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# Role of detailed balance on the phase diagram of frustrated systems; the modified ANNNI model

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Received 31 May 1995

Abstract. We study the effect of removing detailed balance from the axial next-nearestneighbour Ising (ANNNI) model on its phase diagram. Although the concepts of free energy or Gibbsian thermodynamical equilibrium no longer apply, we find numerically that the phase diagram is preserved even when the interactions are completely unidirectional. We also find that the value of the multiphase point varies with the degree of asymmetry in the rules.

#### 1. Introduction

Even after a few decades of study, the understanding of cooperative systems whose dynamics lacks detailed balance remains in its infancy. This situation is not due to lack of effort, but rather is because most of the relatively simple concepts and tools developed for conventional equilibrium statistical mechanics no longer apply. In particular, the long-time asymptotic microstate probability distribution is no longer given by a simple Boltzmann form  $\exp(-\beta H)$ , where H is a simple (energy) function of the microstate and  $\beta = T^{-1}$ is the inverse temperature, nor does one have the concept of the free energy as a quantity whose minimization determines the macrostate.

Detailed balance is always obeyed in closed systems. However, in many situations one is interested in studying only parts of a larger system, for example in biological reactions in the larger biosphere or for many growth problems. In such cases, detailed balance can no longer be assumed to hold generically. In fact, for many systems the effective absence of detailed balance is necessary to achieve complex behaviour; the propulsion of molecular motors is an example which has received attention recently [1]. Since the justification of most concepts in conventional statistical mechanics requires detailed balance, an understanding of the relevance of detailed balance in determining the character of macroscopic dynamical attractors should be very useful if one wishes to apply experience of conventional systems to systems without detailed balance.

One of the key concepts of conventional statistical mechanics is that of phase transitions; that as the control parameters are varied the systems migrate into different macrostates. One of the simplest phase transitions is that of spontaneous symmetry-breaking in which the ergodicity consequential to high stochasticity in local dynamics is broken as the temperature is lowered, as for example in a transition from a paramagnet to ordered magnet. Another is a transition from one ordered phase to another as the interactions between particles are varied, for example ferromagnet to antiferromagnet as the sign of a nearest-neighbour exchange interaction is changed. Examples of both these simple types of phase transitions have also been found in systems without detailed balance; for example in simple cellular automata with directed rules, (i) the paramagnet to ordered transition occurring as the degree of stochasticity is reduced in probabilistic cellular automata [2], (ii) the ordered-ordered transition occurring as the local rule is varied in deterministic coupled-map lattices and cellular automata [3].

Effects of detailed balance appears to be difficult to predict. On the one hand, recent lattice gas automata (LGA) simulations have shown that the absence of detailed balance can lead to spontaneous symmetry breaking [4]. From a random configuration, in a LGA with an asymmetric collision table, stable system-size dynamical patterns form with a symmetry depending on the details of the initial configuration. Interestingly, these patterns are unstable under rules satisfying detailed balance. On the other hand, analytical results of asymmetric SK and related models predict that for a non-zero temperature, any deviation from detailed balance destroys the spin-glass phase [5]. Numerical simulations indicate that this phase is resistant to a finite degree of asymmetry only at zero temperature [6].

In this paper we wish to consider a different type of phase transition, known for conventional systems but, as far as we are aware, unstudied for systems without detailed balance. This concerns transitions between ordered phases as the degree of stochasticity is varied, normally studied for conventional systems by consideration of the minimization of the free energy, a concept which no longer applies in the absence of detailed balance. Such transitions occur in conventional systems when the controlling interactions are frustrated, an example being the axial next-nearest-neighbour Ising (ANNNI) model which exhibits a plethora of different ordered phases. In this paper we consider the behaviour of an analogue of the ANNNI model without detailed balance and show that the phenomenon of transitions between ordered phases as the stochasticity is varied continues to exist.

### 2. Detailed balance

The presence of detailed balance forces is generally taken for granted when one studies physical systems. It has been proven, for example, that for both classical and quantum mechanical systems in isolation, detailed balance is satisfied [7]. It has also been shown that an extended detailed balance can be defined when a symmetry breaking field is introduced. However, a large proportion of phenomena in nature takes place in an open environment, with constant apport of *useful* energy or reactants and elimination of *decayed* energy and other products. This phenomenon is particularly striking in reactions found in biological systems. In such situations, detailed balance is not required. For example, the synapses connecting neurons are thought to give a different weight depending on the direction of the interaction; in other words, the interaction matrix is not symmetric so the problem is not Hamiltonian. Other examples have been discussed recently in the context of propulsion of viruses and bacteria. It has been proposed that in order to be able to move around, these micro-organisms extract energy from the stochastic surrounding using a ratchet-like mechanism [1].

For a system of Ising (two-state) spins,  $\sigma_i = \pm 1, i = 1...N$ , obeying random sequential stochastic dynamics, we can write the master equation

$$\frac{\mathrm{d}p_t(\{\sigma\})}{\mathrm{d}t} = W_{\sigma\sigma'}p_t(\{\sigma'\}). \tag{1}$$

When the transition matrix  $W_{\sigma\sigma'}$  respects the detailed balance condition

$$W_{\sigma\sigma'} p^{\rm e}_{\sigma'} = W_{\sigma'\sigma} p^{\rm e}_{\sigma} \tag{2}$$

where  $p^e$  indicate the equilibrium probability distribution, it can be shown that the set of eigenfunctions is complete with orthogonal eigenvectors and real eigenvalues [7]. From

then, the problem becomes, at least formally, straightforward to solve by applying the techniques of linear algebra. However, for a generic system,  $W_{\sigma\sigma'}$  possesses no particular symmetry and therefore one cannot describe the solution in terms of eigenfunctions, depriving us from many analytical tools for the analysis.

#### 3. A generalized ANNNI model

The model we choose to study is a generalization of the ANNNI model. On a cubic lattice the ANNNI model is characterized by the Hamiltonian

$$H = \frac{1}{2} \sum_{ij\delta} J_0 \sigma_{ij} \sigma_{ij+\delta} + \sum_{ij} \left[ J_1 \sigma_{ij} \sigma_{i-1j} + J_2 \sigma_{ij} \sigma_{i-2j} \right]$$
(3)

where *i* is the layer index while *j* and  $\delta$  represent, respectively, the index and the nearestneighbour directions inside the layers. Frustration is therefore present only along one direction with simple first-neighbour interaction between sites belonging to the same plane. This model was first introduced by Elliott in order to understand modulated magnetic materials [8]. Although there exists no exact solution for the full phase diagram, it has been studied extensively by series expansion, mean-field analysis and Monte Carlo simulations. Its mean-field phase diagram (figure 1) presents an infinite number of commensurate phases separated, above the incommensurate line, by incommensurate phases forming an incomplete devil's staircase (see [9, 10] for reviews).

In the absence of detailed balance, one can no longer write down a Hamiltonian. However, one can consider a dynamics in which the behaviour of any site ij is determined by a local field

$$h_{ij} = \sum_{\delta} J_0 \sigma_{ij+\delta} + J_{1-} \sigma_{i-1j} + J_{1+} \sigma_{i+1j} + J_{2-} \sigma_{i-2j} + J_{2+} \sigma_{i+2j}$$
(4)



Figure 1. Mean-field phase diagram of the ANNNI model in three dimensions (taken from [9]). The notation  $\langle n_1 n_2 n_3 \dots n_l \rangle$  indicates a spin ordering which alternates  $n_1$  layers with average spin up,  $n_2$  down,  $n_3$  up,  $\dots$ ,  $n_l$  (up for l odd, down for l even),  $n_1$  opposite to set l etc. The dotted curve on the diagram indicates a limiting curve above which there are also incommensurate phases, which are not indicated explicitly.

only if  $J_{1-} = J_{1+}$  and  $J_{2-} = J_{2+}$  is the influence of any site on any other symmetric and given by

$$h_{ij} = \frac{1}{2} \left[ H(\sigma_{ij} = 1) - H(\sigma_{ij} = -1) \right].$$
(5)

In particular, we shall consider a Glauber process which yields

$$W_{\vec{\sigma}\vec{\sigma}'} = \sum_{k} w_k(\vec{\sigma}') [\delta(\vec{\sigma}' - F_k\vec{\sigma}) - \delta(\vec{\sigma}' - \vec{\sigma})]$$
(6)

where k now labels a site,

$$w_k(\vec{\sigma}') = \frac{1}{2} [1 - \tanh(\beta \sigma'_k h_k(\vec{\sigma}'))] \tag{7}$$

and  $F_k \Phi(\vec{\sigma}) = \Phi(\sigma_1, \ldots, -\sigma_k, \ldots, \sigma_N).$ 

We parametrize the asymmetry in terms of two measures  $\epsilon_1$ ,  $\epsilon_2$  defined by

$$J_{x\pm} = (1\pm\epsilon_x)\tilde{J}_x \qquad x=1,2.$$
(8)

One can then describe the relative strength of the second-neighbour interaction by the ratio  $K = -\tilde{J}_2/\tilde{J}_1$ . At T = 0 for the perfect ANNNI model, a multiphase ratio  $K_c$  separates the ground state stability of a fully ferromagnetic and the so-called  $\langle 2 \rangle$  phase in which the planes order two up, two down, two up, etc and takes the value  $K_c = 0.5$ .

#### 4. One-dimensional phase diagram

In one dimension, we can argue that the corresponding  $K_c$  varies with  $\epsilon_x$ . In this case, ordered phases exist only at zero temperature but the value of  $K_c$  remains at 0.5 for symmetric interactions. For  $\epsilon_1 > K$ , the sign of the local field is completely determined by the nearest neighbour on the right of each spin. Although the probability of flipping this site is dependent on all first and second neighbours, its preferred orientation is controlled by one neighbour only. Starting with a  $\langle 2 \rangle$  or a random phase, and moving systematically from right to left on the chain, it is easy to see that we end up in a ferromagnetic state. Updating in a random sequential way, we expect the formation of ferromagnetic domains in the long-time limit. As soon as  $\epsilon_1 < K$ , all neighbours contribute in determining the sign of the local field and the equilibrium distribution should be the same as for the detailed balance case. We find similar behaviour for  $\epsilon_2 > 1/K$  where it is the next-nearest neighbour on the right which completely determines the preferred orientation of each spin.

Given that the multiphase point at  $\epsilon_x = 0$  is  $K_c = 0.5$ , and that the  $\epsilon_x$  are limited to a band of values from 0 to 1, only  $\epsilon_1$  is expected to have an impact on  $K_c$ . The phase diagram of the one-dimensional chain at zero temperature is given in figure 2 as a function of the asymmetry parameter  $\epsilon = \epsilon_1 = \epsilon_2$ . From  $\epsilon = 0$  to  $\epsilon = 0.5$ , the multiphase point  $K_c$ remains at the detailed balance value. For larger  $\epsilon$ , it increases linearly with the asymmetry.

Because of the addition of neighbours in the planes, perpendicular to the axial direction and playing a stabilizing role, this result cannot be expected to remain quantitatively valid in higher dimensions. For a Hamiltonian system ( $\epsilon_1 = \epsilon_2 = 0$ ), these neighbours would not change the behaviour of the model at zero temperature, but here the absence of detailed balance creates a dynamic asymptotic state even in this case. Nevertheless, this (one-dimensional) result hints at an asymmetry-dependent multiphase point in the threedimensional model studied in the rest of the paper.



Figure 2. Variation of the multiphase ratio  $K_c = -\tilde{J}_2/\tilde{J}_1$  as a function of  $\epsilon = \epsilon_1 = \epsilon_2$  for a onedimensional chain.

#### 5. Macroscopic solution

It is possible to obtain an expression for the macroscopic magnetization per layer  $m_{\alpha} = 1/N_L \sum_{i \in \alpha} \sigma_i$ , by following the evolution of the probability distribution

$$P_t(\{m_{\sigma}\}) = \sum_{\{\sigma\}} p_t(\vec{\sigma}) \prod_{\alpha} \delta(m_{\alpha} - m_{\alpha}(\vec{\sigma}))$$
(9)

where the sum is over all possible configurations,  $N_L$  is the number of sites per layer, and the layers are identified by the Greek letters. Choosing equation (1) as the dynamics and taking a mean-field approximation, we obtain the usual mean-field dynamical equation [11]

$$\frac{\mathrm{d}m_{\alpha}}{\mathrm{d}t} = \tanh\beta \left(4J_0m_{\alpha} + \sum_{\gamma\neq 0}J_{\gamma-\alpha}m_{\gamma}\right) - m_{\alpha} \tag{10}$$

where the lattice structure and dimensionality enters only via the factor multiplying  $J_0$ . Here, we take a three-dimensional cubic lattice. If static equilibrium is reached, i.e.  $dm_{\alpha}/dt = 0$ , as it would be asymptotically in the case of a detailed balance system, for example, we find the usual equilibrium mean-field relation [12]

$$m_{\alpha} = \tanh \beta \left( 4J_0 m_{\alpha} + \sum_{\gamma \neq 0} J_{\gamma - \beta} m_{\gamma} \right)$$
(11)

but now, not necessarily with  $J_n = J_{-n}$ .

Equation (10) is straightforward to integrate from any particular initial condition. It evolves rapidly to dynamical but spatially periodic solutions in  $m_{\alpha}$  with period depending on the choice of parameters. Its final states are also dependent on the initial configurations. Figure 3 presents snapshots of converged solutions at different temperatures with the same initial configuration, a slightly distorted (2) phase. These phases translate on the lattice at velocities depending on temperature and asymmetry. For all values of  $\epsilon_x$ , solutions of this equation for different parameters give a series of phases similar to those found for the perfect ANNNI model. However, since we lack a quantity to minimize we cannot select amongst the multiple steady state solutions to equation (10) one corresponding to the unique solution to the full model. The only way we have been able to identify the solutions is to use direct microscopic methods, i.e. Monte Carlo simulations.



Figure 3. Mean-field solution for the magnetization as a function of the layer index in a 120-layer system with  $\epsilon_1 = 0.5$ ,  $\epsilon_2 = 1$  and K = 0.55 at  $k_BT/J_0 = (a) 4.0$ , (b) 4.34, (c) 4.44, (d) 4.54 and (e) 5.14. The initial configuration in all cases is a slightly distorted (2) phase.

### 6. Numerical results

The usual method for solving the full ANNNI model with detailed balance, either analytically or numerically, is to calculate the free energy for different phases and to select the phase with the lowest one. Since such a procedure cannot be followed here, we had to resort to brute force numerical study and to try to look at systems big enough that influence of the boundary would be reduced as much as possible. This is, however, non-trivial; even the asymptotic state as the temperature tends to zero cannot be deduced *a priori* from global minimization. Even at finite temperature, when the transition rules are no longer deterministic, nothing guarantees that the system will tend towards a static macroscopic phase, let alone that it will be the same as for the corresponding Hamiltonian model. So the first task is to find the macrostate to which the system converges as we lower T.

Simulated annealing provides us with a convenient procedure. Starting at a temperature high enough that the system is in the paramagnetic phase, we slowly turn the temperature down and let the system settle before continuing the cooling. If we wait a long time, we are guaranteed to find an equilibrium probability configuration and if we find the same final distribution from different starting points, we may consider this state as the unique distribution. We have performed such simulations on a  $10 \times 10 \times 60$  lattice with  $\epsilon_1 = 0$  and  $\epsilon_2 = 1$  at points far away on both sides from K = 0.5 and found that, indeed, as the temperature is decreased the system goes to the ferromagnetic or (2) phase as expected. However, it becomes difficult to use this method very close to the multiphase point because the relaxation times exceed the capabilities of our computers. Nevertheless, around K = 0.5, we can verify the stability of the selected initial phase at low temperature. Imposing the (2) phase for K below 0.5, we find that as we raise the temperature enough to overcome the barriers in the simulation time the system goes to a phase much closer to ferromagnetic than (2). We obtain the opposite behaviour starting with a ferromagnetic layer configuration

for K above 0.5, indicating that for these values of  $\epsilon_x$ ,  $K_c$  represents the low-temperature multiphase point.

If one is concerned only with simulating static equilibrium properties of systems with detailed balance, the specific simulational dynamics is irrelevant as long as it yields the correct asymptotic distribution  $P_{\vec{\sigma}} \propto \exp(-\beta H(\vec{\sigma}))$ . However, in the absence of detailed balance the choice of dynamics may have a non-negligible effect. We have therefore studied simulationally two different types of dynamics for our model, one characterized by the Metropolis algorithm, the other by that of Glauber; with detailed balance both yield the Boltzmann distribution asymptotically. In the Metropolis procedure, single spin flips  $\sigma_k \rightarrow -\sigma_k$  are tested and accepted if  $\exp(-\beta\sigma_k h_k) > p$  where p is a number chosen randomly in (0, 1) at each attempt. For Glauber dynamics, spins k are picked and their value  $\sigma_k$  subsequently chosen randomly with probability  $\frac{1}{2}[1 - \tanh(\beta\sigma_k h_k)]$ . In both cases, the selection of each site to update was made at random. A Monte Carlo timestep is defined as the average time interval before a site is revisited.

Most simulation results presented here were performed on  $10 \times 10 \times Z$  lattices with Z = 60 and a few control runs made with Z = 62 and 120. A large system size was taken in order to allow for the possibility of long periods. The value of the parameters studied was restricted to be relatively close to the multiphase point  $K_c = 0.5$  so that the length of phases would remain much smaller than the period of our box at least for the perfect ANNNI model. Starting at a relatively low temperature, in an ordered phase, we heated up the system slowly, allowing 40 000 Monte Carlo steps/spin (MCS/S) of relaxation before observing over the next 10 000 MCS/S. As explained previously, the absence of detailed balance leads generally to a dynamical equilibrium, to a well defined periodic phase moving on the lattice with definite velocity. One cannot therefore perform a time average over magnetization per layer. We chose rather to average over the absolute value of the spatial Fourier transform of the magnetization per layer which should become constant as the system reaches its long-time state.

Figure 4 shows the spatial Fourier transform at four temperatures for a 60-layer lattice relaxed using Glauber dynamics. At each temperature, only one peak dominates so the phase can be well defined by a single wavevector. The next set of figures presents the maximum wavenumber as a function of temperature in systems with and without detailed balance, updated using Metropolis (figure 5) and Glauber dynamics (figure 6). This quantity is obtained by averaging over the width of the peak shown in figure 4 where the width is taken as the point where the amplitude falls by a factor 1/e. As we vary  $\epsilon_2$  from 0 to 1 while keeping  $\epsilon_1 = 0$ , there is very little change happening with respect to the phase transitions:



Figure 4. Wavenumber spectra of the spatial magnetization modulation in a  $10 \times 10 \times 60$  system at K = 0.55 with  $\epsilon_1 = 0$  and  $\epsilon_2 = 1$ , at four different temperatures (given in normalized units  $k_BT/J_0$ ).



Figure 5. Maximum wavenumber as a function of temperature for Z = 60, K = 0.55. The symbols are for a non-detailed balance system with  $\epsilon_2 = 1$  and  $\epsilon_1 = 0$ . For clarity, simulation results with  $\epsilon_1 = \epsilon_2 = 0$  (the Hamiltonian interaction) are shown as a full line. Results were obtained using the Metropolis algorithm.



Figure 6. Maximum wavenumber as a function of temperature for Z = 60, K = 0.55. The full line is for the Hamiltonian interaction and the full and open symbols are for a non-detailed balance system with  $\epsilon_2 = 1$  and, respectively,  $\epsilon_1 = 0$  and  $\epsilon_1 = 0.5$ . Results were obtained using Glauber dynamics.



Figure 7. Maximum wavenumber as a function of temperature for Z = 60 (full curve), Z = 62 (full circles) and Z = 120 (open circles),  $-\bar{J}_2/J_1 = 0.55$  with  $\epsilon_2 = 1$  and  $\epsilon_1 = 0$ . Results were obtained using the Metropolis algorithm.



Figure 8. Maximum wavenumber as a function of temperature for Z = 60,  $\epsilon_1 = \frac{3}{5}$ , and  $\epsilon_2 = \frac{2}{3}$  using Glauber dynamics. The open circles are for a ratio  $-\tilde{J}_2/\tilde{J}_1 = 0.65$ , the full circles for a ratio  $-\tilde{J}_2/\tilde{J}_1 = 1.05$ , and the open triangles for a ratio  $-\tilde{J}_2/\tilde{J}_1 = 1.70$ . The sets of points end when the system reaches a paramagnetic state.

transitions occur at temperatures very close to those found in the Hamiltonian model and the same plateaux are reached. One can explain this result by the fact that we keep the fundamental feature of the model; depending on the local configuration the first neighbour or the second neighbour interaction can take precedence over the other. We have performed these simulations for other values of  $\epsilon_x$  and what we obtain is qualitatively similar although the transition temperatures to phases with shorter wavenumber tend to be lower as  $\epsilon_1$  is increased while keeping the ratio K constant as we can see in figure 6.

Size effects are examined in figure 7 where the variation of the period as a function of





Figure 9. Maximum wavenumber as a function of the ratio K for  $\epsilon = \epsilon_1 = \epsilon_2 = 0.95$  and T = 1.50 after a relaxation of 100 000 timesteps. The full circles are for (2) initial configurate and the open circles, a ferromagnetic initial state. Lines connecting the points are for clarity and the parallel lines indicate the error margins on the multiphase point  $K_c$ .

Figure 10. Variation of the multiphase ratio  $K_c = as$  a function of  $\epsilon = \epsilon_1 = \epsilon_2$  for a three-dimensional lattice. The error bars are as explained in the text and the curve is for clarity.

temperature is shown for three different sizes (60, 62 and 120 layers) for  $\epsilon_2 = 1$  and  $\epsilon_1 = 0$ . Although the frustration prevents the system with 62 layers from attaining the desired phase (2) at low temperature, the sequence of phases as well as the transition temperature seem to be in good agreement for all the sizes studied indicating that these results are qualitatively size independent.

Exploring the phase diagram at different K's we find that particular periods in the magnetization per layer appear only for particular ranges of this ratio in qualitative accord with the behaviour shown in figure 1 for the system with detailed balance. Figure 8 presents results for  $\epsilon_1 = \frac{3}{5}$  and  $\epsilon_2 = \frac{2}{3}$ .

As mentioned in section 3, we expect that the multiphase point  $K_c$  will be dependent on the level of asymmetry. In one dimension and zero temperature, the value of  $K_c$  remains unchanged for  $\epsilon_1 < 0.50$  and from this point, increases linearly with the asymmetry. The procedure to determine the multiphase point is the following. Starting with a ferromagnetic or a (2) phase, we fix  $\epsilon = \epsilon_1 = \epsilon_2$  and let the system relax for 100000 MCS. Because the phase transition between the two phases is first order, we expect to have some hang-up so that even after long relaxation the final results will depend on the initial configuration. This will be particularly true close to the multiphase point. An example of the type of results obtained is shown in figure 9. Around the multiphase point, the slowing down of the dynamics is such that both phases remain stable, limiting the accuracy with which we can identify this point. For  $\epsilon = 0.95$ , this region is between K = 0.74 and 0.82. Complete results are presented in figure 10. The behaviour of  $K_c$  in three dimensions is therefore qualitatively equivalent to what happens in one dimension although it is quantitatively less affected by the asymmetry. Results plotted in this last figure have been obtained at several different temperatures. As a general rule, the higher  $\epsilon$  is, the lower is the temperature used in the run because the system remains less stable. Too high a temperature and the equilibrium states are no longer the zero-temperature phases but something more complicated from which we cannot extract the information we want. If the relaxation temperature is too low, the region of stability of the two phases widens to a point where it becomes meaningless. Results from figure 10 indicate that even for the completely asymmetric interaction  $\epsilon_1 = \epsilon_2 = 1$ , the system will present a series of commensurate phases as the temperature is varied.

## 7. Conclusion

It is clear that detailed balance is not needed to create complex phase diagrams such as one finds in frustrated systems like the ANNNI model. Even in dynamical systems, the presence of temperature, noise or other external stochasticity can induce phase transition to new ordered states through some competitive process that cannot be easily formalized. Moreover, our studies of a modified ANNNI model have shown that a system with stochastic local-field dynamics, even without the symmetry necessary for detailed balance, can exhibit a sequence of phases close to those of the corresponding Hamiltonian system. The latter can therefore provide useful insight. On the other hand, we also know that new phases, for example cycles and chaotic solutions, are also possible for appropriate models without detailed balance [3, 13, 14], so that many questions still remain concerning the effects of the removal of detailed balance in frustrated systems.

## Acknowledgments

We would like to thank Julia Yeomans for useful discussions. NM would like to acknowledge the Natural Sciences and Engineering Research Council of Canada for a post-doctoral fellowship.

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