, namely:

$$\left\{\boldsymbol{S_{i,\alpha}}, \boldsymbol{S_{j,\beta}}\right\} = \boldsymbol{\delta_{ij}} \sum_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon_{\alpha\beta\gamma}} \boldsymbol{S_{i,\gamma}} \tag{9}$$

where δ_{ij} is the Kronecker delta and $\varepsilon_{\alpha\beta\gamma}$ is Levi-Civita symbol. Using (9) one can express (8) as:

$$\dot{\boldsymbol{S}}_{\boldsymbol{\iota}} = \boldsymbol{S_i} \times \boldsymbol{h_i} \tag{10}$$

$$\boldsymbol{h_i} = -2J(\boldsymbol{S_{i-1}} + \boldsymbol{S_{i+1}}) \tag{11}$$

Here $\mathbf{h_i}$ plays the role of the local magnetic field as seen by spin $\mathbf{S_i}$. These equations involve product of two spins and thus are nonlinear. We can linearize them around the ground state configuration by assuming that ${S_p}^z = S$ and ${S_p}^x, {S_p}^y \ll S$ for all p, as well as neglecting all products, involving ${S_p}^x, {S_p}^y$. The resulting system of equation for spin p reads:

$$\frac{\boldsymbol{dS_{i,x}}}{\boldsymbol{dt}} = \boldsymbol{2JS}\left(\boldsymbol{2S_{i,y} - S_{i-1,y} - S_{i+1,y}}\right) \tag{10.a}$$

$$\frac{dS_{i,y}}{dt} = -2JS\left(2S_{i,x} - S_{i-1,x} - S_{i+1,x}\right) \tag{10.b}$$

$$\frac{dS_{i,z}}{dt} = 0 \tag{10.c}$$

By looking for the solution for this system in the form:

$$S_{i,x} = u\,\exp[i(pka - \omega t)]; \qquad S_{i,y} = v\,\exp[i(pka - \omega t)]$$

We arrive to the following eigenvalue problem:

$$\begin{vmatrix} i\omega & 4JS(1-\cos ka) \\ -4JS(1-\cos ka) & i\omega \end{vmatrix} = 0$$

The resulting dispersion relation is:

$$\boldsymbol{\omega = 4JS(1-\cos ka)} \tag{11}$$

For cubic lattice in higher dimension we simply write:

$$\boldsymbol{\omega = 2JS\left(n - \sum_{\delta} \cos k\delta\right)} \tag{12}$$

where the summation is over the n vectors denoted by δ which join the central atom to its nearest neighbors [7]. We will use this result later in order to verify the validity of the implemented integrator for the dynamic evolution of the system.

D. Experimental description of BEC of magnons.

Group of S. Demokritov conducted a series of experiments of parallel parametric pumping of magnons in YIG thin (2-10 μm) films and claimed the observation of BEC. The YIG thin films are mainly interesting because of slow spin-lattice relaxation (above 1μs) that experimentally manifests itself in larger lifetime of the quasi-equilibrium states. The magnon-magnon thermalization consists of two- and four-magnon scattering processes, and it takes place at a typical time of 100-200 ns. Those scattering processes conserve the number of particles, so that the total number of magnons can be considered as fixed. This means that the chemical potential can take non-zero values. The experimental setup used by Demokritov et al. is illustrated in Figure 1.

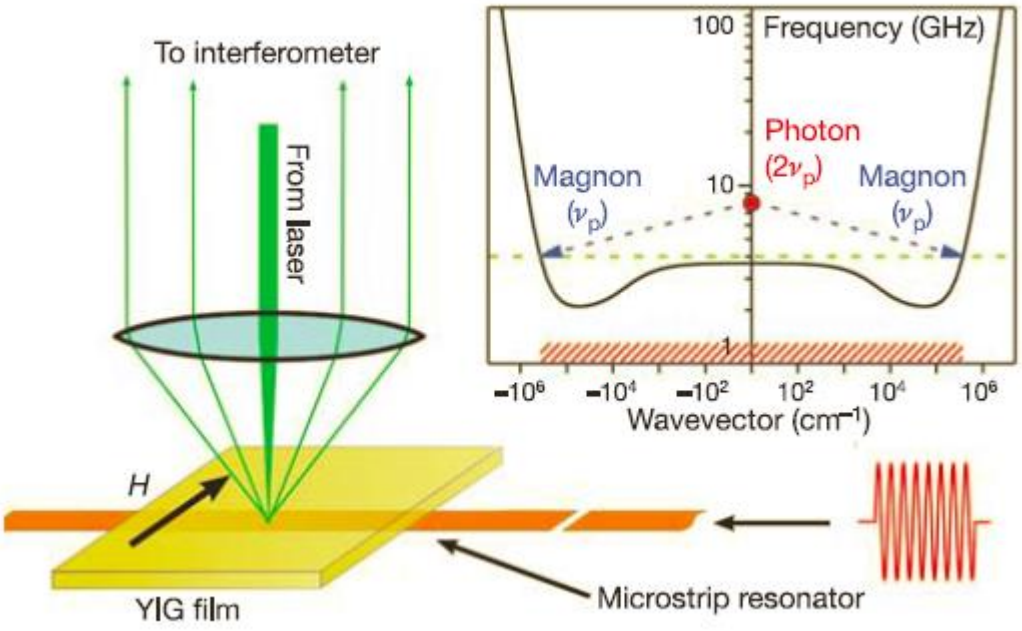

Figure 1 : Experimental setup of Demokritov et al. [2]

A thin YIG film with lateral sizes of 2 mm × 20 mm and thickness of 2-10μm is places in a uniform and static magnetic field as in Figure 1. Magnons with a wave-vector parallel to this field have a characteristic minimum in their spectrum [2]. A microstrip resonator is attached to the surface of the film. The mechanism of parallel parametric pumping can be described as following: the oscillating magnetic field of the microwave radiation is applied parallel to the static magnetization, and since all wave-vectors are confined to the first Brillouin zone, one can apply conservation of momentum and energy to such a system. The speed of light inside the material is several orders of magnitude greater than characteristic group velocity of magnons, therefore we can neglect wave-vector of the microwave radiation: such photons can excite two magnons with the same frequency and opposite wave-vectors. Those primary magnons after relaxation create a gas of quasi-equilibrium magnons. With the increasing power of pumping, chemical potential of such gas also increases and attains the required value. Similarly to the experiment on condensation of classical nonlinear waves, higher pumping rates correspond to the higher strength of nonlinear interaction, for which the distribution function is strongly localized around minimal value of the frequency.

F. Spin model.

From the description of the ferromagnet in terms of electrodynamics of continuous media, it follows that the spectrum with the characteristic minimum can be obtained by

including exchange interaction, interaction with the external field and the dipole-dipole interaction of magnetic moments. For this reason we consider the Hamiltonian of the system of the following form [9]:

$$\widehat{\boldsymbol{H}} = -\boldsymbol{\gamma}\sum_{\boldsymbol{i}} \boldsymbol{S_i}\cdot\boldsymbol{H_0} + -\boldsymbol{J_0}\sum_{\boldsymbol{i,\delta}} \boldsymbol{S_i}\,\boldsymbol{S_{i+\delta}} + \boldsymbol{U_d}\sum_{\boldsymbol{i\neq j}} \frac{\boldsymbol{S_i S_j} - \boldsymbol{3}(\boldsymbol{S_i}\cdot\boldsymbol{n_{ij}})(\boldsymbol{S_j}\cdot\boldsymbol{n_{ij}})}{|\boldsymbol{r_{ij}}|^{\boldsymbol{3}}} \tag{13}$$

Using the same formalism as in previous section, we can obtain the corresponding equations of motion:

$$\dot{\boldsymbol{S}}_{\boldsymbol{\iota}} = \boldsymbol{S_i}\times\boldsymbol{h_i} \tag{14}$$

$$\boldsymbol{h_i} = -\boldsymbol{\gamma}\boldsymbol{H_0} + -\boldsymbol{J_0}\sum_{\boldsymbol{\delta}} \boldsymbol{S_{i+\delta}} + \boldsymbol{U_d}\sum_{\boldsymbol{i\neq j}} \frac{\boldsymbol{S_j} - \boldsymbol{3n_{ij}}(\boldsymbol{S_j}\cdot\boldsymbol{n_{ij}})}{|\boldsymbol{r_{ij}}|^{\boldsymbol{3}}} \tag{15}$$

Where coefficients before the sums are the coupling constants, indices i, j run across the lattice sites and taking values r_i etc., δ corresponds to the summation over the nearest neighbors, $\mathbf{r_{ij}} = \mathbf{r_i} - \mathbf{r_j}$, $\mathbf{n_{ij}}$ - unit vector in the direction of $\mathbf{r_{ij}}$. Since the original work of Demokritov was performed on thin films, where thickness is three orders of magnitude smaller than lateral sizes, which makes the system practically quasi two dimensional, we will investigate the dynamics of the two dimensional spin systems given by above Hamiltonian. We should immediately address several important aspects of the Hamiltonian.

First, in real system, the value of dipole constant is several orders of magnitude smaller than other coupling constants, so this interaction can be considered as weak, however, it is a long range interaction and therefore its contribution becomes important for large system. The calculation of the dipole component in the local field requires knowledge of the spin configuration of the entire system and it is the most expensive calculation. In order to reduce the total computational time, we will consider relatively small system (about 50x50) with the dipole coupling constant of the order of unity to account for the "accumulation" effect.

Second, as it was mentioned in the section 2C, spin waves are solutions for the equations of motion when the magnitudes of the transverse magnetization are much less that the magnitude of the spin, so that we could neglect nonlinear terms in all equation. At the same time, results of the experimental papers on both condensations of classical nonlinear waves as well as BEC of magnons suggest that the process of condensation is more pronounced for the higher values of nonlinear interactions. Therefore, one may doubt the

applicability of the approach based on the use of the spin wave model when the magnitude of the transverse magnetization and dipole constant are not small. Practically, the spin wave model is helpful only for the investigation of the dispersion relation. We can solve the equations of motions numerically, with the initial conditions corresponding to the spin wave with a given wave-vector and then by investigating the precessional motion of a particular spin, obtain a relation between its frequency and wave-vector. It is not important whether the constructed spin wave is an actual eigenmode of the Hamiltonian, but rather that it lies close to the actual solution in the frequency space. To justify this procedure, one can compare dispersion curve obtained by the mentioned procedure with the result of the Fourier transform of the spin precession with arbitrary initial conditions and see that they indeed give close results.

3. Numerical analysis

A. Description of the simulation

The following section describes the numerical procedure and all important steps that are carried in the presented order. Results of the simulations can be found in the next section.

Solution of equations of motion (14-15) requires correct choice of the characteristic time-scale of the system's dynamics. By comparing the units of both sides of equations of motion, it is clear that units of time are equal to the inverse units of effective magnetic field; therefore for the natural timescale for the problem one can choose timescale equal to inverse of the root mean square of this effective field.

Dynamics of the system under consideration is confined to the 2-D lattice with square unit cell, where all spins are fixed in their positions. It is sensible to save in computer memory data that incorporates periodic boundary conditions and store all fixed parameters, needed for calculating the dipole-dipole interaction.

To solve the equations of motion we use 4^{th} order Runge-Kutta (RK4) algorithm, add formulas: This algorithm uses four intermediate steps to calculate the evolution of the system during a single time-step. RK4 integrator has local precision $O(eps^5)$, where eps is the discretization time step. By an appropriate choice of characteristic time and its discretization, we can reach local error to be of the order of a round-off error of the computing device. This is needed to guarantee the stability of the integrator for the nonlinear system. Equations of

motion conserve the magnitude of the spin S, and also the energy of the system, so that the reliability of the algorithm can be tested by how well those quantities are conserved. Another way to verify validity of the integrator is to reproduce the dispersion relation of a simpler problem, which was discussed in section C.

The most computation heavy part of the is the RK4 part, because in order to advance the system by a time step, we need four iterations when we perform calculation of the local magnetic field for a given spin, and due to dipole-dipole interaction in the system, we have to sum it over the whole lattice. The initial code was implemented completely in Python 2.7, but due to the issue with RK4 stated above its effectiveness for long simulation runs was low. Later the integrator and local filed calculator were rewritten in Fortran90. Python being an interpreter language is known to be much slower than Fortran, and because of the global interpretation lock in Python, it is not allowed to use multiple CPUs at once.

Since the advancement of each spin depends only on its current state and local field, this process can be performed in parallel. There are two parts of the algorithm where parallelization could be implemented: in the function that returns local magnetic field and the RK4 itself. Since RK4 calls this function multiple times, we chose to put *OpenMP parallel do* inside the RK4. The part of the Fortran code that does 2nd intermediate step of RK4 is given below:

```
!$omp parallel do shared(sp, f1, f2) private(i,j,temp)
    do i=0, m-1
        do j=0, n-1
            temp = h_local(i,j, sp+0.5_8*eps*f1)
            f2(i,j,:) = f(sp(i,j,:)+0.5_8*eps*f1(i,j,:), temp)
        enddo
    enddo
    !$omp end parallel do
```

There are five such calculations (four for intermediate steps and one for final calculation), so that at each step system calculates some intermediate data and then this data is shared among threads to calculate the next intermediate step.

The system under consideration has symmetric dispersion relation, meaning that we can limit ourselves to the positive values of wave-vectors. The allowed values of wave-vectors k are given by $\frac{\pi b}{na}$, where n is number of cells of length a along the prescribed dimension and b is an integer, such that $k \leq \frac{\pi}{a}$. Further, this set of wave-vectors corresponds to the set of wavelength that can be fit into the discrete system, thus discreteness of the lattice cuts unphysical high frequency modes. Equations of motions with the initial conditions chosen from this set are solved using the RK4 algorithm, and solutions can be fitted by a cosine function, such that the corresponding frequencies are be obtained from the fit. Practically, it is faster not to fit the cosine over several periods, but rather parabola that corresponds to the first order Taylor expansion of the cosine. Since, we are not interested in the precise values of the frequencies, but rather in the shape of the spectrum, this approximation suffices for further analysis. The second method is the Fourier transform (FT) and it will be used in further studies, when we have a superposition of different waves. The approximate cosine function can help us to estimate the upper bound for frequency range, then we can use this value to find the discretization frequency using Niquist Theorem, and then perform the FT of the dynamics. In order to implement the FT, we used Discrete Fourier Transform (DFT) function from the *numpy.fft* package [10] for Python. It should be noted that when one performs a DFT of the signal of final width, the phenomenon of "spectral leakage" might occur. This means that instead of one frequency we would observe a multiple peaks. In order to observe peaks, corresponding to the different spin waves, the width of a Fourier peaks should be smaller than the distance between the adjacent frequency peaks. This can be made by either monitoring dynamics at larger timescales, or using specific window functions for the DFT.

By trial and error, we obtain a set of parameters, namely values of coupling constants and size of the system, such that the obtained dispersion has required characteristic minimum and that we have enough wave-vectors to enable various scattering processes to be allowed by the conservation laws. We also need to check whether spin waves are stable solutions for large time scales, so that they adequately approximate the actual eigenmodes of the system. Once this is done, we investigate to the finite temperature dynamics.

As the configuration of the ground state is known, to obtain finite temperature dynamics one can slightly distort the ground state by randomly tilting the spins, such that they make a small angle with the net magnetization and solving the equations of motion for some time interval. During this time, the system will dynamically thermalize, meaning that at a particular moment it will reach dynamical equilibrium and thus can be described by a certain temperature. One can simulate further this equilibrium dynamics and then decompose the system into the constituent frequencies by the means of DFT. The squares of the expansion coefficients will correspond to the occupation numbers of the energy states. The equilibrium distribution should be of the form (5). When we perform the random spin orientation, we may also excite the spin waves with wave-vector that is perpendicular to the static magnetic field. We should filter them out in order to observe the processes associated with spin waves in the prescribed direction. This can be done by estimating the dispersion curve for those spin waves and then deleting the corresponding Fourier components from the set of frequencies obtained by DFT routine.

The final step is to introduce pumping and dissipation to the system. . The pumping mechanism can be incorporated into the original Hamiltonian by adding time-dependent magnetic field term of the form $h_p \cos \omega_p t$ on top of the static field that can be switched on/off at designated moments of time and has duration t_p. Although we focus only on the dynamic of the magnetic part of the system, there is spin-lattice interaction that can be formally incorporated as additional dissipative term. Since the exchange of energy between spins and lattice is at several orders of magnitude slower that the spin-spin interactions, we can formally account for spin-lattice relaxation by choosing dissipative term that conserves the length of the spin in the form $\boldsymbol{\alpha}[\mathbf{S_i} \times (\mathbf{S_i} \times \mathbf{h_i})]$, where α is a small quantity. Since the lowest energy configuration is the one, where spins are parallel to the magnetic field, the term above effectively decreases the angle between spin and the local field, decreasing the energy exponentially and thus playing the role of dissipation.

B. Numerical results

First, we reproduce the dispersion relation for Hamiltonian (13) in 2D (fig. 2). We see that for the value of transverse magnetization $mag = \frac{1}{20} S$ that is not very small we still get good agreement between dynamical simulation and the spin-wave formalism. If we add

external field on top of the exchange interaction, we simply shift the whole curve by the value of the magnetic field strength, and this result is consistent with general theory [11].

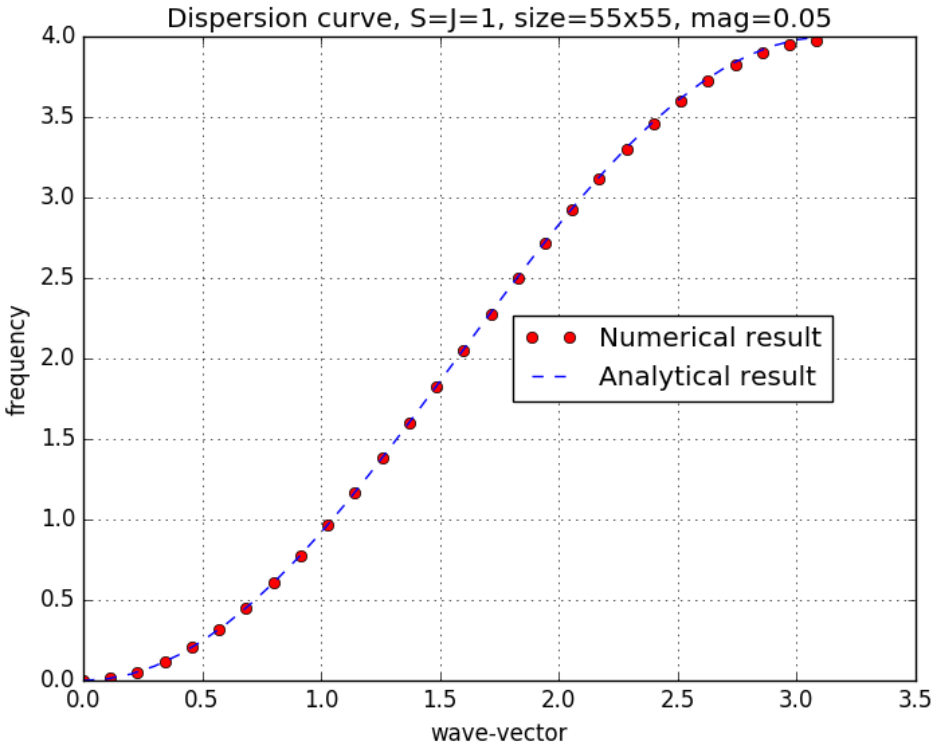

Figure 2: Comparison of the dispersion curves for exchange Hamiltonian in 2D for wave-vectors along x direction.

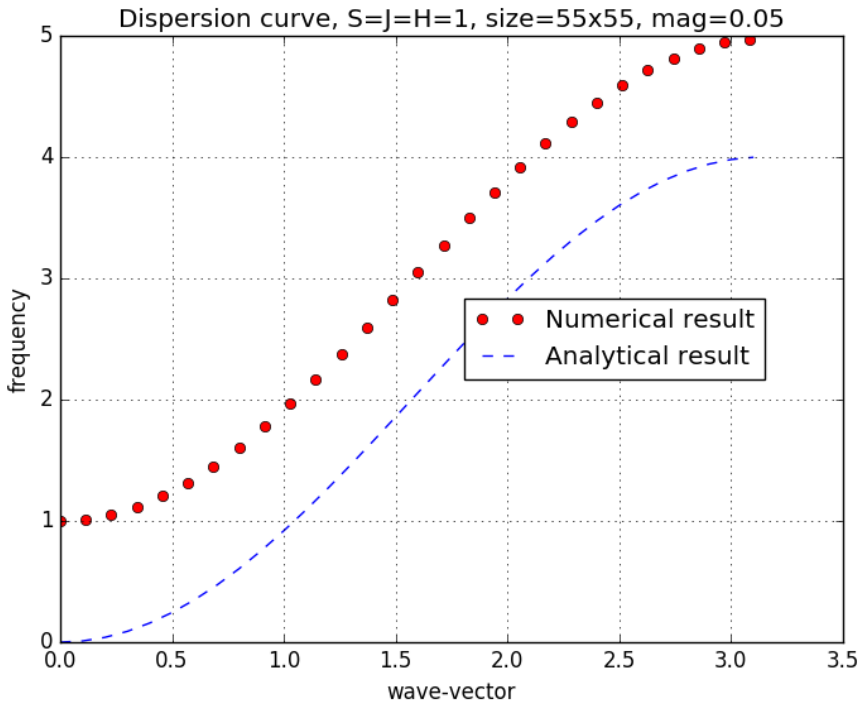

Figure 3: Numerical dispersion curves for exchange Hamiltonian in external field in 2D for wave-vectors along the static field and analytical expression for exchange Hamiltonian.

Our next step is to analyze for which values of transverse magnetization and strength of the dipole-dipole interaction, the formalism of spin waves is still valid. Figure 4 illustrates how the amplitude of the precession of magnetization becomes position dependent, however the frequency of the precession is invariant across the lattice.

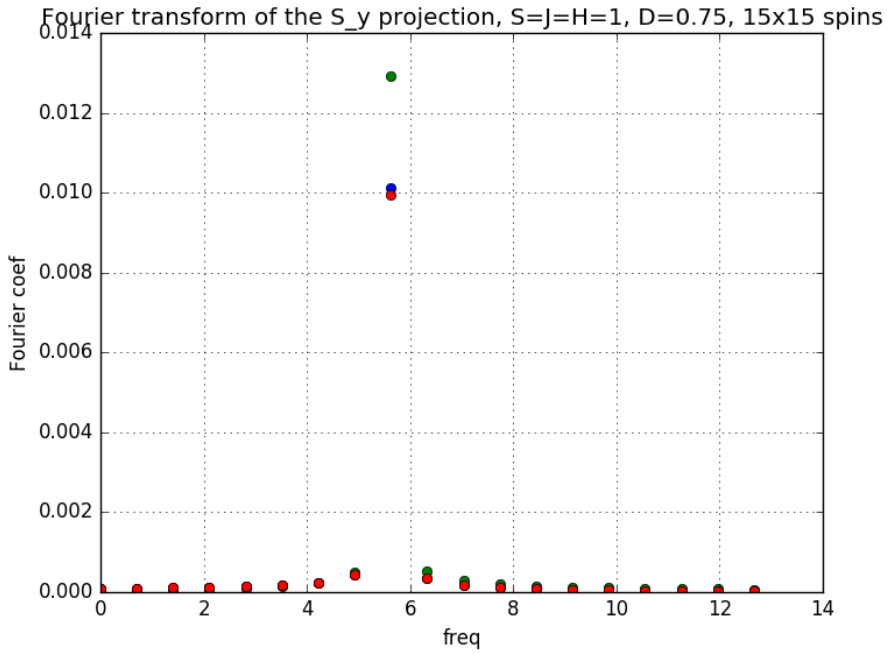

Figure 4: Fourier transform of the S_y projection of the transverse magnetization for various spins in the spin wave

Since for each constructed spin wave we get a single frequency, this means that chosen configuration still can be considered as an eigenmode. Because of this fact, we can trace the dynamics of only one spin, and still obtain all necessary information about the system. From now on, further analysis will be performed for spin with position (0, 0) on the lattice, because it has zero phase shift and can be easily fitted with parabolic approximation for cosine.

Now we want to obtain the dispersion relation with characteristic minimum and see how good is obtained dispersion relation by studying an evolution of the system with random initial conditions and decomposing it into frequency

The resulting dispersion relation for wave-vectors parallel and perpendicular to the static field is given in Figure 5:

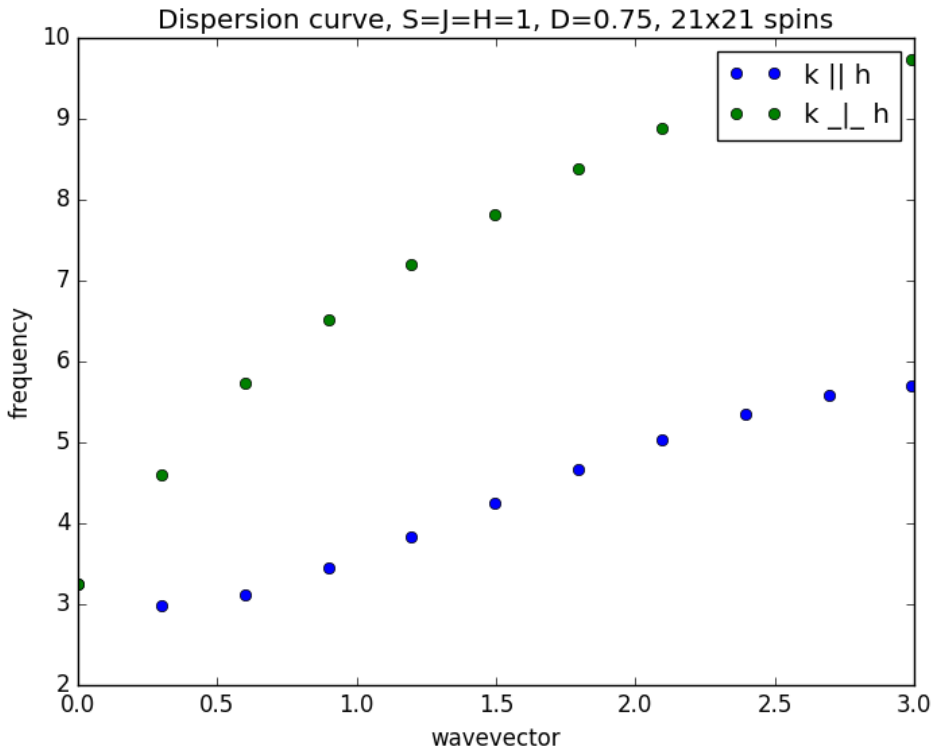

Figure 5: Dispersion curve for Hamiltonian (13) in 2D for wave-vectors parallel and perpendicular to the static magnetic field.

This figure shows that dispersion curve for the spin waves with wave-vectors parallel to the static magnetic field has a minimum for non-zero value of the wave-vector. This result was also checked by Fourier transform of the configuration with randomly oriented spins. One has to play more with the parameters of the system in order to make this minimum deeper and locate it farther from the origin, so that thermalization processes would be faster.

Conclusion

In this thesis we presented numerical analysis of the classical lattice spin-Hamiltonian and showed that spin-wave solution are robust in the presence of the dipole-dipole interaction. We obtained the dispersion relation of the required form, and by the means of the Fourier transform of the spin dynamics with random initial conditions verified its validity.

We need further studies in order to make a comprehensive analysis of the appropriate implementation of the pumping and dissipative mechanism as well as averaging of the dynamics over large number of random initial configurations. We hope to achieve those results in the future work.

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Numerical investigation of an externally driven spin dynamics in search of a classical condensation of waves

Table of Contents

Abstract

The following work is a numerical study of a recently discovered Bose-Einstein condensation of magnons at room temperature by purely classical means. The classical Hamiltonian of the system includes exchange and dipolar interaction as well as interaction with external magnetic field. The system under consideration is a 2-dimentional lattice of classical spins with fixed positions. Classical equations of motions are derived from this Hamiltonian by applying the Poisson-bracket formalism. Equations of motions were solved numerically by the 4^{th} order Runge-Kutta algorithm and obtained spin dynamics is transformed to the frequency space by the means of Fourier transform. This spectral decomposition of the dynamics allows monitoring the occupation of the energy states and observing condensation into the lowest energy state. In this work, we were able to reproduce the dispersion curve with characteristic minimum at non-zero value of the wave-vector by varying parameters of the system. We discuss models for pumping and dissipation, and hope to implement them in the future work.

1. Introduction

The development of experimental condensed matter physics in the last two decades made it possible to investigate exotic phases of matter such as Bose-Einstein condensates and quantum spin liquids. The quantum nature of the majority of those systems makes it difficult to numerically investigate their properties due to exponentially increasing number of eigenstates that scales with the size of the system. Classical or semi-classical picture requires fewer variables to describe the system of interest and therefore it allows one to perform simulations of considerably larger systems. This becomes a great advantage for spin systems, where classical picture provides results close to quantum simulations. One can study the corresponding properties of quantum systems using their classical analogs to address several classes of problems. First example is the investigation of the properties that are also present in classical picture, such as phase transitions and glassy dynamics. The second class consists of 1/Z expansion, where Z is the coordination number [1], and other 'beyond mean field' models that can be used to test various sample Hamiltonians for the emergence of properties of interest. For instance, studying the coherence and correlations, one can hope to find a suitable system for the quantum computer.

In 2006, Demokritov et al. claimed the first observation of the Bose-Einstein condensation (BEC) of magnons at room temperature in yttrium-iron-garnet (YIG) thin films under pumping [2]. Magnon BEC became an attractive topic after recent proposals to employ magnon BEC as qubits for quantum computing [3]. This provides grounds for testing of classical simulation applicability to quantum systems in the following ways. First, knowing that the low energy excitations of the spin system are wave-like, it is interesting, whether it is possible to produce condensation of the classical waves in this system. Second, it is interesting to test the 1/Z method on how robust it is in describing the critical phenomena and try to apply it the BEC. The current work deals only with the simulation of classical dynamics under external drive. It is expected to generalize 1/Z so that it could account for long-range interactions and apply it to the BEC of magnons in future works.

2. Theoretical description

A. BEC of particles and quasi-particles

Bose-Einstein condensation is the one of the most fascinating predictions of quantum theory. This phenomenon leads to the formation of collective quantum state of the integer

spin particles and thus can be characterized by a single wave-function. This happens when at a finite temperature a macroscopic fraction of particles occupies a single particle state. Here we give a brief discussion of the BEC.

Typically, if the size of the system is large, we expect that the spacing between the energy levels approaches zero, so we can change all summations with integrations, and can express the number of particles in the system by the following formula in terms of volume V, one-particle density of states D(E) and Bose distribution function:

$$\mathbf{N = V \int_0^\infty \frac{D(E)dE}{e^{(E-\mu)/kT} - 1}} \tag{1}$$

Since the Bose-distribution function is nonnegative, the value of chemical potential μ cannot exceed the minimal value of energy E. For further analysis, let us consider BEC of an ideal gas in 3-D, then expression (1) reads [4]:

$$\mathbf{\frac{N}{V} = \frac{g(mT)^{3/2}}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty \frac{\sqrt{z}dz}{e^{z-\mu/T} - 1}} \tag{2}$$

The expression under the integral contains parameterized energy distribution function for bosons and one-particle density of states. If we fix the N/V in the equation (2) and keep lowering the temperature, then the value of chemical potential will gradually increase, reaching its maximum value $\mu = 0$ at some temperature T_0. At temperatures $T<T_0$ the value of the N/V is smaller than the expression on the right side of the equation. The occurring contradiction is due to the fact that it is not allowed to replace the sum with the integral under such conditions, and when we do so, we multiply the first term in the sum by $\sqrt{E} = 0$, and it falls out of the sum. It turns out that the above formula will describe only particles in the excited states, while the rest of the particles will condense to the ground state. From this line of thought, it is natural to assume that, when the chemical potential is equal to the minimum value of energy in the system, the macroscopic fraction of the particles occupies the lowest energy state and this leads to the condensation in the momentum space. It is important to realize that the density of states plays an important role in the discussion above. In the case of 1-D or 2-D, the density of states is proportional to $\frac{1}{\sqrt{E}}$ and const. respectively. In both of those cases, the expression (2) diverges on the lower limit, so it does not have a maximum. This means that we can always choose $\mu<0$ and BEC will not occur. This story is different for finite samples, because in finite geometry, ground state is greater than zero, as clearly seen

from the expression for the ground state for the particle in the box: $\frac{\hbar^2\pi^2}{2mL^2}$. Interaction of the system with external potential may also change the density of states; therefore, it is possible to investigate BEC of dilute atomic gases in the traps.

From the expression (2) one can observe that there are two ways, in which condensation can occur: either to decrease the absolute temperature of the sample keeping the density of the gas constant, or to increase the density under the constant temperature. In both of these cases the chemical potential will increase (remaining negative) and will reach its maximum at μ = 0.

The Bose-Einstein condensation of quasi-particles representing collective excitations of the medium is somewhat specific, because for some systems the number of collective excitations is not equal to the total number of particles. When the number of quasi-particles is not fixed, it is determined by the equilibrium condition and the value of chemical potential in this equilibrium. Chemical potential can be defined as a partial derivative of a free energy with respect to number of particles with the fixed temperature and volume:

$$\mu = \left(\frac{\partial \mathbf{F}}{\partial \mathbf{N}}\right)_{\mathbf{T,V}} \tag{3}$$

In the thermodynamic equilibrium, free energy has a minimum; therefore, chemical potential is identically zero. This means that in equilibrium, system chooses how to occupy eigenstate and there is no any constrain that would make macroscopic number of particle fall into the ground state, so that condensation may not occur. This difficulty can be formally overcome by driving the system externally, so that the system will be in some partial equilibrium state. In such a state, chemical potential may differ from zero, so by pumping quasi-particles into the system, one can increase their density keeping the temperature constant, by incorporating a heat sink that would not allow the system to absorb all the energy, and reaching infinite temperature. By this technique, one can attain the correct parameters for the BEC condition, and observe condensation on the timescales of the lifetime of such non-equilibrium state.

B. Condensation of classical nonlinear waves.

Although the BEC condensation is a purely quantum effect, that relies on the corresponding statistics, recent studies of the wave turbulence have indicated that a classical ensemble of waves with random phases can manifest condensation in momentum space

similar to the BEC. The role of collisions in such systems plays four-wave (2 in-2 out) mixing, and maximum entropy principle drives the system towards equipartition of energy, because the classical waves have quadratic dispersion relation. In order to consider the system statistically, one need random ensemble of waves and an interaction between various modes. The evolution of the spectral distribution of modes is governed by Boltzmann-like kinetic equation [5]:

$$\frac{\partial n_{k_1}}{\partial t} = g^2 \int d\mathbf{k}_2 d\mathbf{k}_3 d\mathbf{k}_4 \, W_{k_1 k_2; k_3 k_4} (n_{\mathbf{k}_3} n_{\mathbf{k}_4} n_{\mathbf{k}_1} + n_{\mathbf{k}_3} n_{\mathbf{k}_4} n_{\mathbf{k}_2} - n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} - n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_4}) \tag{4}$$

The kinetic term on the right describes four-wave interaction, g is the strength of the nonlinear interaction, $W_{k_1 k_2; k_3 k_4} = \sigma\delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\delta({k_1}^2 + {k_2}^2 - {k_3}^2 - {k_4}^2)$ is the collision term, and σ is the scattering matrix, which is a constant factor for the case of homogeneous system. The presence of the δ-function is present for purpose of the momentum and energy conservation during the collisions. As in the kinetic theory, where Boltzmann H-theorem states, that evolution of the system is subject to the constraint $\frac{dS}{dt} \geq 0$, where S is the entropy of the system. The equilibrium distribution function is obtained from the condition $\frac{dS}{dt} = 0$, and the constraint on conservation of total energy and power (proportional to the number of particles), so the results reads:

$$n_{\mathbf{k}}^{eq} = \frac{T}{k^2 - \mu} \tag{5}$$

This is Rayleigh-Jeans distribution. Note that as in case of Bose gas, $\mu < E_{min}$. If we substitute this result into expression for total energy and number of particles, we see that they both diverge at the ultraviolet limit $k \to \infty$. Therefore, one need to introduce the ultraviolet cutoff k_c, the physical justification for it is that for numerical simulations it is avoided by spatial discretization of the equation, while in real systems it is absent due to viscosity and diffusion [6]. In this work, we consider the system defined on a lattice with periodic boundary conditions, and therefore all physical wave-vectors are within the first Brillouin zone.

Let us do the similar analysis of the condensation of classical waves in 3D [6]:

$$\frac{N}{V} = 4\pi T k_c \left[1 - \frac{\sqrt{-\mu}}{k_c} \arctan\left(\frac{k_c}{\sqrt{-\mu}}\right)\right] \tag{6}$$

If we fix N/V, and start decreasing the temperature, $\mu = 0$ at T_c and below we can use distribution with $\mu = 0$. The remaining particles will be in the ground state. The cases for other dimensions are also qualitatively similar to BEC results. It is important that in bounded systems condensation in 2D at finite temperature is still possible [5].

Experimental investigation of the condensation of classical light in self-focusing photorefractive crystal showed that the effects of nonlinearity are essential for condensation to occur [5]. By increasing the strength of nonlinearity g, the distribution becomes more narrowly peaked about the minimum value of energy. This result is important for our further analysis, because the resulting classical equation of motion will be nonlinear and by appropriate choice of coupling parameters one can control strength of nonlinearity and potentially the thermalization rate.

C. Magnons.

One interesting property of physical problems is that when one is considering the Hamiltonian, which is a quadratic form in its dynamics variables, the result is analogous to the solution to harmonic oscillator. The recipe is as follows: one solves the classical analog of the system in terms of eigen-frequencies, and then substitutes them to the energy levels of quantum harmonic oscillator. This is applicable to the oscillations of magnetic moment. Quantized version of the spin wave is called magnon and here we will give simplified and a bit unrealistic description of spin waves in the theory of ferromagnetism of 1D-spin chains, because the following results in 1D can be generalized to higher dimensions, where this theory works properly. Since the energy of spin system is written as sum of energies of non-interacting harmonic oscillators $E_i = \omega_i(n_i + \frac{1}{2})$ (where$\hbar = 1$), we see that multiple magnons can occupy single particle state and therefore they are bosons. Consider the following Hamiltonian with periodic boundary conditions [7]:

$$\boldsymbol{H} = -2\boldsymbol{J}\sum_{\boldsymbol{i=1}}^{\boldsymbol{N}} \boldsymbol{S_i}\,\boldsymbol{S_{i+1}} \tag{7}$$

Here J>0 is a nearest neighbor exchange coupling, and **S** is a spin at site i. In this model, spins can be treated as vectors in 3D. This Hamiltonian corresponds to the ferromagnetic state: at zero temperature all spins are aligned in the same direction. Note that at zero temperature there are no magnons, thus their number is generally temperature-dependent. This suggests that they are quasi-particles. The elementary excitations of such a

spin system have wave-like form, where each consecutive spin is slightly misaligned from the previous one. The energy of such configuration is smaller than of the configuration, where only one spin is flipped. The equations of motion for a spin can be obtained by using Poisson-bracket formalism that replaces commutators in quantum mechanics, so that time derivative of the spin variable reads [8]:

$$\frac{\boldsymbol{dS_{i,\alpha}}}{\boldsymbol{dt}} = \left\{\widehat{\boldsymbol{H}}, \boldsymbol{S_{i,\alpha}}\right\} \tag{8}$$

Where index α corresponds to the x, y, z components of the magnetization vector. In order to expand right hand side of (8), we use the commutation relations for the angular momenta variables, namely:

$$\left\{\boldsymbol{S_{i,\alpha}}, \boldsymbol{S_{j,\beta}}\right\} = \boldsymbol{\delta_{ij}} \sum_{\boldsymbol{\gamma}} \boldsymbol{\varepsilon_{\alpha\beta\gamma}} \boldsymbol{S_{i,\gamma}} \tag{9}$$

where δ_{ij} is the Kronecker delta and $\varepsilon_{\alpha\beta\gamma}$ is Levi-Civita symbol. Using (9) one can express (8) as:

$$\dot{\boldsymbol{S}}_{\boldsymbol{\iota}} = \boldsymbol{S_i} \times \boldsymbol{h_i} \tag{10}$$

$$\boldsymbol{h_i} = -2J(\boldsymbol{S_{i-1}} + \boldsymbol{S_{i+1}}) \tag{11}$$

Here $\mathbf{h_i}$ plays the role of the local magnetic field as seen by spin $\mathbf{S_i}$. These equations involve product of two spins and thus are nonlinear. We can linearize them around the ground state configuration by assuming that ${S_p}^z = S$ and ${S_p}^x, {S_p}^y \ll S$ for all p, as well as neglecting all products, involving ${S_p}^x, {S_p}^y$. The resulting system of equation for spin p reads:

$$\frac{\boldsymbol{dS_{i,x}}}{\boldsymbol{dt}} = \boldsymbol{2JS}\left(\boldsymbol{2S_{i,y} - S_{i-1,y} - S_{i+1,y}}\right) \tag{10.a}$$

$$\frac{dS_{i,y}}{dt} = -2JS\left(2S_{i,x} - S_{i-1,x} - S_{i+1,x}\right) \tag{10.b}$$

$$\frac{dS_{i,z}}{dt} = 0 \tag{10.c}$$

By looking for the solution for this system in the form:

$$S_{i,x} = u\,\exp[i(pka - \omega t)]; \qquad S_{i,y} = v\,\exp[i(pka - \omega t)]$$

We arrive to the following eigenvalue problem:

$$\begin{vmatrix} i\omega & 4JS(1-\cos ka) \\ -4JS(1-\cos ka) & i\omega \end{vmatrix} = 0$$

The resulting dispersion relation is:

$$\boldsymbol{\omega = 4JS(1-\cos ka)} \tag{11}$$

For cubic lattice in higher dimension we simply write:

$$\boldsymbol{\omega = 2JS\left(n - \sum_{\delta} \cos k\delta\right)} \tag{12}$$

where the summation is over the n vectors denoted by δ which join the central atom to its nearest neighbors [7]. We will use this result later in order to verify the validity of the implemented integrator for the dynamic evolution of the system.

D. Experimental description of BEC of magnons.

Group of S. Demokritov conducted a series of experiments of parallel parametric pumping of magnons in YIG thin (2-10 μm) films and claimed the observation of BEC. The YIG thin films are mainly interesting because of slow spin-lattice relaxation (above 1μs) that experimentally manifests itself in larger lifetime of the quasi-equilibrium states. The magnon-magnon thermalization consists of two- and four-magnon scattering processes, and it takes place at a typical time of 100-200 ns. Those scattering processes conserve the number of particles, so that the total number of magnons can be considered as fixed. This means that the chemical potential can take non-zero values. The experimental setup used by Demokritov et al. is illustrated in Figure 1.

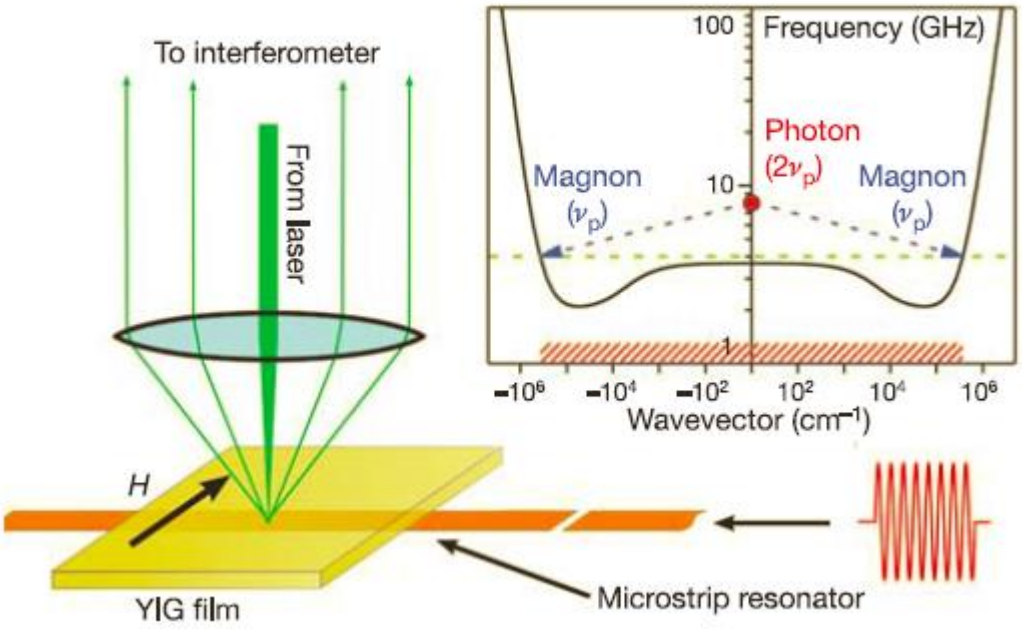

Figure 1 : Experimental setup of Demokritov et al. [2]

A thin YIG film with lateral sizes of 2 mm × 20 mm and thickness of 2-10μm is places in a uniform and static magnetic field as in Figure 1. Magnons with a wave-vector parallel to this field have a characteristic minimum in their spectrum [2]. A microstrip resonator is attached to the surface of the film. The mechanism of parallel parametric pumping can be described as following: the oscillating magnetic field of the microwave radiation is applied parallel to the static magnetization, and since all wave-vectors are confined to the first Brillouin zone, one can apply conservation of momentum and energy to such a system. The speed of light inside the material is several orders of magnitude greater than characteristic group velocity of magnons, therefore we can neglect wave-vector of the microwave radiation: such photons can excite two magnons with the same frequency and opposite wave-vectors. Those primary magnons after relaxation create a gas of quasi-equilibrium magnons. With the increasing power of pumping, chemical potential of such gas also increases and attains the required value. Similarly to the experiment on condensation of classical nonlinear waves, higher pumping rates correspond to the higher strength of nonlinear interaction, for which the distribution function is strongly localized around minimal value of the frequency.

F. Spin model.

From the description of the ferromagnet in terms of electrodynamics of continuous media, it follows that the spectrum with the characteristic minimum can be obtained by

including exchange interaction, interaction with the external field and the dipole-dipole interaction of magnetic moments. For this reason we consider the Hamiltonian of the system of the following form [9]:

$$\widehat{\boldsymbol{H}} = -\boldsymbol{\gamma}\sum_{\boldsymbol{i}} \boldsymbol{S_i}\cdot\boldsymbol{H_0} + -\boldsymbol{J_0}\sum_{\boldsymbol{i,\delta}} \boldsymbol{S_i}\,\boldsymbol{S_{i+\delta}} + \boldsymbol{U_d}\sum_{\boldsymbol{i\neq j}} \frac{\boldsymbol{S_i S_j} - \boldsymbol{3}(\boldsymbol{S_i}\cdot\boldsymbol{n_{ij}})(\boldsymbol{S_j}\cdot\boldsymbol{n_{ij}})}{|\boldsymbol{r_{ij}}|^{\boldsymbol{3}}} \tag{13}$$

Using the same formalism as in previous section, we can obtain the corresponding equations of motion:

$$\dot{\boldsymbol{S}}_{\boldsymbol{\iota}} = \boldsymbol{S_i}\times\boldsymbol{h_i} \tag{14}$$

$$\boldsymbol{h_i} = -\boldsymbol{\gamma}\boldsymbol{H_0} + -\boldsymbol{J_0}\sum_{\boldsymbol{\delta}} \boldsymbol{S_{i+\delta}} + \boldsymbol{U_d}\sum_{\boldsymbol{i\neq j}} \frac{\boldsymbol{S_j} - \boldsymbol{3n_{ij}}(\boldsymbol{S_j}\cdot\boldsymbol{n_{ij}})}{|\boldsymbol{r_{ij}}|^{\boldsymbol{3}}} \tag{15}$$

Where coefficients before the sums are the coupling constants, indices i, j run across the lattice sites and taking values r_i etc., δ corresponds to the summation over the nearest neighbors, $\mathbf{r_{ij}} = \mathbf{r_i} - \mathbf{r_j}$, $\mathbf{n_{ij}}$ - unit vector in the direction of $\mathbf{r_{ij}}$. Since the original work of Demokritov was performed on thin films, where thickness is three orders of magnitude smaller than lateral sizes, which makes the system practically quasi two dimensional, we will investigate the dynamics of the two dimensional spin systems given by above Hamiltonian. We should immediately address several important aspects of the Hamiltonian.

First, in real system, the value of dipole constant is several orders of magnitude smaller than other coupling constants, so this interaction can be considered as weak, however, it is a long range interaction and therefore its contribution becomes important for large system. The calculation of the dipole component in the local field requires knowledge of the spin configuration of the entire system and it is the most expensive calculation. In order to reduce the total computational time, we will consider relatively small system (about 50x50) with the dipole coupling constant of the order of unity to account for the "accumulation" effect.

Second, as it was mentioned in the section 2C, spin waves are solutions for the equations of motion when the magnitudes of the transverse magnetization are much less that the magnitude of the spin, so that we could neglect nonlinear terms in all equation. At the same time, results of the experimental papers on both condensations of classical nonlinear waves as well as BEC of magnons suggest that the process of condensation is more pronounced for the higher values of nonlinear interactions. Therefore, one may doubt the

applicability of the approach based on the use of the spin wave model when the magnitude of the transverse magnetization and dipole constant are not small. Practically, the spin wave model is helpful only for the investigation of the dispersion relation. We can solve the equations of motions numerically, with the initial conditions corresponding to the spin wave with a given wave-vector and then by investigating the precessional motion of a particular spin, obtain a relation between its frequency and wave-vector. It is not important whether the constructed spin wave is an actual eigenmode of the Hamiltonian, but rather that it lies close to the actual solution in the frequency space. To justify this procedure, one can compare dispersion curve obtained by the mentioned procedure with the result of the Fourier transform of the spin precession with arbitrary initial conditions and see that they indeed give close results.

3. Numerical analysis

A. Description of the simulation

The following section describes the numerical procedure and all important steps that are carried in the presented order. Results of the simulations can be found in the next section.

Solution of equations of motion (14-15) requires correct choice of the characteristic time-scale of the system's dynamics. By comparing the units of both sides of equations of motion, it is clear that units of time are equal to the inverse units of effective magnetic field; therefore for the natural timescale for the problem one can choose timescale equal to inverse of the root mean square of this effective field.

Dynamics of the system under consideration is confined to the 2-D lattice with square unit cell, where all spins are fixed in their positions. It is sensible to save in computer memory data that incorporates periodic boundary conditions and store all fixed parameters, needed for calculating the dipole-dipole interaction.

To solve the equations of motion we use 4^{th} order Runge-Kutta (RK4) algorithm, add formulas: This algorithm uses four intermediate steps to calculate the evolution of the system during a single time-step. RK4 integrator has local precision $O(eps^5)$, where eps is the discretization time step. By an appropriate choice of characteristic time and its discretization, we can reach local error to be of the order of a round-off error of the computing device. This is needed to guarantee the stability of the integrator for the nonlinear system. Equations of

motion conserve the magnitude of the spin S, and also the energy of the system, so that the reliability of the algorithm can be tested by how well those quantities are conserved. Another way to verify validity of the integrator is to reproduce the dispersion relation of a simpler problem, which was discussed in section C.

The most computation heavy part of the is the RK4 part, because in order to advance the system by a time step, we need four iterations when we perform calculation of the local magnetic field for a given spin, and due to dipole-dipole interaction in the system, we have to sum it over the whole lattice. The initial code was implemented completely in Python 2.7, but due to the issue with RK4 stated above its effectiveness for long simulation runs was low. Later the integrator and local filed calculator were rewritten in Fortran90. Python being an interpreter language is known to be much slower than Fortran, and because of the global interpretation lock in Python, it is not allowed to use multiple CPUs at once.

Since the advancement of each spin depends only on its current state and local field, this process can be performed in parallel. There are two parts of the algorithm where parallelization could be implemented: in the function that returns local magnetic field and the RK4 itself. Since RK4 calls this function multiple times, we chose to put *OpenMP parallel do* inside the RK4. The part of the Fortran code that does 2nd intermediate step of RK4 is given below:

```
!$omp parallel do shared(sp, f1, f2) private(i,j,temp)
    do i=0, m-1
        do j=0, n-1
            temp = h_local(i,j, sp+0.5_8*eps*f1)
            f2(i,j,:) = f(sp(i,j,:)+0.5_8*eps*f1(i,j,:), temp)
        enddo
    enddo
    !$omp end parallel do
```

There are five such calculations (four for intermediate steps and one for final calculation), so that at each step system calculates some intermediate data and then this data is shared among threads to calculate the next intermediate step.

The system under consideration has symmetric dispersion relation, meaning that we can limit ourselves to the positive values of wave-vectors. The allowed values of wave-vectors k are given by $\frac{\pi b}{na}$, where n is number of cells of length a along the prescribed dimension and b is an integer, such that $k \leq \frac{\pi}{a}$. Further, this set of wave-vectors corresponds to the set of wavelength that can be fit into the discrete system, thus discreteness of the lattice cuts unphysical high frequency modes. Equations of motions with the initial conditions chosen from this set are solved using the RK4 algorithm, and solutions can be fitted by a cosine function, such that the corresponding frequencies are be obtained from the fit. Practically, it is faster not to fit the cosine over several periods, but rather parabola that corresponds to the first order Taylor expansion of the cosine. Since, we are not interested in the precise values of the frequencies, but rather in the shape of the spectrum, this approximation suffices for further analysis. The second method is the Fourier transform (FT) and it will be used in further studies, when we have a superposition of different waves. The approximate cosine function can help us to estimate the upper bound for frequency range, then we can use this value to find the discretization frequency using Niquist Theorem, and then perform the FT of the dynamics. In order to implement the FT, we used Discrete Fourier Transform (DFT) function from the *numpy.fft* package [10] for Python. It should be noted that when one performs a DFT of the signal of final width, the phenomenon of "spectral leakage" might occur. This means that instead of one frequency we would observe a multiple peaks. In order to observe peaks, corresponding to the different spin waves, the width of a Fourier peaks should be smaller than the distance between the adjacent frequency peaks. This can be made by either monitoring dynamics at larger timescales, or using specific window functions for the DFT.

By trial and error, we obtain a set of parameters, namely values of coupling constants and size of the system, such that the obtained dispersion has required characteristic minimum and that we have enough wave-vectors to enable various scattering processes to be allowed by the conservation laws. We also need to check whether spin waves are stable solutions for large time scales, so that they adequately approximate the actual eigenmodes of the system. Once this is done, we investigate to the finite temperature dynamics.

As the configuration of the ground state is known, to obtain finite temperature dynamics one can slightly distort the ground state by randomly tilting the spins, such that they make a small angle with the net magnetization and solving the equations of motion for some time interval. During this time, the system will dynamically thermalize, meaning that at a particular moment it will reach dynamical equilibrium and thus can be described by a certain temperature. One can simulate further this equilibrium dynamics and then decompose the system into the constituent frequencies by the means of DFT. The squares of the expansion coefficients will correspond to the occupation numbers of the energy states. The equilibrium distribution should be of the form (5). When we perform the random spin orientation, we may also excite the spin waves with wave-vector that is perpendicular to the static magnetic field. We should filter them out in order to observe the processes associated with spin waves in the prescribed direction. This can be done by estimating the dispersion curve for those spin waves and then deleting the corresponding Fourier components from the set of frequencies obtained by DFT routine.

The final step is to introduce pumping and dissipation to the system. . The pumping mechanism can be incorporated into the original Hamiltonian by adding time-dependent magnetic field term of the form $h_p \cos \omega_p t$ on top of the static field that can be switched on/off at designated moments of time and has duration t_p. Although we focus only on the dynamic of the magnetic part of the system, there is spin-lattice interaction that can be formally incorporated as additional dissipative term. Since the exchange of energy between spins and lattice is at several orders of magnitude slower that the spin-spin interactions, we can formally account for spin-lattice relaxation by choosing dissipative term that conserves the length of the spin in the form $\boldsymbol{\alpha}[\mathbf{S_i} \times (\mathbf{S_i} \times \mathbf{h_i})]$, where α is a small quantity. Since the lowest energy configuration is the one, where spins are parallel to the magnetic field, the term above effectively decreases the angle between spin and the local field, decreasing the energy exponentially and thus playing the role of dissipation.

B. Numerical results

First, we reproduce the dispersion relation for Hamiltonian (13) in 2D (fig. 2). We see that for the value of transverse magnetization $mag = \frac{1}{20} S$ that is not very small we still get good agreement between dynamical simulation and the spin-wave formalism. If we add

external field on top of the exchange interaction, we simply shift the whole curve by the value of the magnetic field strength, and this result is consistent with general theory [11].

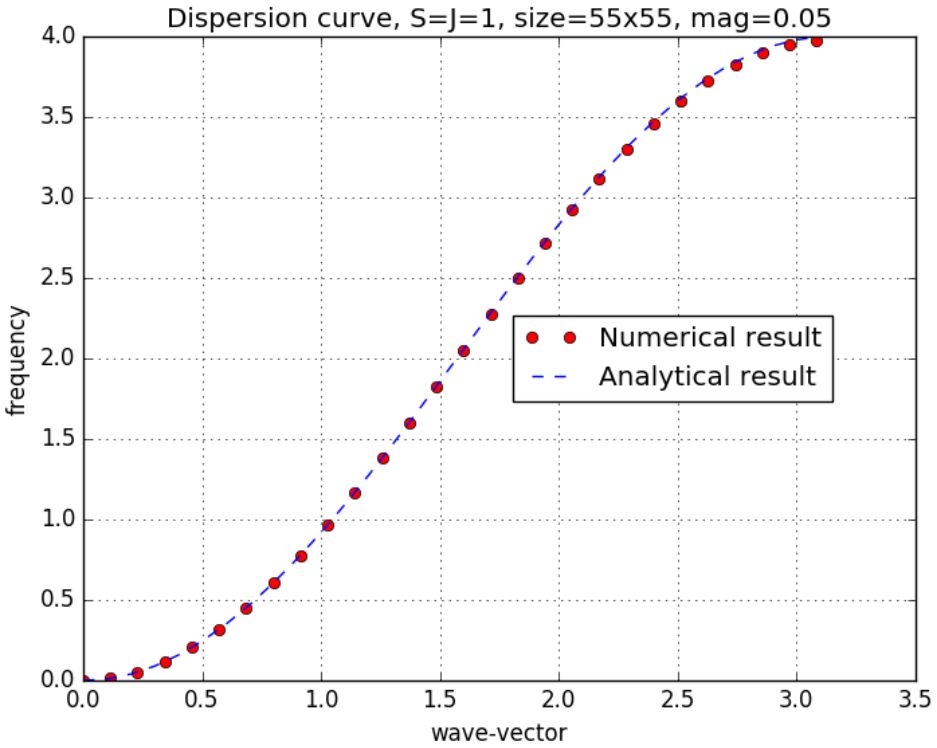

Figure 2: Comparison of the dispersion curves for exchange Hamiltonian in 2D for wave-vectors along x direction.

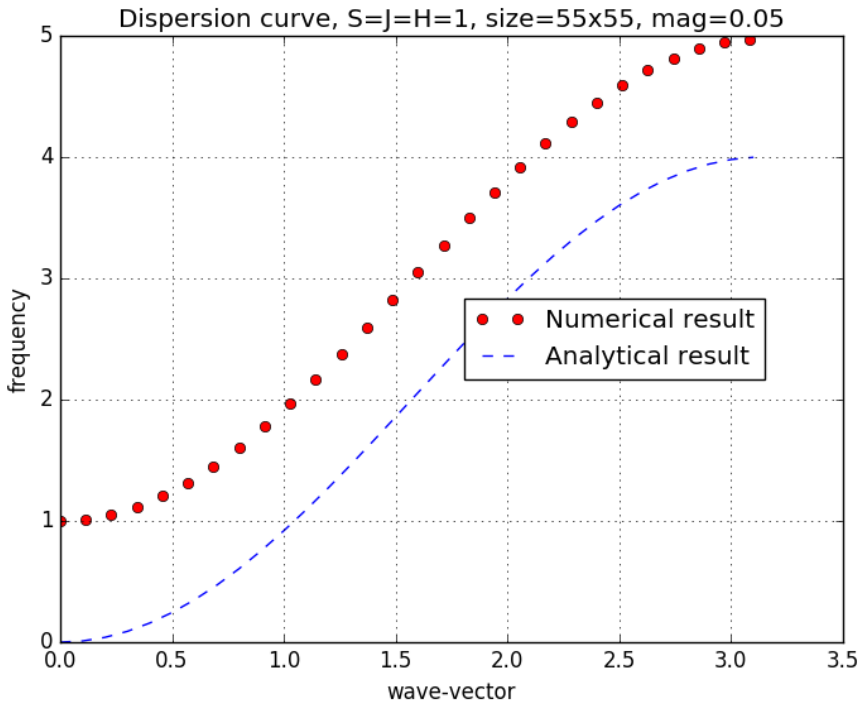

Figure 3: Numerical dispersion curves for exchange Hamiltonian in external field in 2D for wave-vectors along the static field and analytical expression for exchange Hamiltonian.

Our next step is to analyze for which values of transverse magnetization and strength of the dipole-dipole interaction, the formalism of spin waves is still valid. Figure 4 illustrates how the amplitude of the precession of magnetization becomes position dependent, however the frequency of the precession is invariant across the lattice.

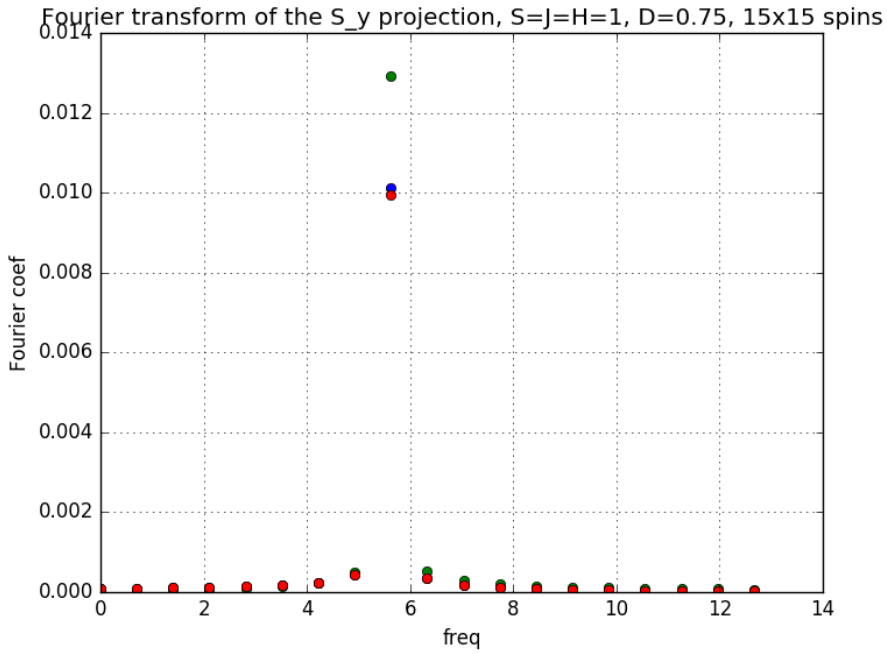

Figure 4: Fourier transform of the S_y projection of the transverse magnetization for various spins in the spin wave

Since for each constructed spin wave we get a single frequency, this means that chosen configuration still can be considered as an eigenmode. Because of this fact, we can trace the dynamics of only one spin, and still obtain all necessary information about the system. From now on, further analysis will be performed for spin with position (0, 0) on the lattice, because it has zero phase shift and can be easily fitted with parabolic approximation for cosine.

Now we want to obtain the dispersion relation with characteristic minimum and see how good is obtained dispersion relation by studying an evolution of the system with random initial conditions and decomposing it into frequency

The resulting dispersion relation for wave-vectors parallel and perpendicular to the static field is given in Figure 5:

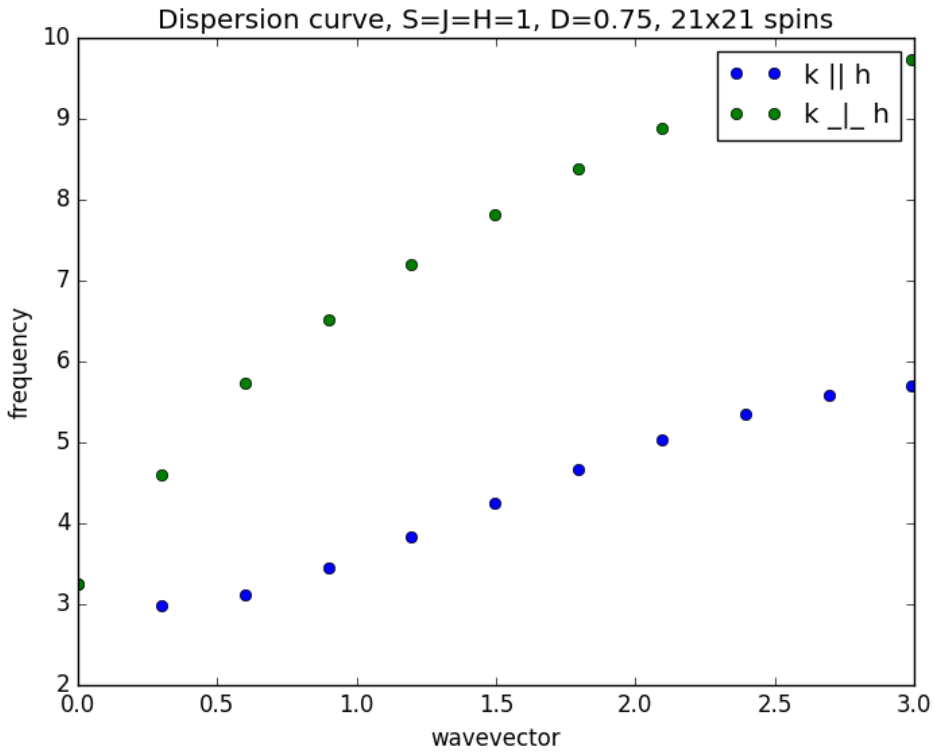

Figure 5: Dispersion curve for Hamiltonian (13) in 2D for wave-vectors parallel and perpendicular to the static magnetic field.

This figure shows that dispersion curve for the spin waves with wave-vectors parallel to the static magnetic field has a minimum for non-zero value of the wave-vector. This result was also checked by Fourier transform of the configuration with randomly oriented spins. One has to play more with the parameters of the system in order to make this minimum deeper and locate it farther from the origin, so that thermalization processes would be faster.

Conclusion

In this thesis we presented numerical analysis of the classical lattice spin-Hamiltonian and showed that spin-wave solution are robust in the presence of the dipole-dipole interaction. We obtained the dispersion relation of the required form, and by the means of the Fourier transform of the spin dynamics with random initial conditions verified its validity.

We need further studies in order to make a comprehensive analysis of the appropriate implementation of the pumping and dissipative mechanism as well as averaging of the dynamics over large number of random initial configurations. We hope to achieve those results in the future work.

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