PH-566 ADVANCED SIMULATION TECHNIQUES

COURSE PROJECT ON ISING MODEL

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1 Introduction to Ising Model

Ising Model named after Ernst Ising is a model to describe and study phase transitions. It can be feromagnet-paramagnet transitions or even water-steam transitions. It consists of a lattice of N-Dimensional grid where spins are arranged either in up or down configurations i.e $\uparrow$ *or* $\downarrow$,generally represented as $+1$ *and* $-1$for computational purposes.Ising model is used to simulate magnetic systems. The general Hamiltonian of ising model is given as:

$$H = \sum_{<i,j>} J_{ij}\sigma_i\sigma_j \; - B\sum_j \sigma_j \tag{1}$$

The first summation considers nearest neighbor interaction between spins and J_{ij} is coupling constant. The second term indicates summation over spins along entire lattice and B is the applied magnetic field. Depending on the spin coupling constant J_{ij} the system can be ferromagnetic or anti-ferromagnetic.

1. If $J_{ij} > 0$,the system is ferromagnetic and the neighbouring spins will tend to align in same direction.
2. If $J_{ij} < 0$,the system is anti-ferromagnetic and the neighbouring spins will tend to align in opposite direction.
3. If $J_{ij} = 0$, no interaction trivial case.

In general we analyse system without applied magnetic field, so the B term drops out of the equation. Thus, final Hamiltonian looks

$$H = \sum_{<i,j>} J_{ij}\sigma_i\sigma_j \tag{2}$$

1.1 Solutions to the Ising Model

Since the model was developed in 1924, a lot of solutions have been there. Ising model can be solved using analytical methods, approximation methods such as Mean Field Theory approaches, numerical(Monte-Carlo methods) etc. Depending on the dimesnion of Ising Model(eg 1-D,2-D..) the complexity of solution also increases. In analytical methods we use Transfer Matrices to find partition function Z and using that we find all other parameters. In mean field approach we consider each spin in an average environment of neighboring spins. We consider a statistical average and deduce further results. But this method doesn't consider correlations and other interactions, hence it is not reliable all times. The Monte-Carlo method is an intuitive and statistical method which uses concepts of probability. Here we start with a random system and tries to minimized its energy by generating random numbers.

We consider the simple case of 1-D Ising Model. As the name says here we have a linear chain of spins. This is the most simple case among all. We will briefly discuss the analytical solution of 1-D Ising model and its important properties. Let us denote partition function Z. In order to find transfer matrix we need to expand Z. We do two simple approximations:

1. We consider periodic Boundary condition where $S_N = S_{N+1}$, thus converting a linear chain into a circular ring.
2. We consider the coupling constant J_{ij} is same for all.

$$Z = \sum_{s_1=-1}^{+1}\sum_{s_2=-1}^{+1} \dots \sum_{s_N=-1}^{+1} \exp(-\beta H\{S_i\}) \tag{3}$$

$$Z = \sum_{s_1=-1}^{+1}\sum_{s_2=-1}^{+1} \dots \sum_{s_N=-1}^{+1} \exp\left[\beta \sum_{i=1}^{N} (JS_iS_{i+1} \; + \; BS_i)\right] \tag{4}$$

After performing summation and some simplifications we get the following form,

$$Z = Tr\,(P)^N \tag{5}$$

where P is given by

$$\begin{pmatrix} e^{\beta(J+B)} & e^{-\beta(J)} \\ e^{-\beta(J)} & e^{\beta(J-B)} \end{pmatrix} \tag{6}$$

By solving the eigenvalues of Z, we get

$$\lambda_{\pm} = e^{\beta J}\left[\cosh(\beta B) \pm \sqrt{\cosh^2(\beta B) - 2e^{-2\beta J}\sinh(2\beta J)}\right] \tag{7}$$

Now when we consider the theromodyncamic limit, i.e $N \to \infty$ only the larger eigenvalue $\lambda_+$is relevant.We will show this by considering the Helmholtz-Free energy F.:

$$-\frac{F}{Nk_BT} = \lim_{N\to\infty}\frac{\ln Z}{N} = \ln\lambda_+ \tag{8}$$

Thus Helmholtz-Free energy is given by:

$$\frac{F}{N} = -k_BT\ln\lambda_+ = -J - k_BT\ln\left[\cosh(\beta B) \pm \sqrt{\cosh^2(\beta B) - 2e^{-2\beta J}\sinh(2\beta J)}\right] \tag{9}$$

We can find other parameters like magnetization as follows,

$$m = \frac{M}{N} \tag{10}$$

$$= \frac{1}{\beta N}\frac{\partial \ln Z}{\partial B} \tag{11}$$

$$= \frac{sin(\beta B)}{\sqrt{\cosh^2(\beta B) - 2e^{-2\beta J}\sinh(2\beta J)}} \tag{12}$$

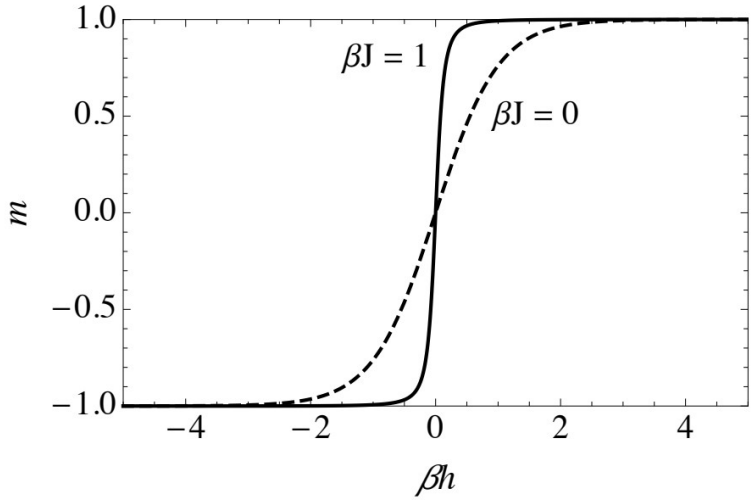

Figure 1: Magnetization per spins vs βB
Image Source: Web. Note: Here B=h

When field is zero, (B = 0), we can see the magnetization is zero for all temperatures. In order to get $0K$ case we can do an expansion of the terms and drop lower order contributions. This means that there is no spontaneous magnetization in 1-D Ising model and it never exhibits ferromagnetism. This is because, the average confiiguration is determined by two opposite and competing tendencies, at any temperature: The tendency towards a complete alignment of spins to minimize the energy, and the tendency towards randomization to maximize the entropy due to thermal fluctuations. The over-all tendency is to minimize the free energy $F = E - TS$. For the 1-D model the tendency for alignment always loses out, due to lack of nearest neighbour interactions. . But, in higher dimensions, there are enough nearest neighbours and a ferromagnetic transition can take place. The trasnfer matrix of a 2-D Ising Model can be found out similarly. But the computation of matrix is quite tedious compared to one dimesnion. So approximation and simplification is necessary. 2-D Ising model have phase transition since it has more number of neighbors compared to 1D, hence it can align overcoming thermal fluctuations.

1.2 Finding Parameters

Once the system is solved we can find all desirable

1. Magnetization:
$$M = \frac{1}{N}\sum_{i=1}^{N}\langle S_i\rangle = -\frac{1}{N}\frac{\partial F}{\partial H} \tag{13}$$
2. Magnetic Suscceptibility:
$$\chi_T = \frac{\partial M}{\partial H}\,|_T = \beta\left(\langle M^2\rangle - \langle M\rangle^2\right) \tag{14}$$

2 Metropolis Algorithm for the Ising Model

We employ the Metropolis algorithm for evolving the 1D and 2D Ising model. The algorithm for 2D is mentioned (can be easily simplified for 1D) below:

- Generate a random array B of size, say n x n with elements 1 or -1 where +1 represent up spin and -1 represent down spin.
- Randomly select a site (i,j) on the array.
- Determine $\Delta E = E_f - E_i$ for the chosen site, using given Hamiltonian. Here, we consider only nearest neighbour interaction.
- Now, if $\Delta E \leq 0$ then flip the spin i.e $B(i,j) \rightarrow -B(i,j)$.
- If $\Delta E > 0$, then spin flips with some probability $e^{\frac{-\Delta E}{K_b T}}$. In order to compute this, generate a random number $r \in (0,1)$, if $r < e^{\frac{-\Delta E}{K_b T}}$ then $B(i,j) \rightarrow -B(i,j)$ else, don't flip.
- Above steps constitute one event, repeat above steps for large number of iterations. After enough iterations system reaches a state of an equilibrium.
- Calculate the physical quantities from the final state. We calculate magnetization and susceptibility, $< M >= \sum_{i,j}\frac{B(i,j)}{N^2}$ and $\chi =< M^2 > - < M >^2$ respectively.

We determine the magnetization and susceptibility for a range of temperature $T \in (0,5)$ in order to see if the phase transition occurs and consequently determine the critical temperature.

However, we faced few challenges in terms of computation which are as follows:

- For small system sizes like 10 X 10 for 2D, magnetization and susceptibility curves with temperature are not very smooth. In order to overcome that we took average of the same for many random initial configurations which does take more time to compile but renders smooth curve which can easily show a phase transition in 2D (as discussed in next section).
- Since J > 1 (coupling constant), we expect our system to align with time, this is readily observed from results as magnetization goes to +1 or -1. But we can't predict if it aligns upwards or downwards. Thus, when we take average over many initial configurations we see that for low temperature T < 1, the average is somewhere between (-1, 1) usually around 0.4. Therefore, we have plotted our graphs for T ∈ (1,5) only.
- For different sizes of systems we have to determine number of iterations in order to attain equilibrium. As expected, we need more iterations for larger system compared to smaller one.

We have averaged the observable for 1000 initial configurations and consequently plotted the graphs using origin.

3 Results and Discussions

3.1 For 1-D Ising Model

For a one-dimensional case ,a linear chain of N=10 sites with arbitrary oriented spins is taken and executed by the metropolis algorithm(Random Walk Metropolis (RWM) is one of the standard Markov algorithms in Monte Carlo).Plotting has been done using origin.We analyze two important parameter

(1)Average magnetisation per spin Vs steps

(2)Average magnetization per spin Vs temperature

3.1.1 Average magnetisation per spin vs Steps

After each step,The graphic indicates that the system's spin alignment gradually increases and leads to an equilibrium state with the least amount of energy. During this process, the initially disordered domains align with each other, and after a specific number of steps, we obtain average constant magnetization.

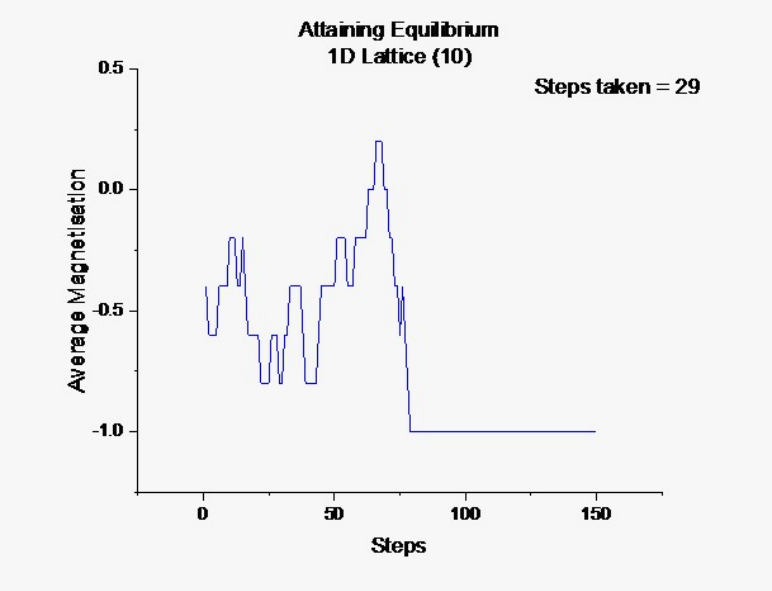

Figure 2: Average magnetisation per spin Vs Steps

Initially, the average magnetization per spin is fluctuating rapidly as the number of steps increases the average magnetization attains a constant value as expected in theory.It took nearly 29 steps in order to attain constant value as lattice point increases the system will take more steps.

3.1.2 Average magnetization per spin vs Temperature

The graph has been plotted at different temperatures against average magnetization per spin.

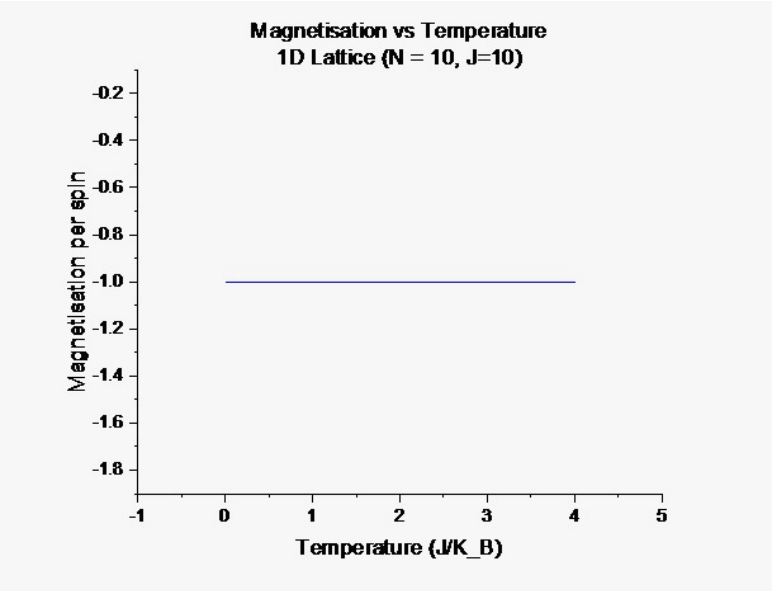

Figure 3: Average magnetization per spin Vs temperature

Theoretically, the average magnetization per spin is constant(1 or -1). Hence there is no phase transition. The susceptibility chi is zero. From the graph, we can see the same i.e no phase transition

3.2 For 2-D Ising Model

3.2.1 Average Magnetisation vs Steps

For a two-dimensional square lattice, an N*N matrix (Here, N=10) matrix with randomly oriented spins is taken and implemented by the metropolis algorithm as given in previous sections. Then after each iteration, the average magnetization per spin is taken down and is plotted against the number of iterations. As the system gets updated after each iteration, the plot signifies that the alignment of spins of the system increases gradually and leads to an equilibrium state, which is the state with maximum alignment. In this process, the domains, which were disordered initially, get aligned with each other and give a resultant non-zero magnetization. The plot is as shown below:

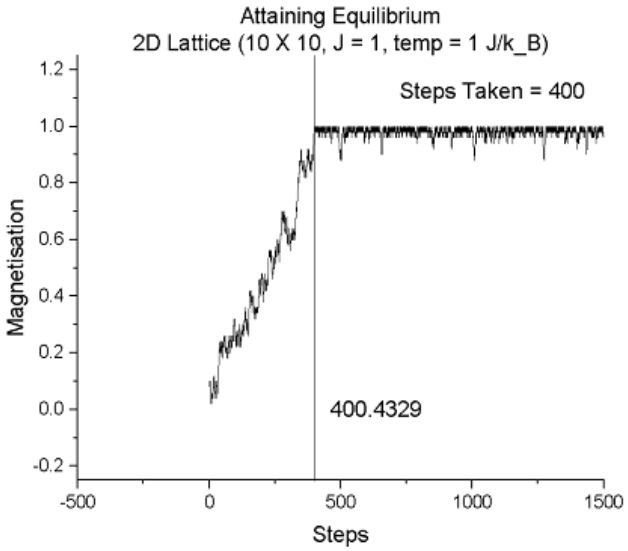

Figure 4: Average Magnetisation per spin vs. steps

From this plot, the required number of sweeps to reach equilibrium for a given size of the initial matrix can be determined and, in this case, found to be 400 for a 10*10 matrix. A larger matrix size requires more sweeps to reach equilibrium and more extensive computation time.

3.2.2 Average Magnetisation vs Temperature

Now repeating this whole process for different values of temperature going from 1 to 4 J/K_B and then plotting the average magnetization with temperature, we get the plot shown in the figure below:

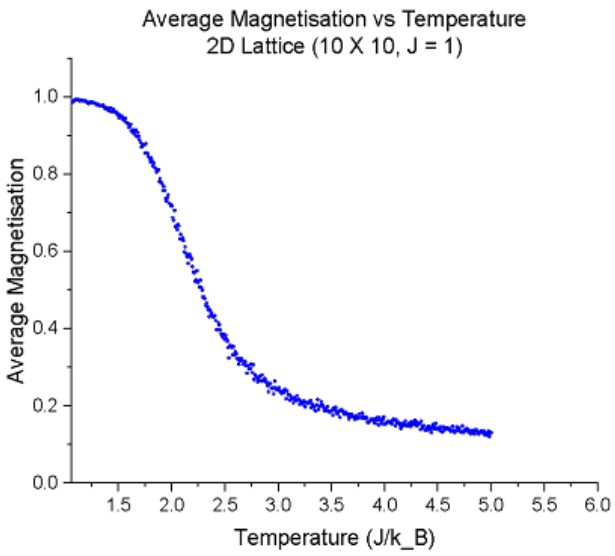

Figure 5: Average Magnetisation per spin vs. temperature

The magnetization value is nearly identical initially, but after reaching a point, it decreases abruptly and approaches zero. This phenomenon can be understood by the fact that increment in the temperature increases thermal motion and hence, leads to disruption in the alignment of the domain, making them disordered. For temperature values higher than T_c, the magnetization remains very small(nearly equal to zero), which shows that the material has undergone a phase transition and has become paramagnetic. The Curie temperature T_c at which this phase transition occurs and below which the material is ferromagnetic is found to be approximately 2.59299 J/K_B. The Curie temperature can be calculated precisely by increasing the system size and number of steps and taking smaller temperature steps.

3.2.3 Average Susceptibility vs Temperature

Along with the average magnetization, the magnetic susceptibility for a series of temperatures is also noted and plotted with temperature. Before the Curie temperature, the susceptibility X grows, reaches a maximum, and then after reaching T_c, it starts to drop gradually.

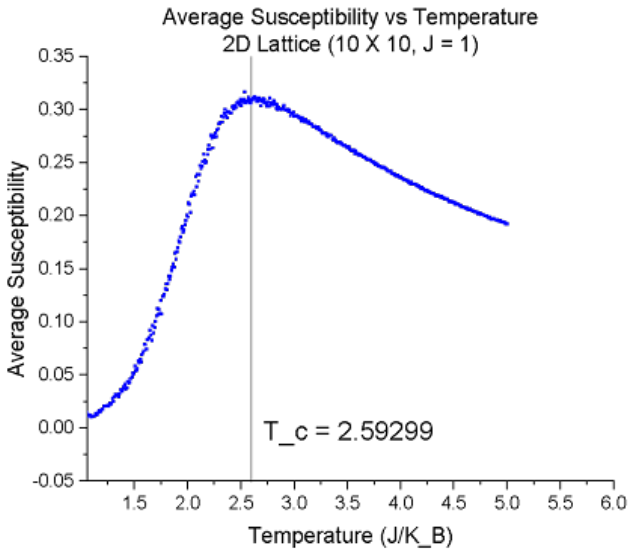

Figure 6: Magnetic Susceptibility vs. temperature

3.2.4 Results for 20×20 Lattice

Now above results for an initial 20*20 matrix is shown:

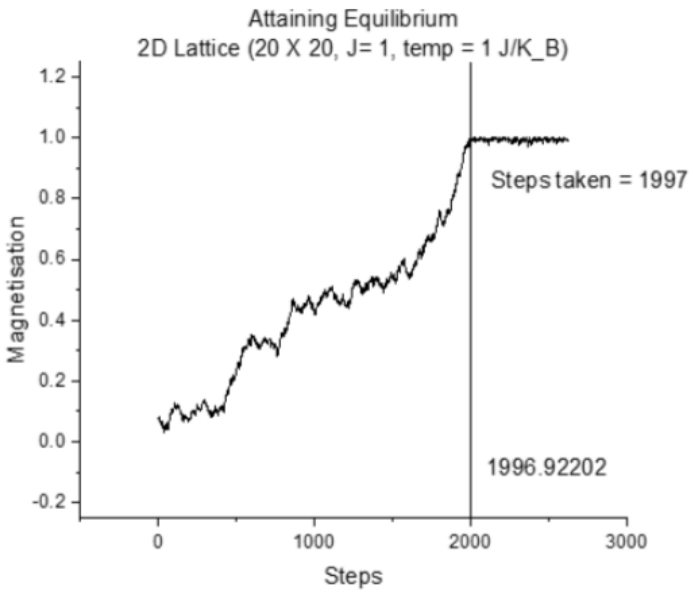

Figure 7: Average Magnetisation per spin vs. steps for 20*20 matrix

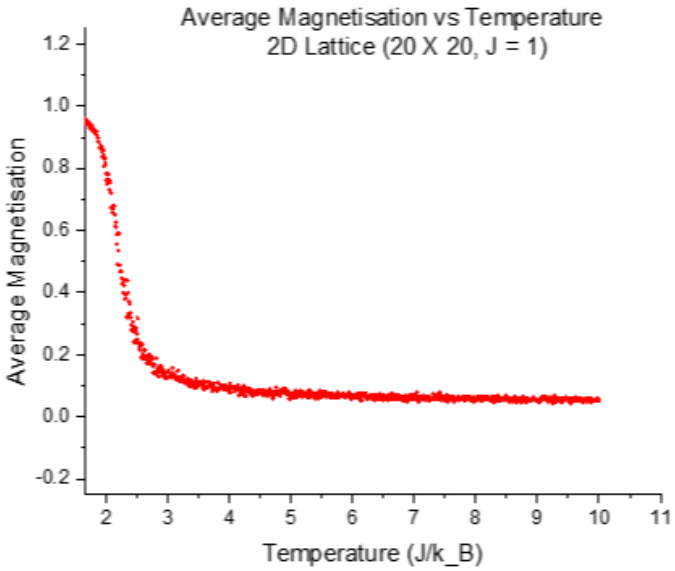

Figure 8: Average Magnetisation per spin vs. temperature for 20*20 matrix

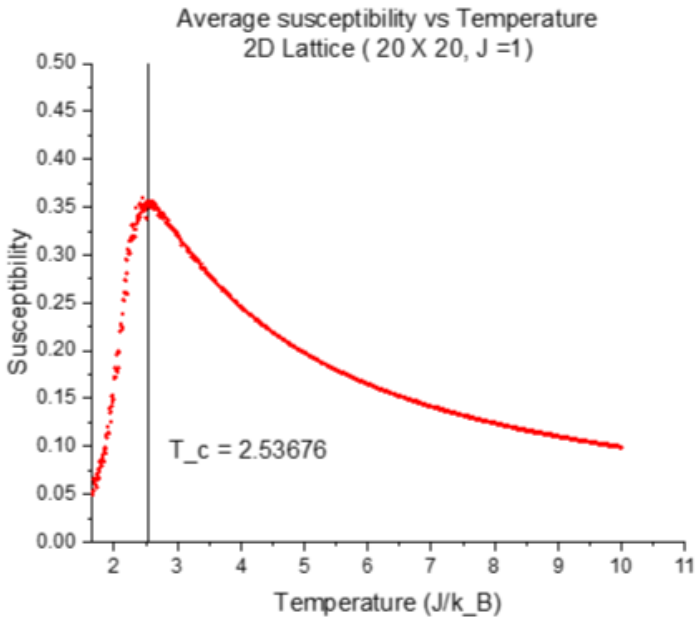

Figure 9: Average Magnetisation per spin vs. temperature for 20*20 matrix

Thus, for a 20*20 matrix the minimum number of steps required to reach equilibrium,are around 2000. The Curie temperature T_c is found equal to 2.53676 J/K_B.

4 Conclusion

In this project we have simulated 1-D and 2-D Ising Model using Metropolis Algorithm. It is interesting to observe that though there is no phase transition in 1-D Ising model but it does emerge in 2-D. In 1D case, magnetization is constant (+1 or -1) with respect to temperature. In 2-D case, the dependence of magnetization and susceptibility with temperature shows that critical temperature is around T_C = 2.6 J/k_B. Specifically, we obtain T_C =2.59 J/K_B from 10 X 10 array and T_C = 2.54 J/K_B from 20 X 20 array. As expected, larger system size attains equilibrium after large number of Monte Carlo steps compared to smaller system size, which we have shown successfully. We have not plotted energy vs temperature because of some computational issue which we are hoping to figure out. We are further trying to visualize the configurations as they evolve in time, which we may present soon. It has been a very educational experience to work on this project while interacting in groups and learning together. We thank Prof.Aftab Alam in guiding throughout the course, which was very helpful here.

5 References

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