ON IMPROVING ANALYTICAL MODELS OF COSMIC REIONIZATION FOR MATCHING NUMERICAL SIMULATION

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ABSTRACT

The methods for studying the epoch of cosmic reionization vary from full radiative transfer simulations to purely analytical models. While numerical approaches are computationally expensive and are not suitable for generating many mock catalogs, analytical methods are based on assumptions and approximations. We explore the interconnection between both methods. First, we ask how the analytical framework of excursion set formalism can be used for statistical analysis of numerical simulations and visual representation of the morphology of ionization fronts. Second, we explore the methods of training the analytical model on a given numerical simulation. We present a new code which emerged from this study. Its main application is to match the analytical model with a numerical simulation. Then, it allows one to generate mock reionization catalogs with volumes exceeding the original simulation quickly and computationally inexpensively, meanwhile reproducing large-scale statistical properties. These mock catalogs are particularly useful for cosmic microwave background polarization and 21 cm experiments, where large volumes are required to simulate the observed signal.

Key words: cosmology: theory – dark ages, reionization, first stars

1. INTRODUCTION

The nature of the epoch of cosmic reionization involves a large dynamic range of scales and various physical processes. An accurate treatment of this epoch requires detailed bookkeeping of the photon budget. Therefore, a good understanding of astrophysics as well as large-scale structure formation and cosmology is a necessity. Indeed, after being emitted by a star, a photon travels through partially neutral interstellar medium and then through intergalactic medium (IGM) populated with Lyman limit systems before it reaches the ionization front. The diversity of these environments makes the study of reionization challenging.

The past two decades have seen the rapid development of analytical (Miralda-Escudé et al. 2000; Furlanetto et al. 2004; Kuhlen & Faucher-Giguère 2012) and numerical (Iliev et al. 2006; McQuinn et al. 2007; Zahn et al. 2007; Croft & Altay 2008; Lee et al. 2008; Shin et al. 2008; Trac et al. 2008; Iliev et al. 2009; Aubert & Teyssier 2010; Friedrich et al. 2011; Ahn et al. 2012; Shapiro et al. 2012; Hutter et al. 2014; Iliev et al. 2014; So et al. 2014; Norman et al. 2015) methods of studying the epoch of cosmic reionization. Nevertheless, they both struggle from various limitations. The growth of computer capabilities gave a great boost to the numerical methods (Trac & Gnedin 2011). However, simulations are limited by the dynamic range, i.e., either smaller boxes with high resolution or large boxes with low resolution. Therefore, either the correlations on large scales are neglected or the crude approximations are adopted for sub-grid models.

On the other hand, the analytical models are computationally inexpensive and can potentially probe the volumes of any sizes. Also, the framework of these models provides a descriptive view on reionization, and, therefore, develops intuition about the significance of each physical process. However, those assumptions, which make the framework so efficient, also cause some limitations. First, it limits physical processes, which can be included in the model. Second, the approximations cause unpredictable accuracy. In particular, one cannot invest more computational power to achieve higher accuracy.

These limitations are reflected in the capabilities of these models to be compared with observations. For instance, in order to match the galaxy luminosity function (star formation history) and escape fractions, one has no other choice but to run a detailed high-resolution simulation; while for the large-scale morphology studies (21 cm tomography), a large number of realizations in cosmological volumes are needed, which can be done only with approximate semi-numerical models.

In this study, we attempt to take the best from both methods. First, in Section 4, we approach the numerical simulation as if it were a product of semi-analytical computation. As a result, we end up with a new kind of statistics based on excursion set formalism, which describes the ionization field on large and small scales. This tool allows one to visualize the dependence of ionization history on the underlying density perturbations in an unusual way.

Then, in Section 5, we test how descriptive the phase-space statistics are that are calculated in Section 4. If it is informative enough, then it will be sufficient for reproducing the reionization history on a different set of initial conditions (IC). In other words, we perform a training (or tuning) of an analytical model on a given numerical simulation and discuss how well it can be done. In contrast to Battaglia et al. (2013), where a similar goal was set, we use the excursion set formalism (Press & Schechter 1974) instead of the bias approach. The performance of the excursion set analytical models versus numerical simulation has been carried out in Zahn et al. (2011), where the authors put the same physics (the efficiency of ionizing photon production) into numerical and analytical models. We adopt a different approach, and try to find any analytical model that would correspond to a given numerical simulation.

The results from this study allow us to make conclusions about the capabilities of the analytical approach, i.e., what physical processes they generally fail to mimic and for which
tasks it can be used. Also, we show how the analytical framework can play a complementary role in the numerical calculations by providing a tool for the visualization of the spatially complicated reionization history.

In addition, we present a semi-numerical code based on excursion set formalism, which emerged from this study. Its main application is the training of an analytical model on a given numerical simulation. Then, this trained model can be used for the rapid generation of mock catalogs for 21 cm experiments.

We start by discussing the motivation in Section 2 and giving a brief overview in Section 3 of the framework of the two main analytical approaches we consider (Section 3.1) and the numerical simulation, which we use as our fiducial model (Section 3.2). This is followed by Sections 4 and 5, where we present and discuss our method. In Section 6, we conclude.

2. MOTIVATION

The value of any theoretical model is its capability to be experimentally tested. The new observational facilities are able to probe for the most interesting reionization range of redshifts $5 < z < 20$. Here, we discuss how these can be estimated in the theoretical models. First, we list those observations, which can be compared versus existing numerical simulations:

1. The integrated optical depth of Thomson scattering on free electrons to the cosmic microwave background provides a glimpse into the history of ionization. The measured value by the Wilkinson Microwave Anisotropy Probe argues in favor of the scenario when reionization began at $z > 15$ (Bromm & Yoshida 2011; Dunlop 2012, p. 223; Hinshaw et al. 2013) with a measured optical depth: $\tau = 0.081 \pm 0.012$. The measured optical depth by Planck Collaboration et al. (2015) is lower: $\tau = 0.066 \pm 0.016$. This observable can be matched with global ionization history. Hence, even models of homogeneous reionization can simulate this quantity.

2. The end of the reionization is probed by the observation of the Gunn–Peterson effect in the spectrum of high-redshift QSOs (Fan et al. 2006; Bolton et al. 2011) and gamma-ray bursts (Chornock et al. 2013), as well as the Ly\(\alpha\) emission from high-redshift galaxies (Stark et al. 2010; Pentericci et al. 2011, 2014; Schenker et al. 2011, 2014; Treu et al. 2013; Tilvi et al. 2014).

3. Another observable is the luminosity function and its derivative star formation rate at high redshift. Current observations by Hubble Space Telescope Ultra Deep allow us to probe the galaxies up to redshift 10. The modern simulations of reionization, including the one we use (Gnedin 2014), are capable of reproducing these luminosity functions.

In contrast to the observations listed above, these cannot be numerically simulated with the same precision due to much larger volumes:

1. The polarization of cosmic microwave background (CMB) caused by reionization allows us to put constraints on its duration and redshift (Zahn et al. 2012; Benson et al. 2014).

2. The most intriguing observation is the 21 cm line, which will allow us to map hydrogen at high redshifts. These include SKA,\(^1\) LOFAR,\(^2\) MWA Tingay et al. (2013), PAPER (Parsons et al. 2010) and HERA.\(^3\)

The data from these types of experiments require Monte Carlo simulations for proper analysis. However, current computational capabilities do not allow us to run multiple simulations in large (1 Gpc) cosmological boxes with fine radiation transfer and galaxy formation. Therefore, semi-numerical models are adopted for these tasks.

3. PRELIMINARIES

3.1. Analytic Models

The analytical models of homogeneous reionization (i.e., Kuhlen & Faucher-Giguère 2012) are beyond the scope of this paper, and so we focus on two of the most popular inhomogeneous models. These are Miralda-Escudé et al. (2000) (MHR00 hereafter) and Furlanetto et al. (2004) (FZH04 hereafter) and their derivatives.

Both models are based on the underlying overdensity field $\delta$. The key concept is the density scale, i.e., the density averaged over some scale $R$. The density $\rho(R)$ can be defined as:

$$\rho(R) = \int_{V_R} \delta dV/V_R, \quad (1)$$

where $V_R$ is the volume of a sphere of a radius $R$, centered at the point of interest. However, in practice, smoothing is performed through filtering in the Fourier space.

If the Gaussian density field is considered, then another useful quantity emerges from the Fourier definition—the variance of density at a given scale:

$$\sigma(R)^2 = \langle \delta(R)^2 \rangle = \int_0^\infty P(k) W^2(kR) \, dk, \quad (2)$$

where $P(k)$ is the power spectrum and $W_R$ is the Fourier transform of a spherical filter:

$$W_R(r) = \Theta(1 - r/R). \quad (3)$$

We do not specify what the scalar field, $\delta$, is that we use in this method. It can be the baryon or dark matter density, the initial Gaussian field or evolved nonlinear field. Also, it can be the halo density field or star formation density.

In the case of the Gaussian field, the distribution of $\rho(R_0)$ in the universe is normal by definition for any $R_0$, and $\sigma(R_0)^2$ calculated with the Equation (2) is its variance. However, for any other non-Gaussian scalar field, the distribution can diverge from normal. Nevertheless, in order to have the plots easily readable and consistent with each other, we normalize the $\rho(R_0)$ to zero mean and unit variance. Even though this operation erases the shape of the distribution function, it essentially affects only visual representation of the figures. Thus, we label those normalized values as “in units of $\sigma^2$” in all the figures.

It is common in the literature to use other variables instead of scale $R$. Among these are the mass, $m$, of a sphere with the radius $R$, or variance, $\sigma^2$, at scale $R$. All three values can be

\(^1\) http://www.skatelescope.org/
\(^2\) http://www.lofar.org/
\(^3\) http://reionization.org/
derived from each other. In this paper, we use only $R$, since it is the most appropriate for our purposes.

3.1.1. MHR00 Model

The MHR00 model was built to describe the later stages of reionization, when only the small patches of hydrogen are left neutral. It describes a process of the ionization background burning into the dense neutral regions, where the recombination and photoionization rates are comparable. The characteristic overdensities of the regions where this effect takes place were studied in Kaurov & Gnedin (2015a) with the same simulation. The result shows that inside the ionized regions the local density is a proxy for the local ionization fraction.

This model uses one specific scale, $R_{\text{MHR}}$, and determines the ionization fraction of a cell based on its local density $\rho(R_{\text{MHR}})$ only. This relatively simple model is capable of describing Lyα forest statistics.

The model is based on the assumption of quasi-static ionization equilibrium, i.e., when the local recombination rate is close to the ionization rate:

$$R_{\alpha}x_{\text{ion}}^2(1+\delta)^2 = \Gamma(1+\delta)(1-x_{\text{ion}}), \quad \text{(4)}$$

where $\delta$ and $x_{\text{ion}}$ are local gas overdensity and ionized fraction, $\Gamma$ is ionizing background, and $R_{\alpha}$ is the ratio of the recombination rate for a homogeneous universe to the Hubble constant, which is order of unity at $z \approx 6$ (see MHR00, Equation (1)). Solving this equation for given ionization background and $x_{\text{ion}} = 0.5$ gives the density threshold above which the gas is neutral.

Even though this model describes the inhomogeneous reionization (some regions are ionized later than others), it still assumes the homogeneous ionization background throughout the universe. Thus, the main limitation of the model is that it does not incorporate any correlation from outside of the $R_{\text{MHR}}$ radius and, therefore, does not depend on the large-scale structure.

3.1.2. FZH04 Model

In contrast to the MHR00, the FZH04 model was developed to describe the morphology of the reionization on the large scales. In order to reproduce the large-scale inhomogeneity, it has to take into account overdensity, not only at a single scale, but on a range of scales.

In the FZH04 model, we assign to each point at position $r$ a one-dimensional function, trajectory $T(r)$, which corresponds to the density of the point defined at different scales $R$:

$$T_r(R) = \frac{\int_{\delta(x)W_r(|r-x|)dx}{\sigma(R)^2}}. \quad \text{(5)}$$

The physical motivation is that the function $T(r)$ can provide an estimate for the fraction of matter collapsed into halos (Press & Schechter 1974). Then, assuming a rate of ionizing photon production in halos, one can derive the total number of ionizing photons in the spherical regions centered at the point of interest. If for any of those regions the number of ionizing photons exceeds the number of hydrogen atoms in the same region, the point is considered ionized.

Various improvements can be made to this model, which allow us to include more sophisticated physics (Furlanetto & Oh 2005; Furlanetto et al. 2006; Alvarez & Abel 2007, 2012; Mesinger & Furlanetto 2007; Mesinger et al. 2011; Zahn et al. 2011; Battaglia et al. 2013; Kaurov & Gnedin 2013, 2014b; Zhou et al. 2013; Sobacchi & Mesinger 2014). However, the main principle remains the same. All physics are combined into the main parameter of the model—the barrier function, $B(R, z)$, which is the function of scale and redshift. The model predicts that the point is ionized at redshift $z$ if its trajectory $T(R)$ intersects with $B(R, z)$.

This model gained popularity, because it is physically justified, based on excursion set framework, which is widely used in structure formation theory, and is computationally efficient. It became a starting point for the development of semi-numerical codes like 21 cm FAST (Mesinger et al. 2011).

The weak part of this family of models is the transition from physical equations to the shape of $B(R, z)$. At this step, a lot of assumptions are made and it is hard to trace how they affect the accuracy of the model. The barrier effectively becomes degenerate, because of the large amount of physical effects contributing to its shape.

3.2. Numerical Simulation

For this study, we use simulations from the Cosmic Reionization On Computers (CROC) project (Gnedin 2014; Gnedin & Kaurov 2014) as a reference numerical simulation. These simulations include a large variety of physical processes, which affect the morphology of reionization in different ways on various scales. For instance, the non-spherically symmetric escape fraction may affect the shape of small bubbles at the earliest stages of reionization, while the bias of galaxy distribution regulates the morphology of ionization fronts on large scales.

The simulation is tuned to match the available observational constraints. These include the galaxy luminosity functions and full distribution function of Gunn–Peterson absorption in the spectra of the high-redshift quasars. However, in this study, we do not need precise tuning of a simulation. We only need a complexity of the ionization bubbles and the shapes of neutral patches, in order to test our methods.

With the use of the Adaptive Mesh Refinement algorithm, CROC simulations achieve a spatial resolution of 125 pc in simulation volumes of up to 40 $h^{-1}$ Mpc, which allows us to consider the IGM and filaments to be well resolved.

In this paper, we use a 40 $h^{-1}$ Mpc realization (run B40.sf1.uv2.bw10.A from Gnedin 2014) as our fiducial set and two other 40 $h^{-1}$ Mpc realizations (runs B40.sf1.uv2.bw10.B,C from Gnedin (2014)) for comparison. The scalar fields, which we extract from the simulation are: the baryon and dark matter density fields, and the ionization fractions of hydrogen.

4. THE FRAMEWORK OF ANALYTICAL MODELS FOR ANALYSIS OF NUMERICAL RESULTS

In this section, we approach a realization of the numerical simulation with the framework of the analytical model.

4.1. Preparing Numerical Simulation

For the following analysis, we use the down-sampled snapshots of 40 $h^{-1}$ Mpc to 256^3 uniform grid (the effective resolution is 156 $h^{-1}$ kpc). Next, for each pixel, we calculate the moment of its ionization. We adopt two thresholds, 10% and 90% weighted by mass. The vast majority of the cells cross these thresholds only once, therefore, we can assign those...
Figure 1. The moment of reaching 10% (left panel) and 90% (right panel) ionization level in a slice from $40h^{-1}\text{Mpc}$ simulation.

Figure 2. The overdensity of initial conditions (left panel) and evolved baryon density field at redshift 6 (right panel) in the same slice as in Figure 1.
values to the grid. In Figure 1, the slices of the redshift of ionization are plotted. In Figure 2, the same slice for the density IC and the evolved baryonic density field at $z = 6$ are plotted.

Immediately, we see that the ionization field is much smoother for the 10% threshold rather than for the 90% threshold. It motivates us to consider the time delay between the moments when a cell reaches the 10% and 90% ionization thresholds as a separate field.

In Figure 3, we plot the distribution of those delays. For the vast majority of the cells, this delay is small compared to the cosmological timescales; however, a fraction of the cells shows big delays. The peak-like structure of the histogram is an artifact due to the characteristic time between the simulation snapshots.

In Figure 4, we plot the delay for the same slice. The cells with long delays are correlated with the overdense cells in the density field. This correlation is caused by the filaments located in denser cells, which stay relatively neutral even when the surroundings are already highly ionized. Therefore, this effect fits into the MHR00 paradigm of the gradual ionization of the overdense regions.

4.2. Random Walk in Numerical Simulation

The trajectory, or random walk, which we described in Section 3.1.2, can also be defined in a numerical approach, i.e., in the simulation box. The smoothing of the scalar field can be performed in the same manner through Fourier space, applying a top-hat filter. The main difference is that the trajectory is not longer a continuous function, and, therefore, we have to discretize it. We choose a number of the physical scales $r_0, r_1, ..., r_N$ in comoving units.

In this paper, we stick with $r$ notation, since we work with different scalar fields, and values of $m$ and $\sigma^2$ are not constant across them. Also, not all scalar fields we use are Gaussian, and those are not described exclusively by the first moment statistics, power spectrum. Therefore, $\sigma^2$ is a less motivated quantity.

We call the barrier a two-dimensional function, $B(r, z)$, which is defined on a uniform grid of scales, $r_i$ and redshifts, $z_j$. The trajectory is a one-dimensional function associated with each cell $x$, $T_i(r_i)$, defined at all scales, $r_i$. It corresponds to the density of the scalar field in the cell after applying a smoothing filter of scale $r_i$.

The analytic theories based on Furlanetto et al. (2004) use the first time crossing as an indication of ionization. The condition of the first time ionization of a cell $x$ can formulated as follows:

$$z_{\text{ion}} = \max \{ z_j \mid \exists i, (T_i(r_i) > B(r_i, z_j)) \}. \quad (6)$$

It summarizes the barrier approach.

In order to translate a numerical simulation to the language of the analytical model, we calculate a random walk for every cell in our simulation box. In order to do this, we use eight log-spaced discrete smoothing scales—from a single cell to the half-box size. This number is found to be sufficient for our purposes, and increasing it does not affect the results. We generate a smoothed density field with every chosen scale. Then, we normalize the resulting scalar fields to the normal distribution with zero mean and unity standard deviation. This operation is performed only to avoid the usage of physical units (which differ from field to field) and better visualization of trajectories in figures. Skipping this step does not affect the final results. Finally, we assign to each cell eight numbers that correspond to the normalized overdensities for eight smoothing scales.

The method described above can work with any scalar field. In this paper, we consider only the IC density field (linear) and...
evolved matter density field (nonlinear). We leave the star density and halo density fields beyond the scope of this paper; however, both of these fields potentially can significantly improve the results.

For now, let us consider the IC, which is a Gaussian field, and the redshift of 10% ionization. We want to determine whether there is a correlation between the trajectories and the redshifts of ionization. We consider the cells that were ionized within some redshift interval and plot the density distribution of their trajectories along with the median in Figure 5. The deviation from zero tells us that, indeed, there is a dependence.

Next, we repeat this operation for all redshift intervals. We consider two density fields (IC and evolved DM density) and two ionization thresholds (10% and 90%). Thus, we have four possible combinations. The median trajectories for all of them are plotted in Figure 6. Also, for completeness, we study delays with the same approach and evolved density field (see Figure 7).

4.3. Discussion

The median trajectories in Figures 6 and 7 clearly show redshift dependence. In this section, we discuss the observed patterns and the physical reasoning behind them.

First, we have two figures which relate to the 10% ionization threshold with the IC and the evolved density fields. They both display a gradual decrease of a barrier from overdense to underdense, which confirms the inside-out scenario. The physical explanation for this observation is simple: the dense regions host galaxies, which produce the ionizing radiation, and, therefore, reionization starts from the overdense regions and ends inside the underdense—voids.

All the trajectories reach zero at the maximum smoothing scale, which is the expected box effect. However, the same behavior is expected in the real world, since cosmic variance is supposed to reach zero at some scale. Since the largest box we have access to is 40 h⁻¹ Mpc, we cannot distinguish these two effects.

On the other hand, at the smallest scales, there is also a reduced correlation between density and ionization field. For the IC density it is caused by the fact that the position of galaxies is not identically correlated with density peaks in the IC. For the evolved density field, the reasoning is different. The evolved density field correlates with galaxy positions much better; however, it also correlates with dense filaments, which require more intense flux of ionizing photons to ionize.

The phase plots show that the highest correlation (largest amplitudes of the trajectories) is achieved at scales 0.5–2 h⁻¹ Mpc. This might be interpreted as the range of scales where the majority of the information about the ionization field is contained. As mentioned above, due to the lack of larger boxes, we can only speculate regarding the upper bound of such a range. However, we can be more confident in the lower bound, because the resolution of the numerical simulation (0.6 h⁻¹ kpc) is much higher than the down-sampled grids (156 h⁻¹ kpc), which we used for this analysis.

Another feature that can be observed is the scale of the largest correlation amplitude. It increases from just below 1 h⁻¹ Mpc at redshift 15 to a few h⁻¹ Mpc scale at redshift 6. It can be associated with the growth of the characteristic bubble size.

The most important observation from these phase-space plots is that the median trajectories are distinguishable and, therefore, they contain information about the reionization history. It confirms the applicability of the excursion set framework for describing the reionization morphology.

Now, we consider the figures related to the 90% threshold. The main difference is located at lower redshifts, where the median trajectories are going up again. These correspond to the regions correlated with the local density, which we mentioned in Section 4.1. The IC density phase plot shows weaker upturn than the evolved density because, again, the density peaks in the IC are less correlated with filaments than in the evolved field.

This upturn reveals the transition between the two regimes FZH04 and MHR00. By design, the MHR00 model describes the late stages of reionization. It shows that denser regions will be ionized at later times. It is what we can see as growing trajectories in the phase plot. The scale of the largest correlation for this regime is the smallest in our analysis.

The question is if the trajectories can be associated with the redshift of ionization one to one. We see in Figure 6 that for the 90% ionization threshold some trajectories are indistinguishable from one another. However, the phase space of delayed field in Figure 7 does not have intersecting trajectories. It means that by splitting the 90% ionization threshold field into 10% ionization field and delays, we can avoid degeneracy in the phase space.

Another way of thinking about it is that the MHR00 model is valid not only at late stages of reionization, but at any redshifts inside the ionized bubbles. While the FZH04 model only describes the ionization fronts at low-ionization thresholds (10% in our case).

5. TRAINING THE ANALYTICAL MODEL ON A NUMERICAL SIMULATION

In Section 4, we applied the framework of the analytical model (the excursion set formalism) to the numerical result.
The measured trajectories behave as expected, which makes us more confident about the analytical approach. Hence, in this section, we study how well the analytical model can match a simulation.

One could try to construct an analytical model, which would incorporate the physics identical to the numerical simulation, and then compare both results. Instead, we consider a different approach. We question how well the analytical model can describe a given ionization field without relying on the underlying physics. We perform a sort of reverse engineering of the numerical result, trying to find the barrier in the analytical model, which can produce this ionization field.

Then, in Section 5.1, we describe our method of training the analytical model and in Section 5.2 we describe the method of extracting a barrier from the phase space.

The question which immediately emerges when we talk about training or fitting is what is the criteria of goodness. We provide an overview of them in Section 5.3.

Figure 6. The phase space of median trajectories color-coded with redshift and defined for the IC and 10% ionized threshold ionization field (top-left panel); IC and 90% (top right panel); evolved density field and 10% (bottom left); evolved density and 90% (bottom right).
5.1. Building a Model

As was shown in Section 4, there is a non-negligible delay between a pixel approaching the 10% and 90% ionization levels. While the trajectories, which correspond to the 10% ionization level, are distinct, those for the 90% level intersect with each other. It means that the random walk by itself is not informative enough to predict 90% ionization in some regions. However, it was also shown in Section 4 that the median trajectories, which correspond to the delay are distinguishable, and, therefore, can be described by a trajectory.

Thus, we propose to consider the ionization field as consisting of two components: the redshift of crossing the 10% ionization threshold and the delay to the 90% threshold crossing. Both of these fields are well distinguishable in the trajectory phase space.

These two components can be considered as a combination of the FZH04 and the MHR00 models. The FZH04 model describes the morphology of ionized patches at large scales, while the MHR00 is responsible for neutral patches inside ionized volume, which take longer to ionize.

5.2. Barrier Estimation

In Section 4, we operate with median trajectories; however, the excursion set formalism model, the FZH04 model, relies on barriers. Nevertheless, the median trajectories are useful, because they are easy to define and give a good sense of the overall behavior of the trajectories.

Now, if we imagine a simulation generated using excursion set formalism, then it would be possible to derive the barrier by simply calculating a ~99.9% percentile line, instead of the median in Figure 5. This will work for the analytical model, because all of the trajectories that were ionized in the redshift interval \([z_i, z_{i+1}]\) cross the barrier \(B(z_{i+1}, r)\) and do not cross \(B(z_i, r)\). Since it is not the case for a real numerical simulation with radiative transfer, because we have at least some noise in the phase plot, we need to come up with a more robust algorithm.

In Figure 5, the two-dimensional density of trajectories is plotted for a given redshift. In fact, the phase plot is three-dimensional, where the third dimension is the redshift. In this space, the series of barriers at different redshifts is represented by a surface.

The simplest algorithm would be the brute-force, i.e., to probe all possible barriers and find the one that allows us to achieve the best concordance with the reference simulation. This would be the most robust, but not an effective algorithm. We can optimize it by making an initial guess of a good barrier, and then only brute-force all barriers close to it.

In order to make a good initial guess for the barrier, we consider the gradients along the redshift axis. The collection of points with the highest gradients defines the surface, which is our best guess. Note that for the scale equal to our box size all gradients along the redshift axis will be zero, because the trajectories are not distinguishable on this scale. Consequently, the maximum gradient cannot be found and the barrier is not defined at this scale (see Figure 8).

No matter what is the training algorithm, it should rely on some sort of goodness criteria, which we discuss in Section 5.3. Here, we choose to optimize the cross-correlation coefficient (see Equation (7)) on all scales. The resulting barriers for the given simulation and 10% ionization threshold are presented in Figure 8. Depending on the application, one can choose a different criterion, for instance limit the scales of interest, and have a slightly different best fit.

The shape of the barriers can be qualitatively explained as follows. At the largest scales all median trajectories are indistinguishable. Therefore, there is not much information at those scales in the phase space and the barrier approach is not effective. Thus, the barrier should be high at those scales in order to have negligible effect. The same logic can be applied for the smallest scales, where median trajectories for the 10%
ionization threshold also approach zero. The majority of information is contained at intermediate scales. Therefore, in order to capture it, the barrier has to be lower in the middle. The slices of the numerical simulation and the result of our trained analytical model at redshift 8 are shown in Figure 9. The model is trained to match the power spectrum of neutral hydrogen; however, even visually we can establish that the analytical model mimics the large-scale structure of ionization fronts.

5.3. Goodness Criteria

The comparison between the numerical and analytical models had been carried out before in Zahn et al. (2011) and Battaglia et al. (2013). Here, we outline possible criteria and discuss why some of them are not applicable in our case.

*Global ionization fraction*, or optical depth averaged over the whole sky, does not trace any information about morphology and inhomogeneity of reionization. Therefore, it can be used only for estimating the total number of emitting photons, neglecting recombination (which in a general case can significantly depend on the morphology).

*Bubble distribution* has a few definitions. The first one is robust and based on smoothed scalar fields. It is equivalent to the power spectrum. On the other hand, if a bubble is defined as an ionized volume, which is not connected with other bubbles through ionized patches, then it becomes much harder to define it algorithmically. If the bubbles are defined as the largest spherical volume with some given ionized fraction (Zahn et al. 2007), then in our case it is not clear how to define bubbles for the dense semi-neutral filaments and for the cells right near them.

*Pixel-by-pixel* comparison, which was made in Battaglia et al. (2013), is the most powerful in the case where we expect a perfect match. However, if we expect some deviations, we will face a few uncertainties. First, as mentioned before, the redshift of ionization of a cell is not a well defined quantity. It depends on the threshold, and also the process of ionization cannot be instantaneous. Second, one should ask which areas are more important to match. For instance, at redshifts below 6 most of the observed signal comes from neutral patches, which occupy small volume. Therefore, pixel-by-pixel comparison has to take it into account weighting pixels by their contribution to the observed quantities.

*Topological quantities*, such as the Minkowski functional are used for the statistical analysis of the reionization and distribution of cosmological objects (Friedrich et al. 2011; McDonough & Brandenberger 2013). However, these quantities are not directly observed.

*Power spectrum* is the most common statistics for describing fields on large scales. Also, it is a direct observable, which will be measured with 21 cm experiments. In a vanilla FZH04 model, where only excursion set formalism and the Gaussian IC are used, the barrier and the power spectrum (as well as bubble distribution) are directly interconnected and one can be derived analytically from another. However, when we modify the model by using nonlinear density field and adding the neutral patches inside the ionized regions\(^4\) this convenience vanishes and we have to perform all calculations numerically.

\[ r_{XD} = P_{XD}/\sqrt{P_{XX}P_{DD}}. \]

Cross-correlation coefficient between the neutral hydrogen in the numerical simulation, \(D\), and analytical model, \(X\), defined as (Zahn et al. 2011):

In this study we consider only the last two statistics, because these are directly related to the observable quantities and do not have uncertainties in the definition. The result of training is shown in Figure 9 with black lines. The analytical model matches the numerical simulation within 10\% of percent level, which is consistent with the similar study in Zahn et al. (2011). In contrast to that study, we consider smaller scales and semi-neutral filaments, and as a result, we have a different shape of \(r_{XD}\) as a function of \(k\). The largest deviation from unity reaches 0.2 at scales \(\sim 2 \text{ } h^{-1} \text{ Mpc}\); the deviations at the same scales can be visually distinguished in Figure 9.

Besides the realization that has been used for training (realization A), we have two others with the identical physics, but different IC (B and C). We apply the same analytical model to these two realizations and compare the power spectrum and cross-correlation coefficients in Figure 9. The model performs equally well. Therefore, we can conclude that we did not overtrain the model.

Also, in Figure 9, we show the power spectrum of the analytical model applied to a 160 \(h^{-1}\) Mpc box, for which we do not have a numerical result. It illustrates how the analytical model can be expanded to larger volumes.

The three stages captured in Figure 9 represent the beginning, middle, and very end of reionization. The first one is characterized by individual bubbles with only a few galaxies within them. The model can reproduce the power spectrum; however, visually many bubbles are placed in the incorrect places. It happens, because in this study we used only density fields. The model can be significantly improved if the halos are considered as well. The second stage with overlapping bubbles corresponds to the global ionization fraction reaching \(~50\%). At this stage, the bubbles contain multiple galaxies, and, therefore, the location of each individual halo becomes less important. We found this stage to be the most difficult to mimic (the deviations in the correlation coefficient are the largest). Finally, the third presented stage shows the moment right after the reionization was complete. Only filaments remain partially neutral. At this stage, the most uncertain are the small scales. It shows the limitations of our approach in which overdensities are directly linked with ionization fractions.

In Section 4.3, we speculated that the shape of the estimated barriers tells us that most of the information lies in the range of scales \(0.5–2 \text{ } h^{-1} \text{ Mpc}\). However, here we showed that the largest deviations occur on the scales just above this range. We interpret it as the limitation of the barrier approach. Since the excursion set formalism is only an approximation to the numerical simulation, it is only capable of capturing the correlations partially.

6. CONCLUSIONS

In this paper, we limit ourselves to the approach based on the excursion set formalism. However, having all of the available information from the phase space, we could construct any mathematical model, for instance, based on the likelihood to the given median trajectories. The advantage of the barrier approach is the similarity with the existing and widely used...
Figure 9. The ionization fraction in the numerical simulation (the first row of panels) and trained analytical model (the second row) in the same slice as in Figures 1, 2, and 4. The power spectrum of the neutral hydrogen in the numerical simulations (dashed lines) and our model (solid) is shown in the third row of panels. The correlation coefficient (see Equation (7)) is shown in the forth row. Black is the realization A, blue and red are realization B and C. Solid lines correspond to the same analytical model, which is fitted only to realization A. The green solid line corresponds to the power spectrum calculated with the same analytical model in a 160 $h^{-1}$ Mpc box. The columns correspond to three different moments in time: early stage of reionization with 5% ionized fraction; intermediate stage with 50% ionized fraction and interloping bubbles; and late stage, when only the filaments remain partially neutral.
analytical models. The excursion set formalism is not the only analytical method that can be fitted into numerical simulation.

We have performed a detailed comparison between the numerical high-resolution simulation and approximate analytical methods. We studied how the framework of the analytical model (excursion set formalism) can help to statistically describe ionization fronts in the numerical simulation. We have shown that it is possible and have highlighted some physical properties, which are usually lost or cannot be easily seen in other statistics like power spectrum.

The statistics we developed is descriptive enough to be able to reproduce reionization history from density field. It allows us to build a model, which combines the framework of excursion set formalism Furlanetto et al. (2004) for describing the large-scale structure of ionization fronts and the threshold approach Miralda-Escudé et al. (2000) for small-scale neutral patches—filaments—inside ionized bubbles. We perform training of the model into a given numerical simulation, using the power spectrum as our main criterion. The fitted model is capable of reproducing the power spectrum of other simulation realizations, which were not used during the fitting.

Ideally, a theoretical model should be able to describe all of the mentioned observations, as discussed in Section 2. Our approach allows us to build a single model, and compare it versus all available observations.

We propose the following work flow. First, one runs a simulation with any physics included. The box might be relatively small and number of realization can be low. Such a numerical simulation allows one to model the Thompson optical depth, $\tau_{\text{Th}}$, and galaxy luminosity function. Then, the semi-analytical model is trained on this numerical simulation using the described method. The resultant model can generate as many mock catalogs as needed in boxes with sizes exceeding the size of the original simulation. These extended boxes are suitable for generating mock catalogs for $21$ cm experiments and to generate polarized CMB signal.

We made our code publicly available, and further details are available on [https://bitbucket.org/kaurov/211mm](https://bitbucket.org/kaurov/211mm).

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