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Slow coarsening in a class of driven systems

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Abstract. The coarsening process in a class of driven systems is studied. These systems have previously been shown to exhibit phase separation and slow coarsening in one dimension. We consider generalizations of this class of models to higher dimensions. In particular we study a system of three types of particles that diffuse under local conserving dynamics in two dimensions. Arguments and numerical studies are presented indicating that the coarsening process in any number of dimensions is logarithmically slow in time. A key feature of this behavior is that the interfaces separating the various growing domains are macroscopically smooth (well approximated by a Fermi function). This implies that the coarsening mechanism in one dimension is readily extendible to higher dimensions.

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 05.70.Ln Nonequilibrium and irreversible thermodynamics – 05.70.Np Interface and surface thermodynamics

1 Introduction

The study of phase separation and coarsening processes has been a subject of broad and growing interest in recent years [1]. Following a quench into an ordered phase from a disordered one the typical linear size of domains of the ordered phase, $\ell(t)$, grows in time. Usually, at late times the system enters a scaling regime characterized by a single length scale $\ell(t)$ that grows as $\ell(t) \sim t^n$. The value of the exponent *n* depends on the symmetry of the order parameter and on the conservation laws of the system. In two dimensions and above it has been argued that for a scalar order parameter *n* is either 1/3 [2,3] or n = 1/2 [4, 5] depending on whether or not the dynamics conserves the order parameter, respectively.

In one dimension and for short-range interactions the situation is different due to the absence of long-range order at any temperature T > 0. An exact solution of the non-conserving Glauber dynamics at zero temperature gives the expected scaling $\ell(t) \sim t^{1/2}$ [6–8]. On the other hand, at zero temperature under Kawasaki dynamics where the order parameter is conserved, the system gets trapped in metastable states with isolated domain walls and coarsening is arrested. Studies of such conserving one-dimensional models in a small T limit have shown that the growth law $\ell(t) \sim t^{1/3}$ still persists [9,10]. However, for both conserving and non-conserving dynamics a solution of the deterministic continuum Ginzburg-Landau equations gives rise to a different answer. In these cases the domain walls interact with each other at large distance through exponen-

tially small forces which in the absence of diffusion leads to the growth law $\ell(t) \sim \log(t)$ [11].

Another situation where a logarithmic growth law arises is when energy barriers proportional to the domain size have to be surmounted during the coarsening. A specific example of this is a three-dimensional Ising model with next nearest neighbor interactions [12]. However, in this model the slow coarsening is lost in two dimensions.

Coarsening processes in driven systems are less well understood. Here the dynamics does not obey detailed balance. This gives rise to many phenomena which do not occur in thermal equilibrium [13,14]. For example, several one-dimensional driven systems have been shown to exhibit long-range order and spontaneous symmetry breaking even when the dynamics is local [15,16]. A study of the coarsening process in a one-dimensional Ising model with conserved order parameter has shown that for a small driving field the average domain size grows as $t^{1/2}$ in contrast to the $t^{1/3}$ behavior of the non-driven case [17,18]. However, in the coarsening of the two-dimensional conserved driven Ising model there is some evidence to suggest that after defining a properly rescaled isotropic domain size the growth law $\ell(t) \sim t^{1/3}$ is retained [19].

Recently, several one-dimensional driven systems have been shown to exhibit coarsening and phase separation of a novel kind [20–26]. The phase separation does not rely on microscopic rates tending to zero (as is the case for equilibrium systems in the limit of zero temperature). Instead the phase separation is achieved through a drive which stabilizes certain domain walls and allows ordered domains to be stable if the number of species of domains is greater

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than two. The mechanism (to be reviewed below) leads to a slow coarsening process in which $\ell(t) \sim \log(t)$ [21].

In this paper we consider the coarsening dynamics of an extension of one of these models to two and higher dimensions. We show that the slow, logarithmic, coarsening is retained. In the ordered phase the various states are separated by domain walls, which in one dimension are point-like objects. On the other hand in higher dimensions these interfaces are fluctuating extended surfaces. The evolution of the coarsening domains may depend on the roughness of these surfaces. It would thus be of interest to explore this issue in some detail. An analysis of the model introduced in this paper shows that the width of the interfaces is finite even for infinitely large systems. Such interfaces are traditionally referred to as smooth. In fact, it is found that the interface profiles are described by a Fermi function with a linear potential (see Eq. (6)). This is expected to be a generic feature for the class of models under consideration.

The one-dimensional version of the model we study is defined on a ring of length L where each site is occupied by one of the three types of particles A, B or C [20]. The model evolves under a random sequential update procedure which is defined as follows: at each time step two neighboring sites are chosen randomly, and the particles at these sites are exchanged according to the rates

$$AB \stackrel{q}{\leftarrow 1} BA$$
$$BC \stackrel{q}{\leftarrow 1} CB$$
$$CA \stackrel{q}{\leftarrow 1} AC.$$
$$(1)$$

The model conserves the number of particles $N_{\rm A}$, $N_{\rm B}$ and $N_{\rm C}$ of the three species. When q = 1 the particles undergo symmetric diffusion and the system is disordered. For completeness we now review the explanation of why the system coarsens logarithmically in time for any $q \neq 1$ [21]. This argument will provide a starting point for the analysis in higher dimensions. To be explicit we consider the case q < 1. Due to the bias, an A particle prefers to move to the left inside a B domain and to the right inside a C domain. Similarly the motion of the B and C particles in foreign domains is biased. Consider the evolution of the system starting from a random initial condition. The configuration is composed of a random sequence of A, B and C particles. Due to the bias a local configuration in which an A domain is located to the right of a B domain is unstable, and the two domains will exchange places on a relatively short time scale linear in the domain size. Similarly, AC and CB domain walls are unstable. In contrast domain walls of the type AB, BC and CA are long lived. Thus, after a short time the system will rearrange into a state of the type ... AABBBCCAAABBCCC ... in which only stable domain walls are present. The evolution of this state will proceed by slow diffusion against a bias in which, for example, an A particle crosses an adjacent C domain. The time scale for such a process to occur is $q^{-\ell}$ where ℓ is the typical domain size in the system. This suggests that the average domain size in the system grows as $\ln t / |\ln q|$.

Eventually the system will phase separate into three domains of the three species of the form A...AB...BC...C with small density fluctuations around the domain walls, leaving the bulk of the domains pure. In another model in the class this has been referred to as strong phase separation [23]. In the thermodynamic limit these domains do not remix, implying breaking of translational invariance. For the specific case where the number of particles of each species is equal it was shown that the local dynamics obeys detailed balance with respect to a long-range Hamiltonian. Indeed, using this Hamiltonian it was rigorously proved that the model is completely phase separated into pure domains in the steady state [20,21].

The model we study is the simplest generalization of the above one-dimensional model to higher dimensionality. To be explicit, we consider the model in d = 2 dimensions but the results presented in this paper are also valid in higher dimensions. We introduce a second lattice direction in which the particles perform unbiased diffusion. That is we study an $L_x \times L_y$ lattice, with periodic boundary conditions, in which at each time step two neighboring sites are chosen at random. If the two sites lie along the x axis the particles perform a biased diffusion defined by equation (1) while if they lie in the y axis the particles perform an unbiased diffusion. Thus, along the y axis the dynamics is defined through the rates

$$AB \stackrel{1}{\leftarrow 1} BA$$
$$BC \stackrel{1}{\leftarrow 1} CB$$
$$CA \stackrel{1}{\leftarrow 1} AC.$$
$$(2)$$

Here for simplicity the transition rates are taken to be 1, although choosing a different rate for hops in the y direction would not affect the results obtained in this paper. We expect other generalizations of the model, where the motion in the y direction is biased in a manner similar to that in the x direction, to have the same generic behavior. We return to this point in the discussion.

The model conserves the total number of particles of each species. As will be demonstrated below, in two dimensions the rates do not satisfy detailed balance for $q \neq 1$ irrespective of the number of particles of each species. Thus the system is generically far from thermal equilibrium.

In the following we show, by numerical and analytical methods, that the slow logarithmic coarsening persists in the two-dimensional model and also, we argue, in higher dimensions. In two dimensions the system forms on short time scales stripes of A, B and C particles which are aligned along the y direction and are ordered along the x direction in the form ... AABBBCCAAABBCCC... Thus the interfaces between three phases are lines whose fluctuations must be considered. If the interfaces are smooth the argument suggesting a logarithmic coarsening in the one-dimensional model should also apply in the twodimensional model. That is, the average tunneling time of a domain would be exponentially large in the average domain size. However, if the interfaces are rough such that they can come close to each other it might be that different behavior would prevail. Thus, an important question is: how rough is the interface? What we find is that the interfaces are indeed smooth and the typical size of a stripe grows as $\ell(t) \sim \log(t)$.

The paper is organized as follows: it is first shown in Section 2 that detailed balance cannot be satisfied in two dimensions (in contrast to the one-dimensional case). In Section 3 the coarsening of the model is studied numerically and a simple interface model which captures the essential physics of an interface between two phases is formulated. The model is solved and shown to have a smooth interface. In Section 4 we discuss the generality of the results both to other two-dimensional models and to higher dimensions.

2 Lack of detailed balance in the model

To argue that the model presented above does not satisfy detailed balance (except for q = 1) we first review the situation in the one-dimensional version of the model. In this case it was shown [21] that when the number of particles of each species is equal, that is when $N_{\rm A} = N_{\rm B} = N_{\rm C}$, detailed balance is satisfied by the rates given in equation (1) for arbitrary q. However, when the number of particles of two species are not equal, say $N_{\rm A} \neq N_{\rm B}$, detailed balance is not satisfied. To see this consider an arbitrary set of configurations 1, 2..., k. Let $W(i \rightarrow j)$ be the transition rate from configuration i to j. A necessary and sufficient condition for the existence of detailed balance [14] is that for any given set of k states the following equality is satisfied:

$$W(1 \to 2)W(2 \to 3) \dots W(k \to 1) =$$

$$W(1 \to k)W(k \to k-1) \dots W(2 \to 1) . \quad (3)$$

That is for any closed loop in configuration space the product of rates going along one direction should be equal to the product of rates going in the opposite direction.

We now apply this criterion to show that in d = 1 detailed balance is not satisfied when the three densities are unequal. Consider for simplicity the fully phase separated state A...AB...BC...C. Take the rightmost A particle and move it to the right until it has traversed both the B and the C domains. The resulting configuration is a fully phase separated state translated by one lattice unit with respect to the starting configuration. Repeating this process N times one returns to the starting configuration. The product of the microscopic rates involved in this process is $q^{NN_{\rm B}}$. Carrying out a similar process but in the reverse direction leads again to the starting configuration. For this path the product of rates is $q^{NN_{\rm C}}$. Thus according to the criterion (3) detailed balance is not satisfied when $N_{\rm B} \neq N_{\rm C}$, or when any two of the densities are not equal. It is not difficult to show that when $N_{\rm A} = N_{\rm B} = N_{\rm C}$ detailed balance is satisfied [20, 21].

Next, consider the two-dimensional model. In this case whatever the number of particles of each species one can always choose as a starting configuration a state where on one of the rows the numbers of particles of each species are not equal. Repeating the argument above, given for the one-dimensional model, by considering particle exchanges along this row we immediately see that due to the unequal number of particles detailed balance does not hold.

Therefore, in contrast to the one-dimensional model, whatever that number of particles of each species detailed balance is never satisfied in two dimensions. It is straightforward to see that this argument also implies lack of detailed balance in higher dimensional generalizations of the model.

3 Coarsening in two dimensions

To study the dynamics of the model in two dimensions we first show numerically that on a short time scale, the system indeed evolves into a striped state composed of sequences of A, B and C aligned in the x direction. We then study the slow coarsening process of these stripes and argue that the typical length scale increases logarithmically with time.

3.1 Monte Carlo simulation

In order to study the short time behavior of the model and demonstrate the flow into a striped state, Monte Carlo simulations were performed for various values of L_x and L_y . Starting from a random initial condition we studied the case with equal densities of particles of each species. A typical evolution of a system is presented in Figure 1 for a lattice with $L_x = 300$ and $L_y = 80$ with q = 0.15. One can clearly see that on short time scales a striped structure evolves in which stripes along the y direction develop. As expected, the stripes are ordered in sequence A, B, C along the x direction. On short time scales, when the distance between neighboring domain walls is comparable to their width, the stripes are strongly fluctuating. At this stage the evolution of the structure through the formation of topological defects is relatively fast. As time progresses the asymptotic regime where the stripes are smooth is reached. In this regime the dynamics is dominated by the slow coarsening mechanism described in this paper. Due to the slow time scales involved in the simulations of the coarsening process our data does not allow us to demonstrate quantitatively that the coarsening is logarithmic in time. However in the next section arguments will be presented which support this growth law.

To analyze the data we have calculated the Fourier transform of the density profile along the x direction for each value of y:

$$a_y(k) = \sum_{x=0}^{L_x - 1} \tilde{a}_y(x) \exp\left(\frac{-2\pi \mathrm{i}kx}{L_x}\right). \tag{4}$$

Here $\tilde{a}_y(x)$ is equal to -1, 0 or 1 if the site (x, y) is occupied by an A, B or C particle respectively. It thus corresponds to the density difference of the A and C species.



Fig. 1. On the left hand side one can see from top to bottom the evolution of a typical system for $t_0 = 0, t_1 = 30, t_2 = 66, t_3 = 146, t_4 = 920, t_5 = 383000$ Monte Carlo sweeps when q = 0.15. The different species of particles are represented as different gray scales. On the right hand side the first 50 Fourier components of $\langle |a(k)| \rangle$ averaged over a hundred simulations for the same times are presented and the same value of q. Similar results were obtained for different values of q.

We then calculated $\langle |a(k)| \rangle$, the average of $|a_y(k)|$ for all values of y and over one hundred simulations. The results are also presented in Figure 1. One can clearly see that stripes of a characteristic size form. This is accompanied by the emergence of a typical Fourier mode. As time progresses the k value of the typical Fourier mode decreases as expected in a coarsening system.

It is of interest to examine the considerations presented above for the existence of phase separation and slow coarsening in one dimension and to check whether the argument can be extended to two and higher dimensions. In d dimensions the A, B, C domains are separated by fluctuating (d-1)-dimensional surfaces. For the argument for slow coarsening to go through unmodified, we require that these surfaces are smooth, that is of finite extent in the growth direction. Otherwise, if they were rough, the fluctuating distance between neighboring surfaces might significantly affect the coarsening process. Therefore, we have studied numerically the smoothness of the interfaces in this model. To do this we consider the density of, say, A particles near the AB domain wall. In Figure 2 such profiles obtained from Monte Carlo simulations of the three species model are presented. The simulations were performed for a given q at fixed value of L_x and varying L_y . They were obtained by extracting the density profile of a given species of particles near a domain wall and averaging over 40 sets of data. One can see that the interface

is smooth since the density profile reaches a steady-state form of finite extent in the x direction, as L_y is increased.

We have thus established numerically that the model evolves towards a striped state and that the interfaces between the phases are smooth. Next, an interface model which captures the essential statistical properties of an interface is studied and shown to predict a smooth interface whose profile agrees very well with the numerics.

3.2 Interface model

To construct a simple model that well approximates the behavior of the actual interfaces we begin by assuming that the system is already in a striped configuration in which interfaces are well separated. The density of, say, the C particles near an AB interface is then negligently small. This assumption will be shown to be consistent with a smooth interface. Also any current of particles is exponentially small in the domain size and can be neglected, implying that the average velocity of the interface vanishes. We may thus study the interface properties by considering only A and B particles placed on a lattice with closed (reflecting) boundary conditions in the direction of the bias. As we will show such a model reduces to a model of particles with excluded volume interaction placed in a gravitational-like field in the x direction. For such systems



Fig. 2. Profiles obtained from Monte Carlo simulations for $L_x = 300$ and $L_y = 40, 80, 160, 320$ and q = 0.15. Δ is the distance from the center of the profile. The simulation results for each L_y value is averaged over 40 profiles. Similar results were obtained for different values of q.

the interface is smooth for any $q \neq 1$. This allows us to derive an exact form for the density profile near an interface which is valid for all dimensions. As will be argued later this result applies to a wide variety of models considered previously and is not specific to the model studied here. For example a similar profile is obtained in [23] for a one-dimensional model.

We define the interface model on an $l_x \times l_y$ lattice with periodic boundary conditions in the y direction and closed boundary conditions in the x direction. That is, the model is defined on a lattice with closed boundary condition in the direction of the bias. We choose the densities such that half the lattice sites of the lattice are occupied by A particles and the others are occupied by B particle. Therefore the center (average x position of the interface) of the AB interface is at $l_x/2$. The dynamics of the model is identical to that of the three species model (see Eqs. (1, 2)). However, all dynamics in which C particles participate are irrelevant as there are no such particles present.

In this model an A can be thought of as a particle while a B as a vacancy. Within this picture we have particles, placed on a lattice, which are biased to move in a preferred direction along x. Due to the closed boundary conditions, which imply a zero current, it is easy to show that the model satisfies detailed balance with respect to the steady state weight (unnormalized probability)

$$W(\mathcal{C}) = q^{\sum_{x,y} x A_{x,y}},\tag{5}$$

where $A_{x,y} = 1$ (0) if, the site (x, y) in configuration C is occupied (empty), and the sum runs over all lattice sites. The steady state weight describes particles placed in a linear potential with an excluded volume interaction. Note



Fig. 3. A comparison of the profiles obtained from the interface model and the toy model with no overhangs with the profile obtained from Monte Carlo simulations for $L_x = 300$ and $L_y = 320$. $\Delta = x - l_x/2$ is the distance from the center of the profile.

that the above expression is valid whatever the rates for exchange A and B in the y direction.

The solution of the density profile is obtained in straightforward analogy to a Fermi gas. Since each lattice site (x, y) can be occupied by only a single particle it can be considered as a state of a Fermion with energy $\epsilon_{x,y} = x$. The mean number of particles at site (x, y), $n_{x,y}$, is given by the Fermi distribution with a temperature $T = 1/|\ln q|$:

$$n_{x,y} = \frac{1}{q^{-(x-l_x/2)}+1} \,. \tag{6}$$

As expected the distribution is independent of y. Here $l_x/2$ plays the role of a chemical potential marking the center of the profile. It is easy to check the condition that the average density in indeed 0.5, namely $\sum_{x,y} n_{x,y} = l_x l_y/2$. To see that this is satisfied for any value of q one uses the relation

$$n_{l_x/2+\Delta,y} + n_{l_x/2-\Delta,y} = 1 \tag{7}$$

where $\Delta = x - l_x/2$. The density profile of the interface is given by $P(x) = n_{x,y}$. It has a finite width, $1/|\ln q|$, as expected for a smooth interface.

A comparison of P(x) of the interface model and the profile of the Monte Carlo simulations is given in Figure 3. One can see that the interface model agrees very well with the simulations.

We have thus established that the interfaces in the model are smooth. This in turn implies that the argument which was presented for the one-dimensional version of the model is valid and predicts a logarithmic growth law for the domain size. The interface studied above includes configurations with bubbles and overhangs. In the study of interfaces it is often assumed that bubbles and overhangs may be neglected without affecting the macroscopic properties, so that the interface may be described by a single valued function. In the present context we can study the validity of such an approximation since the profile both with (see Eq. (6)) and without (see below) bubbles and overhangs can be computed. Thus we consider only those configurations in which the particles fill the left part of the system, up to a 'height' h_y which is the number of particles in row y.

By performing the sum in equation (5) for each value of y one obtains the following weight function:

$$W(\mathcal{C}) = q^{\frac{1}{2}\sum_{y} h_{y}^{2}},$$
(8)

where a term of the form $\sum_{y} h_{y}$ has been neglected, as it is a constant equal to the total number of particles in the system.

The properties of the interface can easily be obtained by working in the grand canonical ensemble. We thus introduce a chemical potential to respect the constraint that the total height of the system $\sum_{y} h_{y} = l_{x}l_{y}/2$. The weight of a configuration in this ensemble is thus

$$W_{gc}(\mathcal{C}) = q^{\frac{1}{2}\sum_{y}(h_y - l_x/2)^2}.$$
 (9)

The profile of the density along the x direction is then given by

$$P(x) = \sqrt{\frac{2|\ln q|}{\pi}} \int_{x}^{\infty} \mathrm{d}h \, q^{\frac{1}{2}(h-l_{x}/2)^{2}}, \qquad (10)$$

where the continuum limit is assumed and the upper limit of the integral was taken to be infinity. This gives

$$P(x) = \frac{1}{2} \operatorname{erfc}\left((x - l_x/2)\sqrt{|\ln q|/2}\right), \quad (11)$$

where erfc is the complementary error function. As expected the model with no overhangs also predicts a smooth interface.

In Figure 3 the resulting profile is compared with the one obtained by the numerical simulations. It is evident that although the two profiles agree in general, the fit is not as good as that with the Fermi function profile. This is to be expected since, for example, in the regions where the density of particles is low, the no overhang assumption becomes a less accurate approximation. In these regions excluded volume does not play an important role. Due to the linear potential the profile decays as $P(x) \simeq q^{(x-l_x/2)} \propto \exp(-\alpha x)$ with α a constant. However neglecting overhangs gives rise to a decay of the form $P(x) \propto \exp(-\beta x^2)$ with β a constant.

4 Discussion

In this work we have studied a generalization to two dimensions of the ABC model for phase separation [20,21]. We have shown that the slow logarithmic coarsening of the one-dimensional case persists. Further, we have shown that the interface between the slowly coarsening domains is smooth and can be described by a Fermi function with a linear potential (see Eq. (6)).

We next turn to the question of the generality of our results. First note that in the generalizations of the ABC model to more than three species [21], and in the models introduced by Lahiri *et al.* [22, 23] and by Arndt et al. [24, 25] the mechanism which leads to coarsening in the system is the same as in the ABC model. Namely, the presence of stable domain boundaries is due to a bias which drives particles of one species towards their own domain with a constant velocity. In the model of Lahiri et al. which comprises two coupled rings each containing two species one has four different types of domain. The dynamics is then governed by four stable interfaces separating these domains, in analogy with the model considered in the present work. In the model of Arndt et al. there are three types of domain separated by three interfaces. (One of the stable domain walls corresponds to q > 0 in equation (6) and the other two correspond to q = 0, *i.e.* a zero temperature Fermi function.) Therefore, we expect that the analysis of the present paper is applicable to extensions of these models to higher dimensions. This would imply that coarsening processes in these models are logarithmically slow.

The generalization of the model considered so far is highly anisotropic in the sense that the dynamics along the x and y direction are qualitatively different: while the diffusion is biased in one direction it is symmetric on the other. It is of interest to examine the case where the diffusion along both axes (or all axes in higher dimensions) has some bias. Let us consider such a generalization of the ABC model to two dimensions where the exchanges along the y direction have rates

$$AB \xrightarrow{r} BA$$
$$BC \xrightarrow{r} CB$$
$$CA \xrightarrow{r} AC,$$
$$(12)$$

while the exchanges along the x axis are as in equation (1). On some coarse grained scale (where lattice effects may be ignored) the dynamics is effectively uniaxial. The preferred direction in the x-y plane for exchange of particles is at an angle $\theta = \arctan\left(\frac{1-q}{1-r}\right)$ with respect to the y direction. The effective exchanges in the normal direction are symmetric. The effect of this would be for stripes to form perpendicular to the preferred direction. At large scales the model reduces to the model which we have studied in this paper. Similarly, generalizations of the ABC model in higher dimensions are effectively uniaxial and domains form with interfaces which are (d-1)-dimensional hyperplanes orthogonal to the preferred direction.

To test this scenario we carried out Monte Carlo simulations of the model in two dimensions with r = q. In Figure 4 the coarsening process is illustrated. One sees



Fig. 4. Characteristic configurations during the evolution of a system with q = r = 0.15 for $t_0 = 0, t_1 = 30, t_2 = 66, t_3 = 146, t_4 = 4440, t_5 = 383\,000$ Monte Carlo sweeps and $L_x = L_y = 300$. The different species of particles are represented as different gray scales. Similar results were obtained for different values of q.

that after a transient time stripes oriented perpendicular to the (1,1) direction are formed confirming the above picture.

Studies of phase separation and coarsening in driven systems such as that of the present paper and the works reviewed in the introduction, have suggested that the processes involved are rather diverse. They range from relatively fast power law to slow logarithmic coarsening. For further examples of coarsening in related systems see [27– 29]. It would be very interesting to construct a more general framework within which all these coarsening processes could be understood and classified.

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