Exercise 2, TFY4235 Computational physics

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Introduction

This report documents the simluation of magnons, as described in [1].

Theory

The Hamiltonian in question is, in units of the coupling constant J,

$$\mathcal{H}(S; d_z, a, B) = -\frac{1}{2} J \sum_{\langle i,j \rangle, a} S_{i,a} S_{j,a} - d_z \sum_j (S_{j,3})^2 - \sum_{j,a} B_{j,a} S_{j,a}.$$

S are the spins, the dynamical variables, $i \in \{1, ..., N\}$ is the site index, a is vector component index. d_z, a and $B_{i,a}$ are respectivley the inisotropy strength, the coupling strength, the magnetic moment and the external magnetic field. The magnetic field is given in units of $\mu/J[B_0]$, where μ magnetic moment. These appear as parameters in the Hamiltonian. The dynamics of the system at zero temprature is governd by the Landau-Lifshitz-Gilbert equation,

$$\frac{\mathrm{d}}{\mathrm{d}t} S_{j,a} = -\frac{1}{(1+\alpha^2)} \left[\sum_{bc} \varepsilon_{abc} S_{j,b} H_{j,c} + \alpha \sum_b (S_{j,b} S_{j,b} H_{j,a} - S_{j,b} H_{j,b} S_{j,a}) \right],$$

$$H_{k,b} = -\frac{\partial \mathcal{H}}{\partial S_{k,b}} = \frac{1}{2} J \sum_{\langle i,j \rangle, a} (S_{i,a} \delta_{j,k} \delta_{a,b} + S_{j,a} \delta_{i,k} \delta_{a,b}) + 2 d_z \sum_j S_{j,3} \delta_{b,3} \delta_{j,k} + \sum_{j,a} B_{j,a} \delta_{k,b}.$$

The time units are given by γ. The triple product identity $\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{B}) \vec{C} - (\vec{A} \cdot \vec{C}) \vec{B}$ has been used for the convinience of implementation. The first sum of the H-term can be written as

$$\frac{1}{2} \sum_{\langle i,j \rangle, a} (S_{i,a} \delta_{j,k} \delta_{a,b} + S_{j,a} \delta_{i,k} \delta_{a,b}) = \frac{1}{2} \sum_{\langle i,j \rangle} (S_{i,b} \delta_{j,k} + S_{j,b} \delta_{i,k}) = \frac{1}{2} \sum_{\langle j,i \rangle} 2 S_{i,b} \delta_{j,k} = \sum_{j \in \mathrm{NN}_k} S_{j,b},$$

where NN_k are the set of nearest negihbours of lattice point k. This gives the expression for the effective field

$$H_{k,b} = J \sum_{j \in \mathrm{NN}_k} S_{j,b} + 2 d_z S_{k,3} \delta_{k,3} + B_{k,b}.$$

References

[1] Exercise 2, 2021, tfy4235 computational physics.