Day 3 VAMPIRE Workshop : Customised unit cell files; Application for skyrmions;

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0.1 Inclusion of DMI interaction into the exchange tensor; Theory aspects;

The exchange Hamiltonian can be written in terms of a general exchange tensor $\mathcal{J}_{ij}^{\alpha\beta}$:

$$\mathcal{H}_{exch} = -\frac{1}{2}\sum_{i\neq j} \mathbf{S}_i^{\alpha}\, \mathcal{J}_{ij}^{\alpha\beta}\, \mathbf{S}_j^{\beta}\ ,\quad \alpha,\beta = x,y,z \tag{1}$$

The exchange tensor can be decomposed into three terms:

$$\mathcal{J}_{ij} = J_{ij}\mathbf{I} + \mathcal{J}_{ij}^{S} + \mathcal{J}_{ij}^{A} \tag{2}$$

The term J_{ij} represents the isotropic part of the exchange tensor ($\mathbf{I}$ represents the unit tensor), $\mathcal{J}_{\mathbf{ij}}^{\mathbf{S}}$ the symmetric anisotropic exchange and $\mathcal{J}_{\mathbf{ij}}^{\mathbf{A}}$ is given by the antisymmetric exchange. The antisymmetric exchange corresponds to the Dzyaloshinskii-Moriya Interaction (DMI). The isotropic, symmetric and antisymmetric exchange can be easily deduced from the exchange tensor using the following:

$$J_{ij} = \frac{1}{3}Tr(\mathcal{J}_{ij})\ ,\ \ \mathcal{J}_{ij}^{S} = \frac{\mathcal{J}_{ij}+\mathcal{J}_{ij}^{t}}{2} - J_{ij}\mathbf{I}\ ,\ \ \mathcal{J}_{ij}^{A} = \frac{\mathcal{J}_{ij}-\mathcal{J}_{ij}^{t}}{2}, \tag{3}$$

where $\mathcal{J}_{\mathbf{ij}}^{\mathbf{t}}$ is the transpose of the exchange tensor.
The energy corresponding to the antisymmetrical exchange is given by:

$$\mathcal{H}_{DM} = \mathbf{D}_{ij}\cdot(\mathbf{S}_i \times \mathbf{S}_j) \tag{4}$$

The D_{ij} vector can be easily expressed from the antisymmetric part of the exchange tensor:

$$D_{ij}^{x} = \frac{\mathcal{J}_{ij}^{yz}-\mathcal{J}_{ij}^{zy}}{2}\ ,\ \ D_{ij}^{y} = \frac{\mathcal{J}_{ij}^{zx}-\mathcal{J}_{ij}^{xz}}{2}\ ,\ \ D_{ij}^{z} = \frac{\mathcal{J}_{ij}^{xy}-\mathcal{J}_{ij}^{yx}}{2} \tag{5}$$

Using eq.5, the antisymmetric exchange tensor $\mathcal{J}_{\mathbf{ij}}^{\mathbf{A}}$ can be written as:

$$\mathcal{J}_{\mathbf{ij}}^{\mathbf{A}} = \begin{bmatrix} 0 & D_{ij}^{z} & -D_{ij}^{y} \\ -D_{ij}^{z} & 0 & D_{ij}^{x} \\ D_{ij}^{y} & -D_{ij}^{x} & 0 \end{bmatrix} \tag{6}$$

From the Moriya symmetry rules, the DMI vector for a specific atomic layer k can be described [1]:

$$\mathbf{D}_{ij}^{k} = D^{k} \cdot (\mathbf{z} \times \mathbf{u}_{ij}) \tag{7}$$

where $\mathbf{z}$ and $\mathbf{u_{ij}}$ are the versors pointing along z direction and from site i and j respectively.

0.2 Generating skyrmions in a sc lattice (toy model)

Exercises

1. Calculate the isotropic exchange in this way in which the critical temperature of the system is under 20K (for faster simulations). An approximation of the Curie Temperature is given by Garanin [2] and for a sc lattice has the following form:

   $$T_C = \frac{\epsilon z}{3} \frac{J}{k_B} \approx 1.44 \frac{J}{k_B} \tag{8}$$

   where T_C represents the Curie Temperature, J the exchange constant, k_B the Boltzmann constant. The exchange value should be around 1meV. You can check the critical temperature by running a Curie temperature simulation.

2. Write a simple code to create a sc system with PBC (periodic boundary conditions) and calculate the nearest-neighbours interaction list for the 1 atom unit cell.

3. Based on equation (6) and (7) assign to each interaction an exchange tensor. Build the exchange tensor in this way that the ratio between isotropic exchange and DMI strength can be varied.

   The exchange tensor looks like:

   $$\mathcal{J}_{\mathbf{ij}} = \begin{bmatrix} J_{xx} & D_{ij}^{z} & -D_{ij}^{y} \\ -D_{ij}^{z} & J_{yy} & D_{ij}^{x} \\ D_{ij}^{y} & -D_{ij}^{x} & J_{zz} \end{bmatrix} \tag{9}$$

4. Create the $file.ucf$ that you will afterwards use for the simulations. For a sc monolayer the unit cell should have 1 atom and 4 nearest-neighbours interactions. Consider the ratio between DMI strength and exchange 1.

5. Run a zero field cooling simulation to calculate the ground state of the system. Start with a system of 20x20 atoms for fast simulations. Start from the paramagnetic state ($T > Tc$) and cool the system for at least 100ps.

6. Apply a strong field (3-4T) and check the ground state of the system. You should obtained now skyrmions.

7. Change the ratio between DMI and isotropic exchange, the applied field, anisotropy etc. What effect have these parameters on the skyrmions?

The small system size and critical temperature was chosen in this way that the simulation time is very small. For better results, realistic parameters need to be used.

References

[1] Hongxin Yang, André Thiaville, Stanislas Rohart, Albert Fert, and Mairbek Chshiev. Anatomy of dzyaloshinskii-moriya interaction at co/pt interfaces. *Physical review letters*, 115(26):267210, 2015.

[2] DA Garanin. Self-consistent gaussian approximation for classical spin systems: Thermodynamics. *Physical Review B*, 53(17):11593, 1996.