A classic dipole-dipole model interaction.

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Introduction

The interactions, are the key of any being life. They can arise, interesting and unexpected scenarios, nowadays studied in the subject named complexity. In this report, I reported some results, about the simulation of the classic dipole-dipole magnetic interaction, how a good example of cooperation through simple mathematics rules. I decided to propose some specific cases as summary of this topic, to show effects, such as the sensibility at perturbations and cooperative effects.

The motion equations.

The motion equation, takes in consideration three different interactions. The first interaction is concerning, the classic magnetic dipole interaction described by the hamiltonian terms, reported in the bottom,

$$H_{int} = -\sum_{j>i} \vec{\mu_i} \cdot \vec{B_j} \tag{1}$$

with the magnetic filed equal to

$$\vec{B} = \frac{\mu_0}{4\pi r^3}[3(\vec{m} \cdot \hat{r})\hat{r} - \vec{m}] \tag{2}$$

The second term, is the Heisenberg dipole-dipole, interaction,

$$H_{int} = \sum_{j>i} -J(\vec{r_i} - \vec{r_j})k_1 \vec{S_i} \cdot \vec{S_j} \tag{3}$$

with,

$$J(\vec{r} - \vec{r'}) = \frac{\mu_0 \mu_B^2}{4\pi ||\vec{r_i} - \vec{r_j}||^\alpha} \tag{4}$$

with μ_B the Bohr magneton equal to, $\frac{e\hbar}{2m_e}$. The third interaction is an anisotropic interaction, and it is represented by the following equation:

$$H_{int} = \sum_{j>i} -J(\vec{r_i} - \vec{r_j})k_2 \vec{S_i} \cdot \vec{Sz_j} \tag{5}$$

The motion equation resulting from the mathematics relations written, is the following,

$$\begin{aligned} \dot{\vec{\mu_i}} = \vec{\mu_i} \wedge \sum_{i \neq j} \vec{B_j} + J(\vec{r_i} - \vec{r_j})k_1 \vec{S_i} \wedge \sum_{i \neq j} \vec{S_j} + \\ J(\vec{r_i} - \vec{r_j})k_2 \vec{S_i} \wedge \sum_{i \neq j} \vec{Sz_j} \end{aligned} \tag{6}$$

The equation 5, was solved using RK4 numerical method.

System setting

The spins are placed in a cube, with a virtual grid where the spins can be placed. Into the program it is possible to choose the interaction we want to insert. Several initial conditions, can be set, such as, random spins, all spins in z direction, and a slight perturbation of one dipole in all aligned spins, configuration. The distance between the sites in the grid can be set in nanometers. In all cases considered, it was set with $1\mathring{A}$. The α coefficient was set to 2, whether no specific notes were written. The units used are the seconds for the time, $\frac{J}{T}$ for the bohr magneton and Tesla for the magnetic field, with the grid spaces in meters (in the program the setting is in nm, but converted automatically in m).

Results

The first solution showed, is that one where the spins are aligned in z direction, on a two-dimensional plane excepted one slightly perturbed spin, with the only first interaction switched on (equation 6). The perturbation, carries the system in a disordered configuration, shown in figure 8. The dipole was perturbed slightly, from the z direction, changing the x and y components from zero to 9×10^{-26}. Similar simulation was carried out for the three dimensional case, plotting the total spin components, for the case of all aligned spins in z and comparing it with the single perturbed spin, in the same method used in the first simulation carried out with a 90% of the sites occupied by spins. How the figures 2 and the figure 3 show, after few seconds, we can see the dynamics to be different.This means that the minimal perturbation has a remarkable effect on the evolution of the considered system. This difference is probably the sum of initial perturbation effect and the error propagation, despite RK4 is a stable method. Another interesting case is when the spins initialy are not aligned and they interact by only the second term of the motion equation (the Heisenberg interaction). In this case, the spins rotate, keeping steady the total x,y,z magnetic spins. The third simulation, was split in three different scenarios. All scenarios, started with the aligned spins in z direction, interacting with the two first term of the interactions 6 and with a 90% of the sites occupied by spins. In the first configuration, the coupling coefficient k_1 was set

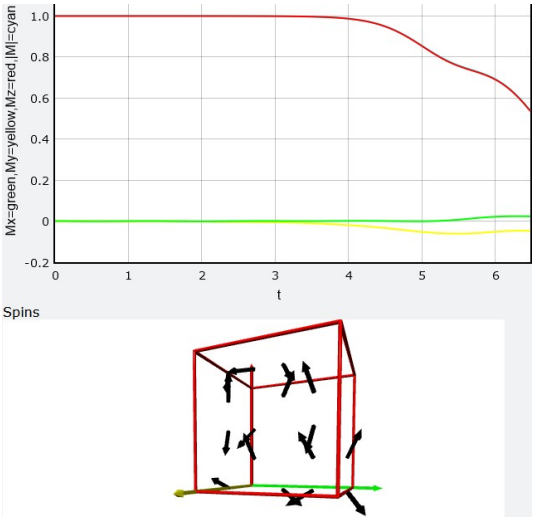

Figure 1: Perturbed single dipole effect on a two dimensional spins system, interacting only by the first interaction of the equation 6.

to 2. With this interaction setting, any spins moved together, moving away from the initial position, but ever pointing in the same direction. This means, that the second interaction, helped the spins to point together in the same direction, giving a cooperating behaivor. Same simulations were repeated, setting the coefficient equal to $k_1 = 1$, obtaining a similar behavior of the previous simulation. Finally reducing the coupling coefficient to $k_1 = 0.5$, they lose the cooperation, starting to point in different directions, how the figure 7 shows. Therefore, we expect a cooperation loss, for a coupling value between 1 and 0.5. The simulation with $k_1 = 2$ was repeated for a time equal to $100s$, showing a rotation of all dipoles of 540 degrees and keeping the same cooperation showed in the previously simulation with same parameters, but running for a shorter time. The fifth simulation was decided to keep on only the second and third terms of the motion equation, starting from a random configuration of spins. In this case the coefficients were set with the values of $k_1 = 2$ and $k_2 = 1$, for two different α values set to 0.1 and 0.5. In the first case, a periodic behavior of the x and y component of the total magnetic dipole moment was observed (figure 9), whereas in the second case it was destroyed after the first 5 seconds (figure 10). This means that a small α, therefore a more intensive interaction allowed the spins to keep a similar behavior, during the simulation.

Technical details

The simulation was coded, with Python allowing us the use of graphs plots and a 3D representation of the dynamics, thanks the Vpython library. The simulations, were carried out on a laptop with 4 Gb ram, and a I7 intel processor. The devices and tools used were enough to reach the wanted goal.

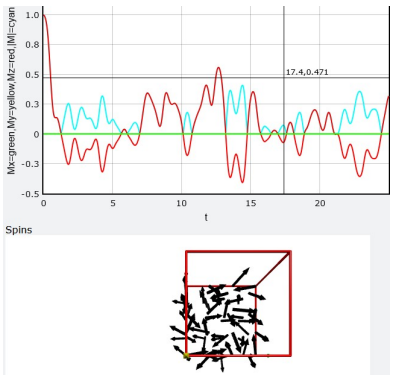

Figure 2: The spins are initially aligned in z direction. The ordered structure is lost almost immediatly, with the only first perturbation on.

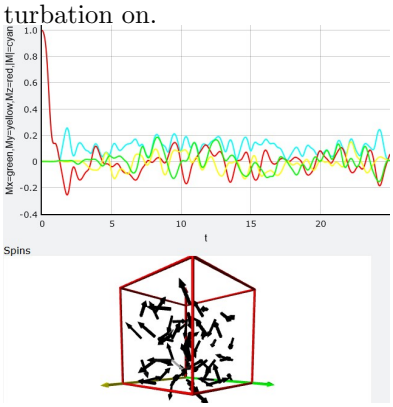

Figure 3: The spins are initially aligned in z direction, with a slighty perturbation on a dipole. The structure results, different after few second, compared the configuration without the perturbation.

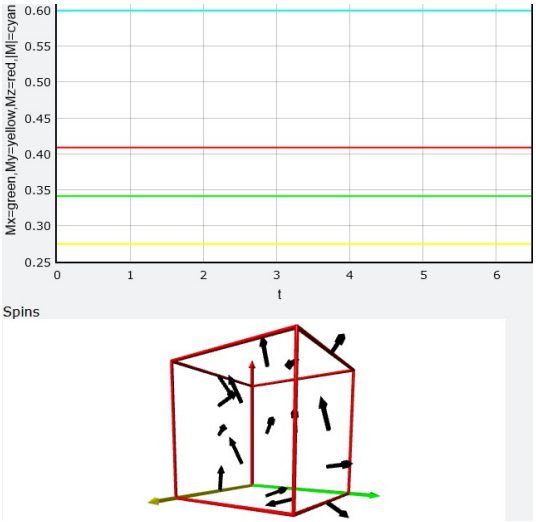

Figure 4: Random spin configuration, interacting by only the second term of the motion equation. In spite of, the movement of the spins, the total components stays steady.

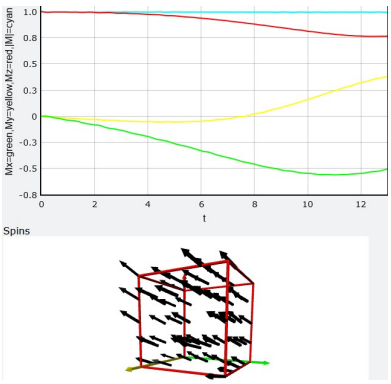

Figure 5: The spins positions after 13 seconds, starting from a completly aligned configuration spins in z direction. The coupling coefficient k_1 was set 2, with $\alpha = 2$.

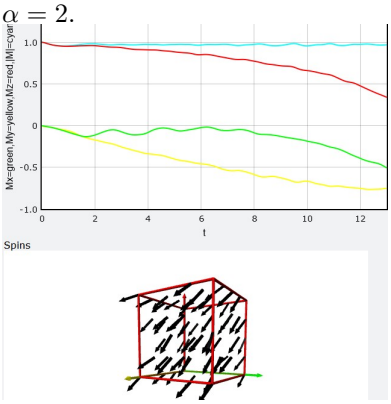

Figure 6: The spins position after 13 seconds, starting from a completely aligned configuration, spins in z direction. The coupling coefficient k_1 was set 1 with $\alpha = 2$.

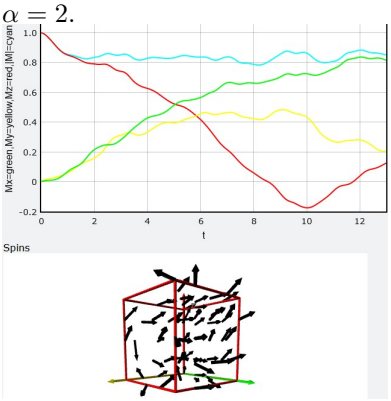

Figure 7: The spins position after 13 seconds, starting from a completely aligned configuration, spins in z direction. The coupling coefficient k_1 was set 0.5 with$\alpha = 2$.

Conclusions

Dipole-dipole interactions were shown how an interesting example of cooperative dynamics. Through this

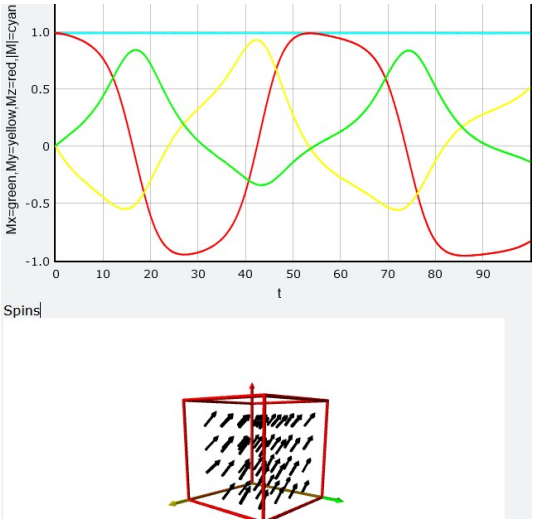

Figure 8: The spins positions after 100 seconds, starting from a completly aligned configuration spins in z direction. The coupling coefficient k_1 was set 2, with $\alpha = 2$.

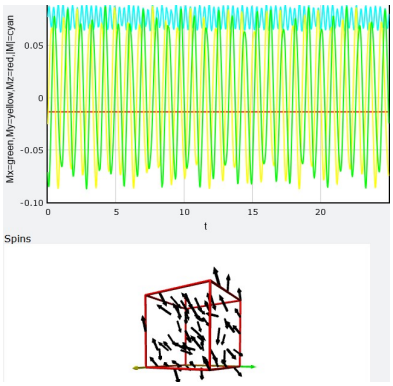

Figure 9: The spins are initially set randomly. The second and third interactions are on with the coefficients set $\alpha = 0.1$, $k_1 = 2$ and $k_2 = 1$.

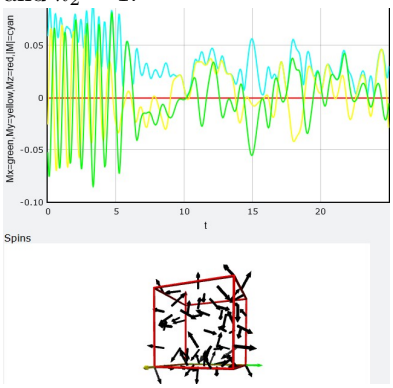

Figure 10: The spins are initially set randomly. The second and third interactions are on with the coefficients set $\alpha = 0.5$, $k_1 = 2$ and $k_2 = 1$.

classic topic of physics studied also from graduating students, we saw some cases where using only simple mathematics rules, coordinated movement were observed. Here only some cases were shown, but other trials can be carried out, modifying parameters, such as, lattice distance or using the same initial conditions and same parameters, perturbing one single dipole and looking for chaotic effects, calculating them by liyauponov coefficient. However, there are no restrictions, on the new interacting terms in addition, trying to find new possible interesting results.

References

[1] https://github.com/paolopoli1980/missp

[2] Ashcroft/Mermim Solid State Physics

[3] Griffiths Electrodynamics