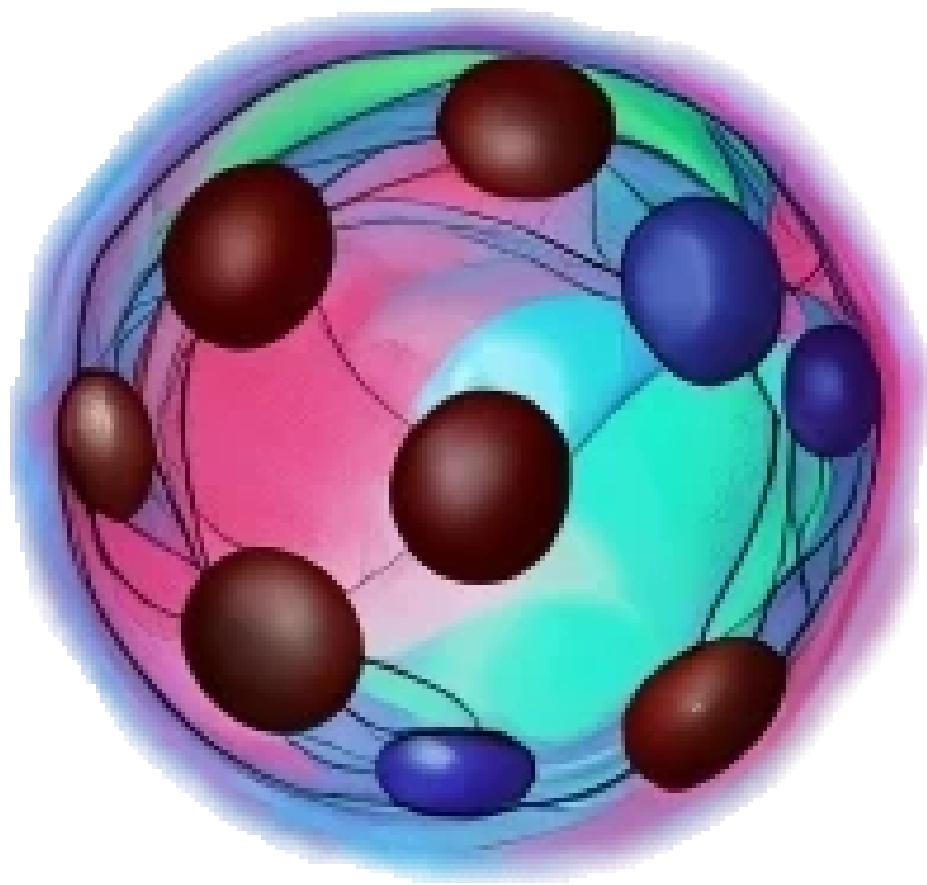


**LOGO**

# Project Spinhamiltapp

**Interactive visualisation of interactions**



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## Abstract

Aspinmate is an interactive program for visualising the influence of the parameters in a Heisenberg model on the figures of merit in the field of molecular magnetism.

The goal of aspinmate is to be user-friendly and provide insights into the underlying theoretical model which comes at the expense of limiting the number of possibilities. Therefore I recommend preferring simple and small systems to isolate the influence of the varying parameters. The video output is, in my opinion, one of the best techniques for tracking changes in the figures of merit as parameters are changing. It includes the most common terms of spin Hamiltonians and offers a wide range of ways to modify them.

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# 1 Getting Started

Aspinmate is available as an open source python script. Therefore you have to install Python in order to use the application if you do not already have Python on your computer. The app should work for python3.7 or newer but surely for python(3.09, 3.10, 3.11, 3.12). For the installation of Python go to <https://www.python.org/> and follow the instructions. If Python is installed you need to download 3 packages: *numpy*, *matplotlib* and *customtkinter*. For users who are new to Python and want to try it on their computer/laptop, the following instructions are a quick guide. Everyone who is already able to install the above packages can skip the following lines.

If you have Python installed you can type `python3 --version` (or maybe just `python`) into your command line to make sure you have installed python on your system. You can now add packages to your Python installation by typing `python3 -m pip install numpy` and after installation repeat that line with `matplotlib` and `customtkinter` (`pip` is a file manager included in Python). If you have the installation confirmation of all 3 packages you are ready to start the program with `python3 aspinmate.py`. (Make sure you are in the directory of the script otherwise change directory: `cd <path to directory>`)

## First Menu



Figure 1.1: First menu of the application. It defines the spins and if dipolar interaction is included.

1. Type in the doubled spin values (in order to be integer values). If you want less than 4 spins just fill the other entries with 0. Remember: calculation time grows rapidly (exponentially) with higher spin numbers and more of them. Keep it small.
2. Here you can include the dipolar interaction. So in the next window you can select the typical length scale of the system.
3. Proceed to the next menu.

## Second Menu



Figure 1.2: Second menu of the application. It defines the structure of your spin system and the video

1. It displays your choice of spins in the most common form.
2. You can choose the distance  $d$  [ $\text{\AA}$ ] (main length scale) of your system. (ring: radius, chain: spacing between consecutive spins, tetrahedron: distance between spins, butterfly: shorter diagonal - longer diagonal is  $1.3 \cdot d$ )
3. Choose the system you want: ring, chain, tetrahedron, butterfly (The latter two only selectable if your system has 4 spins). They are depicted in Fig. 2.1 with their numbering and the Cartesian coordinate system.
4. Choose the variable you want to change throughout the video.  $J_{ij}$ ,  $D$ ,  $\vartheta$  Notice: The ZFS ( $D$ ,  $\theta$ ) has NO qualitative effect on the figures of merit on spins with  $s = 1/2$ .
5. How much do you want to change the chosen variable? The starting point will be selected in the next window, e.g. initial value=-5 and range=10  $\rightarrow [-5, 5]$
6. The number of frames that are produced. Normal range: (50-100). (Choose one more to get nice values, i.e. 51,61,101,... Remember: This has an impact on the calculation time (linearly))
7. Proceed to the next menu

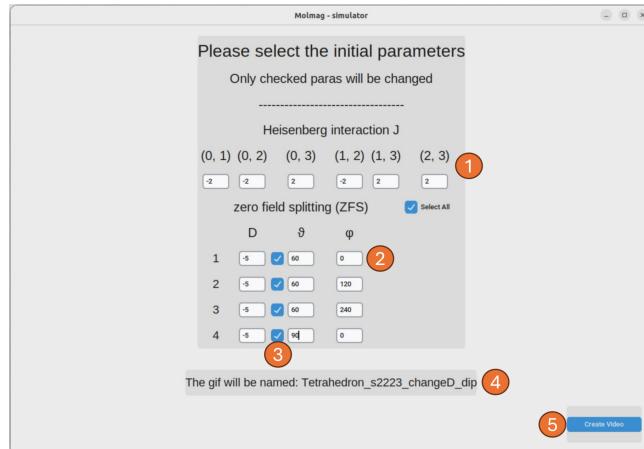


Figure 1.3: Third menu of the application. It defines the initial values for the parameters

### Third Menu

1. Fill in the initial exchange interactions [Kelvin]. The above describes which spins interact beginning with 0 for the first spin <sup>1</sup>. Notice: Too big values can result in a numerical overflow and hence in an error. S
2. Fill in the zero field splitting (ZFS) [Kelvin] in spherical coordinates with angles in degrees [°].  $D < 0$  for an easy axis along  $\epsilon_i(\vartheta, \varphi)$ . The figures of merit all point in z-direction which is equal to  $\vartheta = 0$ . Therefore rotating everything with  $\varphi$  around the z-axis does not change anything in the output. A placeholder value of 0 appears if  $s = 1/2$  because ZFS has no influence in that case
3. The tick boxes appear next to the variables you have chosen to change (in the 2. menu). Select all to change all variables simultaneously, or select only a few changes while the others stay fixed.
4. The name of the gif is generated automatically and appears in the subfolder *spin\_gifs* of the folder with your python script. An equally named text file is also created in that subfolder. There you can look up all the parameters you have chosen.
5. This button creates the video (after clicking the pop-up window). The window is then frozen until the calculation finishes. You can interrupt it by pressing the X-button. (It may appear that Windows shows a warning: *no response*, but the application is still calculating in the background. If you are irritated by that try a very small system to proof that it is calculating.)

<sup>1</sup>Because i bowed down to the conventions used by the computer scientists I discuss too much with.

When the calculation finishes you will get the message 'Video created!' in the window. Now you can close the application and take a look at your produced video in the subfolder. If you are quite familiar with the programming language Python, you can take a look at the Jupyter notebook. You are welcome to modify the notebook to further increase the number of possibilities for the GIF creation.

### 1.0.1 The output

When playing the GIF you see an output looking like Fig. 1.4. This is a small ferromagnetic dimer with  $\vec{s}_i = 1$  and easy axis that are aligned nearly perpendicular. You can see 4 figures of merit of the investigated spin system in equilibrium, namely the zeeman diagram, entropy difference, magnetisation and susceptibility

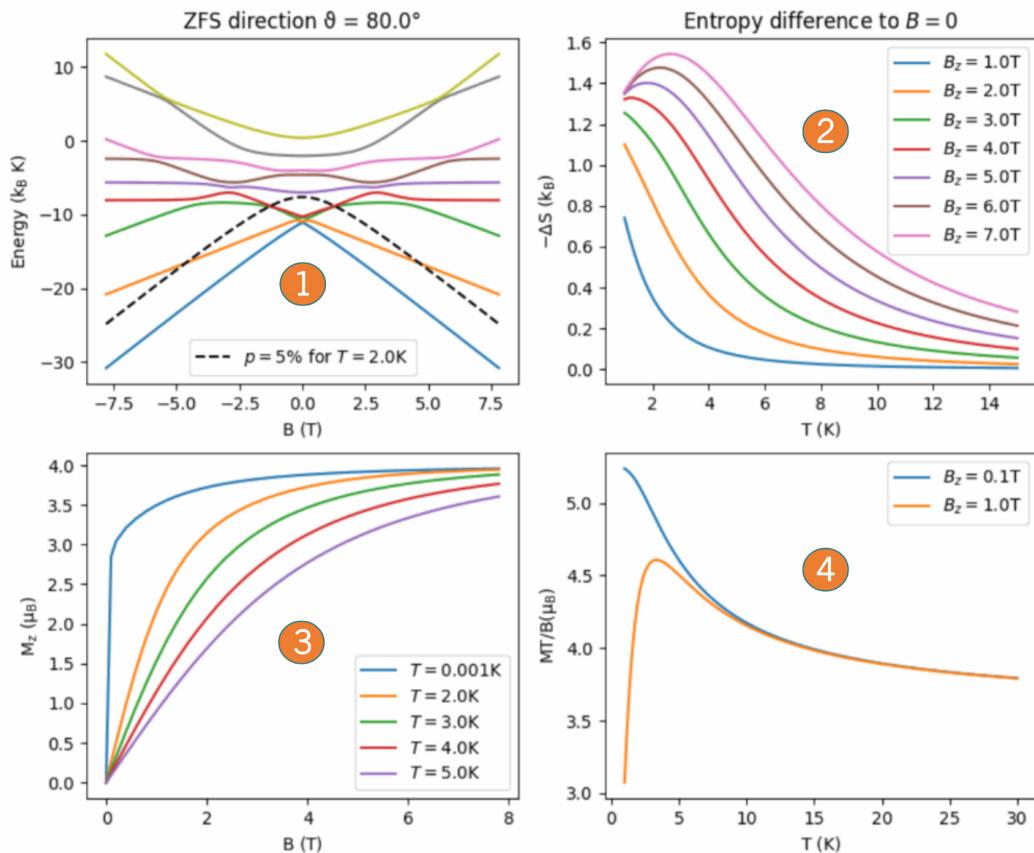


Figure 1.4: A possible output of aspinmate. System is a  $\vec{s}_i = 1$  dimer where one of the anisotropy axis (easy axis with  $D_0 = D_1 = -5\text{ K}$ ) is tilted away by  $\theta_1 = 80^\circ$  from the z-direction and the other one aligned to the z-axis ( $\theta_2 = 0$ ). The exchange interaction is  $J_{12} = -2\text{ K}$  (ferromagnetic).

1. The zeeman diagram where the dashed line indicates the probability of occupancy of 5% at a temperature  $T = 2$  K (cf. Eq. 2). Following illustration shows the colour sequence and therefore the colour of the  $i$ th state beginning at  $i = 0$  for the ground state.



The graph shows the 16 lowest energy eigenvalues or all eigenvalues if the Hilbert space dimension is smaller.

2. The entropy difference  $-\Delta S(T, B)$  in units of the Boltzmann constant  $k_B$  plotted against the temperature. It is plotted for every integer magnetisation till  $B_z = 7$  T.
3. The magnetisation  $M$  in z-direction plotted against the magnetic field for 5 different temperatures  $\{0.001, 2, 3, 4, 5\}$  K.  $M$  is plotted in units of the Bohr magneton  $\mu_B$ .
4. The approximate susceptibility (times temperature)  $\frac{M}{B}T$  in z-direction plotted against the temperature. It is plotted for  $B = \{0.1, 1\}$  T. Remember that this resembles the differential  $\chi T$  curve only if the slope is linear from  $B = 0$  T to  $B = \{0.1, 1\}$  T.

## 2 Theoretical scope

The model used in aspinmate is the heisenberg model for spins where the indices  $i, j$  can run from 0 to  $spincount - 1$ .

$$\begin{aligned} \tilde{H} = & \sum_{i < j} J_{ij} \vec{s}_i \cdot \vec{s}_j + \sum_i D_i (\vec{e}_i \cdot \vec{s}_i)^2 + g\mu_B \vec{B} \sum_i \vec{s}_i \\ & + \frac{\mu_0(g\mu_B)^2}{4\pi} \sum_{i < j} \frac{1}{r_{ij}^3} (\vec{s}_i \cdot \vec{s}_j - 3\vec{s}_i \cdot \vec{e}_{ij} \otimes \vec{e}_{ij} \cdot \vec{s}_j) \end{aligned}$$

The first term is the (Heisenberg) exchange interaction in which a  $J < 0$  corresponds to a ferromagnetic interaction,  $J > 0$  corresponds to an antiferromagnetic interaction, respectively. The sum is chosen such that every interaction is counted just once. The zero-field splitting in the second term is restricted to a simple hard or easy axis, depending whether  $D > 0$  or  $D < 0$ . The  $\vec{e}_i$  defines the global direction of that axis and has to be plugged in in spherical coordinates. The third term describes the zeeman splitting of the system where  $g = 2$  is fixed for the sake of simplicity. The last term describes the dipolar interaction where  $\mu_0$  is the vacuum permeability and  $r - ij$  is the connecting vector of the spins  $i$  and  $j$  in angstrom [Å]. The dipolar interaction is the term introducing the position of the spins to the model. Therefore the chosen system (spin arrangement) without dipolar included just indicates which spins are interacting with each other and a collective (global) rotation around the z-axis does not change any physical property (cf. [1]).

The probability cutoff line in the zeeman diagram shows the probability of occupancy 5% for  $T = 2$  K. This should help the user to estimate the number of energy levels contributing to the thermodynamic properties. The probability cutoff is defined by

$$\text{co}(T, P)/k_B = T(-\ln(P) + \ln(Z)) \quad (2.1)$$

where  $k_B$  is the Boltzmann constant,  $P$  is the probability and  $Z$  is the canonical partition function given by

$$Z(T, B) = \text{Tr}(e^{-\beta \tilde{H}}) = \sum_{\nu} e^{-\beta E_{\nu}}. \quad (2.2)$$

$\beta = 1/(k_B T)$  is the inverse temperature and  $E_{\nu}$  are the eigenvalues of the Hamiltonian. The magnetic field restricted to a scalar notation here because aspinmate just includes homogeneous magnetic fields in z-direction. From the partition function we can derive the thermodynamic

observables via the Gibbs free energy

$$G(T, B) = -k_B T \ln(Z(T, B))$$

which gives rise to

$$S(T, B) = -\frac{\partial G(T, B)}{\partial T} \quad (2.3)$$

$$M(T, B) = -\frac{\partial G(T, B)}{\partial B} \quad (2.4)$$

$$\chi(T, B) = -\frac{\partial^2 G(T, B)}{\partial T^2} = \frac{\partial M(T, B)}{\partial B}. \quad (2.5)$$

Due to the numerical instability of derivatives aspinmateis implemented using the summation expressions

$$S(T, B) = -\frac{1}{ZT} \sum_{\nu} E_{\nu} e^{-\beta E_{\nu}} + k_B \ln(Z) \quad (2.6)$$

$$M(T, B) = -\frac{g\mu_B}{Z} \sum_{\nu} M_{\nu} e^{-\beta E_{\nu}} \quad (2.7)$$

$$\chi(T, B) = \frac{(g\mu_B)^2}{k_B T} \left[ \frac{1}{Z} \sum_{\nu} M_{\nu}^2 e^{-\beta E_{\nu}} - \left( \frac{1}{Z} \sum_{\nu} M_{\nu} e^{-\beta E_{\nu}} \right)^2 \right] \quad (2.8)$$

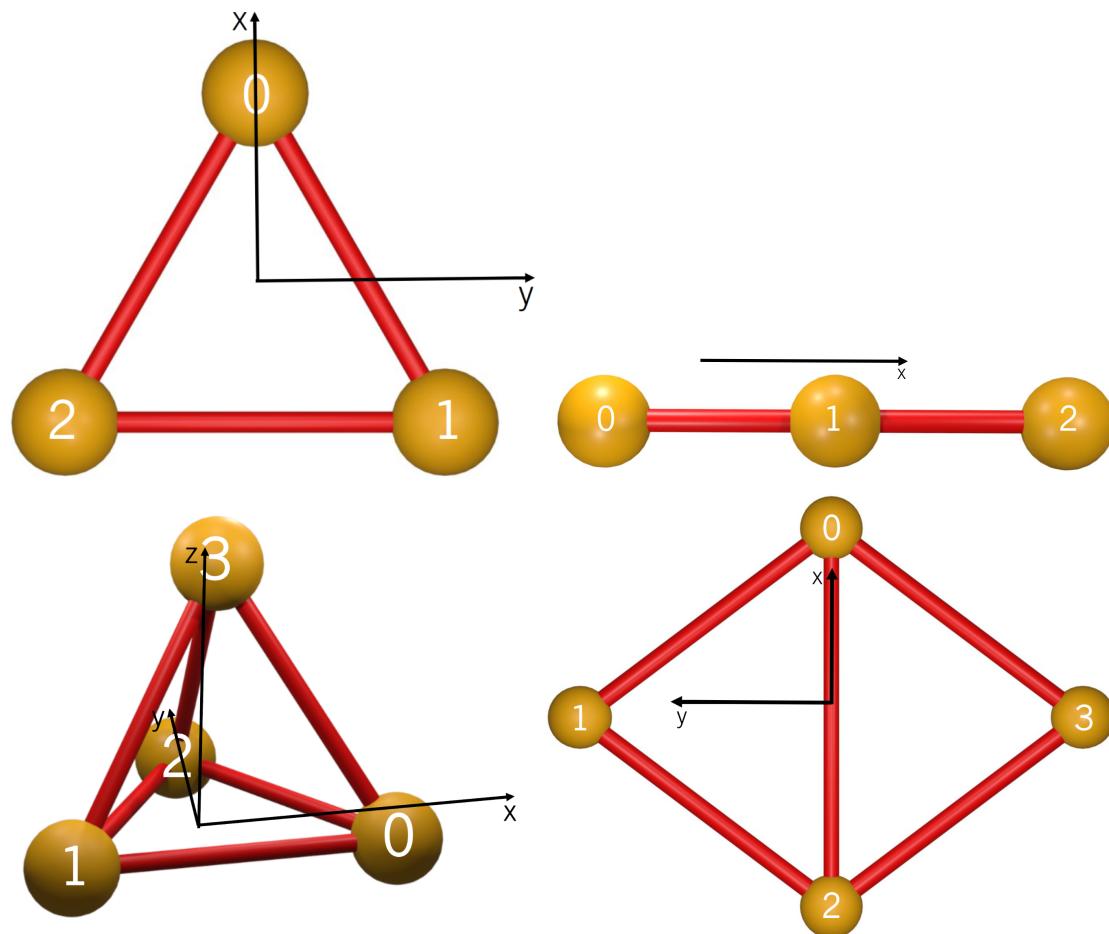


Figure 2.1: The 4 possible structures with the numbering of the spins and the coordinate system are indicated by the important axes. The spins are coloured brown and the exchange interactions are coloured red.

## Bibliography

- [1] D. Pister, K. Irländer, D. Westerbeck, and J. Schnack, “Toroidal magnetic molecules stripped to their basics,” *Physical Review Research*, vol. 4, p. 033221, Sept. 2022.