One Dimensional Spin Dynamics Simulation

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April 12, 2017

Introduction

For this project a one-dimensional spin dynamics simulation was carried out with a lattice of size L and periodic boundary conditions. At each site of the lattice there was a classical spin vector with unit length such that $|\vec{S}_i| = 1$. The size of L was determined by the quantity of spins used for each simulation, i.e. for 10 spins L = 10. Each spin interacted with its nearest-neighbors via the Hamiltonian:

$$H = -J \sum_i \vec{S}_i \vec{S}_{i+1}$$

Here $\vec{S}_i$ is the dimensionless unit spin vector at site *i*, $\vec{S}_{i+1}$is the nearest-neighbor of $\vec{S}_i$, and J the interaction parameter that describes the interaction of the spin system (ie. Antiferromagnetic or ferromagnetic). Utilizing this Hamiltonian, a spin-dynamics program was created to model and determine the time-displaced nearest-neighbor spin-spin correlation functions at temperature, T = ∞.

The equation of motion that determines the rotations of the spins in time is given by:

$$\frac{d\vec{S}_i}{dt} = -\vec{S}_i \times \vec{H}_{eff}$$

Once again $\vec{S}_i$is the dimensionless unit spin vector at site *i*, and $\vec{H}_{eff}$ is the effective field of nearest neighbor interactions acting upon $\vec{S}_i$. $\vec{H}_{eff}$ is given by the formula:

$$H^K_{eff} = -J \sum_{j=NN(i)} S^K_j$$

Here K describes the Cartesian component in consideration (either x, y, or z), $S^K_j$is the nearest-neighbor (NN(i)) of spin i, and J is once again the interaction parameter.

Using this equation of motion, multiple simulations were carried out for different step times and lattice sizes then compared using the time-displaced nearest-neighbor spin-spin correlation function and dynamic structure factor, S(**q**,w).

Methods

To create the lattice, values where chosen for the x-,y-, and z-components of each spin by randomly generating a value between -1 and 1 using the Box-Muller transform and then normalized to be of unit length. Integration was performed by taking the Taylor series expansions of $\vec{S}(t+\tau)$, such that:

$$\vec{S}(t+\tau) = \vec{S}(t) + \frac{d\vec{S}(t)}{dt}\tau$$

Here τ is the time step for integration which was changed throughout the project and compared in the results section. Careful note was taken when choosing the time step. If the time step is too big then the change in the spin-components might be too large causing a translation of the component instead of a smooth rotation. This translation will cause the length of the spin vector to increase.

After the integration was complete the time-displaced nearest-neighbor spin-spin correlation function was determined for each simulation. The function is determined by the following formula:

$$C^K(r-r',t) = < S_i^K(0) S_{i+r'}^K(t) > \; - < S_i(0) >< S_{i+r}(t) >$$

Here <…> represents an ensemble average and K is the x-,y-, and z-components of the spin. The first term is an ensemble average over the time correlation of nearest neighbors. Each time ensemble average can be further averaged by changing the when time of the initial S(0), making the statics more robust. Furthermore, the x-,y-, and z- components in this one dimensional simulation should all show the same correlations and can be used in the correlation function averages.

From the correlation function the Dynamic Structure Factor can be determined. The Dynamic Structure Factor is a Fourier transform over time and space of the correlation function. The Dynamic Structure Factor is given by the following formula:

$$S^K(\vec{q},w) = \sum_{r,r'} e^{q(r-r')} \int_{-tmax}^{tmax} e^{iwt}\, C^K(r-r',t)dt$$

Here **q** is the wave vector defined by $\vec{q} = \frac{2\pi n}{L}$ where n ranges from -L to L, w is the frequency, and (**r**-**r'**) is the separation distance between two spins which is always 1 for the purposes of this project. The integral ranges from -tmax to tmax to account for the sliding window over which the time and space correlation function is averaged. Since this project is for a one-dimensional chain the vector **q** and the separation vector (**r**-**r'**) are parallel to each other.

Results

For each plot in the results section a total of five separate trails were run to calculate the correlation function. The mean of the five trails was found and error bars representing one standard deviation from this mean were also plotted. The proximity of the error bars in these plots seem to form one thick solid line but in the center of each a darker line can be seen which represents the mean value. The Dynamic Structure Function plots where determined from the mean values of each correlation function.

The first three plots (**Figures 1-3**) each show simulations for the time step t = 0.1, each with different numbers of spins, 10, 24, and 74 respectively. Each of the Correlation Function plots show the same general trend. Each simulation begins with a mean correlation value near or less than 0. This is expected since the starting positions for the spin components where chosen randomly. The correlation values then begin to rise abruptly at the beginning of the functions as the effective fields of the neighboring spins begin to affect each other causing the time steps to become more correlated. The max values of **Figure 1-3** correlations are 0.1505, 0.1897, and 0.2088 respectively. After each correlation function reaches its maximum it then begins to trail off toward zero again as correlation due the effective fields begin to lessen. Random fluctuations in the correlation can be seen along the tail end of the functions due to the temperature of the simulation being infinite.

Overall, we see that with larger time separations the spins are uncorrelated with a lack of periodicity in the correlation function. By increasing the number of spins we see an increase in the maximum correlation value and a decrease in error. The average standard deviation from each is 0.0328 for **Figure 1**, 0.0284 for **Figure 2**, and 0.0272 for **Figure 3**.

In the accompanying dynamic structure factor (**q** = 2π) plots we see no peaks in the middle of the plots due to a lack of periodicity in our correlation function. The peaks at either end of the plots are due the correlation function not smoothly reaching zero on both ends of the plot, effectively being a FFT of a step function.

The last figure (**Figure 4**) shows the correlation function and dynamic structure factor for a spin chain simulation of 10 spins but with a reduced time step of t = 0.01. This was done to compare how the step size in integration effects the overall simulation. The correlation function plot in **Figure 4** shows the same trend as the previous correlation function plots, an increase from zero to a max of 0.1606 then a trailing off due to equilibrium. This simulation showed the greatest average standard deviation of all with a value of 0.0924, compared to the larger time step of t = 0.1. Again, in the accompanying dynamic structure factor (**q** = 2π) plot we see no peaks due to a lack of periodicity in our correlation function.

Figure 1: L = 10, TimeStep = 0.1

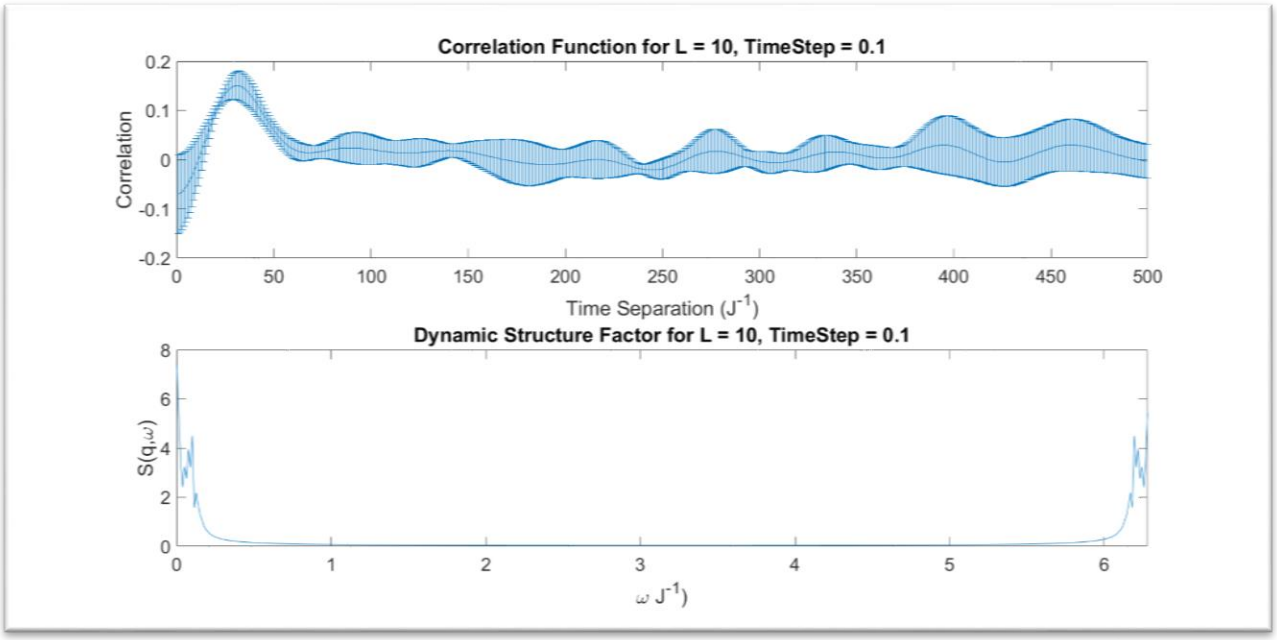

Figure 2: L = 24, Time Step = 0.1

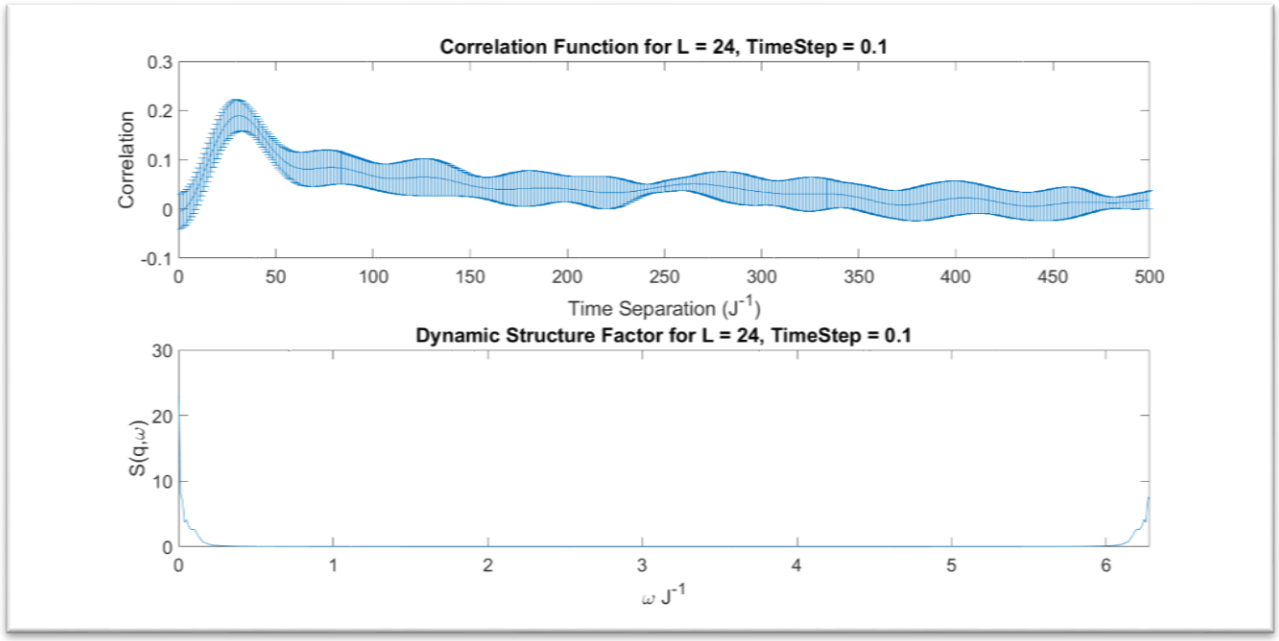

Figure 3: L = 74, Time Step = 0.1

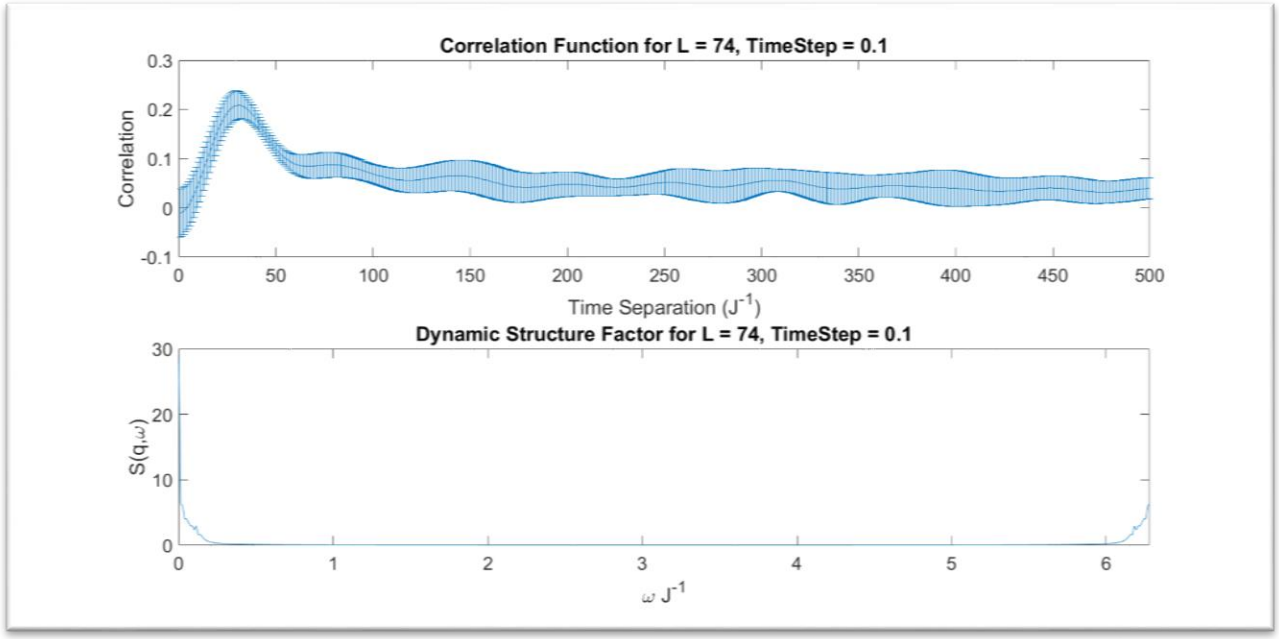

Figure 4: L = 10, Time Step = 0.01