A SYSTEMATIC STUDY OF L\textsubscript{\textalpha} TRANSFER THROUGH OUTFLOWING SHELLS: MODEL PARAMETER ESTIMATION

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ABSTRACT

Outflows promote the escape of Lyman-\textalpha\ (L\textalpha) photons from dusty interstellar media. The process of radiative transfer through interstellar outflows is often modeled by a spherically symmetric, geometrically thin shell of neutral gas that scatters photons emitted by a central L\textalpha source. Despite its simplified geometry, this “shell model” has been surprisingly successful at reproducing observed L\textalpha line shapes. In this paper, we perform automated line fitting on a set of noisy simulated shell-model spectra in order to determine whether degeneracies exist between the different shell-model parameters. While there are some significant degeneracies, we find that most parameters are accurately recovered, especially the \textit{H} \texti column density (N_{\text{\textit{H} \texti}}) and outflow velocity (v_{\text{exp}}). This work represents an important first step in determining how the shell-model parameters relate to the actual physical properties of L\textalpha sources. To aid further exploration of the parameter space, we have made our simulated model spectra available through an interactive online tool.

Key words: galaxies: high-redshift – galaxies: ISM – ISM: clouds – line: formation – radiative transfer – scattering

1. INTRODUCTION

Lyman-\textalpha\ (L\textalpha) emission enables us to both find and identify galaxies out to the highest redshifts. Whether or not a distant galaxy has a L\textalpha emission line appears to be closely connected with the presence or absence of outflows (Kunth et al. 1998; Atek et al. 2008). Partially coherent scattering of L\textalpha photons off the outflow provides an efficient way of shifting them into the wing of the line profile, where the galaxy is optically thin. Recent near-IR spectroscopic measurements have confirmed that the L\textalpha spectral line is systematically redshifted with respect to other non-resonant nebular lines (e.g., Steidel et al. 2010; McLinden et al. 2011; Kulas et al. 2012; Schenker et al. 2013; Erb et al. 2014; Shibuya et al. 2014; Song et al. 2014; Hashimoto et al. 2015; Rivera-Thorsen et al. 2015; Willott et al. 2015), which provides further support for the important role of (interstellar) outflows on the L\textalpha transfer process.

The theoretical modeling of L\textalpha spectra has been the subject of many studies, both purely analytical (Harrington 1973; Neufeld 1990, 1991; Loeb & Rybicki 1999; Dijkstra et al. 2006) and numerical (e.g., Loeb & Rybicki 1999; Ahn et al. 2000; Zheng & Miralde-Escudé 2002; Dijkstra et al. 2006; Hansen & Oh 2006; Tassis, 2006; Verhamme et al. 2006; Laursen et al. 2013; Behrens et al. 2014; Duval et al. 2014; Verhamme et al. 2015). The latter uses L\textalpha Monte Carlo radiative transfer simulations, with the ultimate goal of understanding the L\textalpha spectra emerging from galaxies. The simulations can broadly be split into two categories.

1. In the first class, the galactic environment is modeled as realistically as possible, mostly using hydrodynamical simulations (e.g., Tassis, 2006; Laursen & Sommer-Larsen 2007; Zheng et al. 2011; Verhamme et al. 2012; Behrens & Braun 2014; Smith et al. 2015). It is worth stressing that this is a challenging task as simulating the distribution and kinematics of neutral gas in feedback driven outflows—which play key roles in the L\textalpha transfer process—require a sub-parsec spatial resolution (compare, e.g., Figures 10 and 11 in Fujita et al. 2009).

2. The second approach is to simplify the complex topography of galaxies enormously and to use an abstract geometrical setup instead. This approach is computationally cheap, which allows model L\textalpha spectra to be generated for a large set of parameters.

A particular example from the second group, which has been very successful in reproducing observed L\textalpha spectra, is the shell model (Ahn 2004; Verhamme et al. 2006; Schauer et al. 2011). This model consists of a central L\textalpha source surrounded by an outflowing thin, spherical shell of hydrogen and dust. The shell model has six model parameters: the equivalent width of the emitting source, EW; the intrinsic width of the L\textalpha spectrum, \sigma; the hydrogen column density, N_{\text{\textit{H} \texti}}; the dust optical depth, \tau_d; the temperature, T; and the outflow velocity, v_{\text{exp}}.

Due to its simplicity, and the ability to reproduce a number of observed spectra, the parameters of the shell models have been frequently used to constrain galaxy properties (e.g., Verhamme et al. 2006, 2008; Tapken et al. 2007; Kulas et al. 2012; Chonis et al. 2013; Wofford et al. 2013; Shibuya et al. 2014; Hashimoto et al. 2015; Martin et al. 2015). These previous studies rely on either visual inspection, and are thus affected by subjectivity, or they use a discrete set of models from which they choose the best-fitting spectrum based on \chi^2 values. A systematic study of shell models and their physical relevance has yet to be performed, however. A number of open questions include the following.

1. Is there a unique mapping between shell-model parameters and L\textalpha spectra, or can several different parameter combinations—with different physical implications—produce indistinguishable spectra? If the latter is true, two equally good fits to an observed spectrum could be found that have very different physical meanings, and so caution must be exercised when drawing conclusions from shell-model parameter fits.

2. How uncertain are the parameters obtained from the model fitting procedure? The best-fitting shell-model
parameters to observed spectra are often quoted without estimates of uncertainties.

The two questions are clearly related to one another: question (1) focuses on the intrinsic degeneracies between parameters, while question (2) concerns specific example spectra with some measurement uncertainty and the effect this has on the accuracy with which the model parameters can be recovered. Both must be understood if we are to use the observed spectral line shapes of Lyα to infer the physical properties of outflowing gas. This is especially important if one considers that at high-z, Lyα is likely the only line that will allow us to put any constraints on outflows of atomic hydrogen gas.

The goal of this paper is to address these questions and to develop a procedure to automatically fit shell-model parameters to “realistic” (i.e., noisy) Lyα spectra. The paper is structured as follows. In Section 2, we explain our method for constructing simulated Lyα spectra and describe the fitting procedure we use. We present the results of applying this procedure to a range of simulated spectra in Section 3 and discuss the implications of our results in Section 4. We then conclude in Section 5.

2. METHOD

We briefly describe the Lyα radiative transfer calculations in Section 2.1 and present our application to the shell model in Section 2.2. Our fitting procedure is then described in Section 2.3.

In the following, log denotes the logarithm to base 10, and ln is used for the natural logarithm. The wavelength is given in units of velocity offset from line center, \( v = c(\lambda/\lambda_0 - 1) \), where \( \lambda_0 \approx 1215.67\text{Å} \) corresponds to the wavelength at line center.

2.1. Lyα Radiative Transfer

We use the Lyα Monte Carlo (MC) radiative transfer code tlaα, which was previously used in Gronke & Dijkstra (2014). We briefly summarize the main points of the algorithm here. For a more detailed review, we refer the reader to Dijkstra (2014).

In a radiative transfer MC code, the photons are represented by individual particles (or, rather, photon packets) whose paths of propagation in real and frequency space are tracked throughout the simulation domain. We repeat the following steps for each photon in the MC simulation.

1. A photon is emitted in direction \( k_i \), with intrinsic frequency \( v_i \) drawn from some Lyα source emission pdf, \( f(v) \).

2. A number \( \tau \) is drawn from an exponential distribution, quantifying the distance \( d \) the photon will travel. Here, \( d \) is given by \( \tau = \int_0^d (\sigma_1 n_1(s) + \sigma_2 n_2(s))ds \), where \( n_X \) and \( \sigma_X \) represent the number density and the cross section of dust (\( \sigma_d \)) or hydrogen (\( \sigma_H \)), respectively.

3. The position of the photon is updated to \( p \rightarrow p + kd \). At the new position, the photon is either scattered by hydrogen (probability of \( n_H/(\sigma_1 n_1(s) + \sigma_2 n_2(s)) \), or absorbed by dust.\(^2\) In the former case, a new direction is drawn from the proper phase function (i.e., the angular redistribution function), and a new frequency is drawn from the frequency redistribution function (which depends on direction; see Dijkstra & Kramer 2012).

4. Steps (2) and (3) are repeated until the photon escapes the simulation domain or is absorbed.

If the photon escapes the simulation domain, its frequency and other properties are recorded. This procedure is repeated until the desired total number of photons is reached. Their combined frequencies then yield the simulated Lyα spectrum.

2.2. Implementation of the Shell Model

As discussed in Section 1, the shell-model parameters consist of: (a) the source properties—namely, the equivalent width of the emitting source EW and the intrinsic width of the Lyα spectrum \( \sigma_1 \); and (b) the shell properties, i.e., its hydrogen column density \( N_1 \), its dust optical depth \( \tau_d \) along a path that passes radially through the shell (the dust is confined to the neutral shell), temperature \( T \), and the outflow velocity \( v_{exp} \). In order to cover a particular domain of the parameter space with as few simulation runs as possible, we split these six parameters into two sets: the simulation parameters \( (v_{exp}, N_1, T) \) and the post-processing parameters \( (EW, \sigma_1, \tau_d) \). The simulation parameters change the spectrum in a complex way. We therefore discretize these parameters on a grid and run our radiative transfer simulation at each combination of parameter values. This results in a grid of Lyα spectra with parameters presented in Table 1. The exact discretization was chosen so that the grid is fine enough to allow for an accurate likelihood analysis, i.e., so that the likelihood functions of our simulated spectra are sufficiently well sampled.

The post-processing parameters do not require explicit simulations, but can be modified a posteriori. This considerably reduces computational cost and allows the parameters to be varied continuously (i.e., they are not restricted to discrete values on a grid). Each photon has its own unique weight in our

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**Table 1**

| Simulation Grid for Shell Model Parameters |
|------------------------------------------|
| **Symbol** | **Values** | **Units** |
| \( v_{exp} \) | (0, 2, 5, 8, 10, 15, 20, 30, 40, ..., 400) | km s\(^{-1}\) |
| \( \log N_1 \) | (17.0, 17.2, ..., 21.8) | log(cm\(^{-2}\)) |
| \( \log T \) | (3.0, 3.4, 3.8, ..., 5.6) | log(K) |
| \( \sigma_1 \) | [1, 800] (continuous) | km s\(^{-1}\) |
| \( \tau_d \) | [0, 5] (continuous) | ... |
| EW | [1, 150] (continuous) | Å |

**Notes.**

\(^1\) Expansion velocity.
\(^2\) Hydrogen column density.
\(^3\) Temperature.
\(^4\) Width of intrinsic spectrum.
\(^5\) Dust optical depth.
\(^6\) Intrinsic equivalent width.
simulations which is given by
\[ w = \frac{f_e(v_i)}{f_r(v_i)} e^{-\Delta N_{\text{HI}}/N_{\text{HI}}} \]
where \( v_i \) is the velocity at which we inject the photon and \( \dot{N}_{\text{HI}} \), is the hydrogen column density actually encountered by the photon in the simulation.\(^3\) Furthermore, \( f_e \) denotes the emission pdf that we used in our MC simulation (characterized by a Gaussian emission line with \( \sigma = 800 \text{ km s}^{-1} \) plus continuum; see below), while \( f_r \) denotes the emission pdf that we wish to simulate in post-processing (which is also a Gaussian with standard deviation \( \sigma_r \) plus continuum). This means \( f_e \) and \( f_r \) are of the form
\[ f(v_i) = \begin{cases} \frac{1}{\eta + 1} \left( \frac{\eta}{\Delta v} + G(v_i|\sigma) \right) & \text{for } |v_i| < \frac{\Delta v}{2} \\ 0 & \text{otherwise} \end{cases} \]
where \( G(v|\sigma) \) denotes a normalized Gaussian with standard deviation \( \sigma \) centered at \( v = 0 \), \( \Delta v \) is the bandwidth of the spectrum, and \( \eta = \Delta v \lambda_{\text{Ly}\alpha}/(c \text{EW}) \), where \( \lambda_{\text{Ly}\alpha} \) is the emission wavelength of \( \text{Ly}\alpha \). We stress that each photon is assigned an individual weight. This means the post-processing parameters also affect the shape (and not only the normalization) of the resulting spectrum. We tested our method by comparing several post-processed spectra with “real” spectra, where \( \tau_{\text{esc}}, \sigma_r, \) and \( \text{EW}_i \) were given as fixed input parameters in our MC radiative transfer code. Note that in this framework it is possible to vary the escape fraction \( \alpha \) and to avoid tying our results to a particular observational configuration, we chose \( n_i \) to be Gaussian, with zero mean, constant variance, and no correlations between frequency bins. The frequency binning was chosen so that the noise rms \( v = [−2500, 2500] \text{ km s}^{-1} \), with a simple tophat bandpass and no smoothing. This corresponds to a relatively high (but plausible) resolving power of \( R = c/\Delta v \sim 6000 \), which lies within the capabilities of, e.g., the IRCS instrument on the Subaru telescope.\(^8\) We discuss the impact of changing the binning in Section 4.2.

Following our assumption of uncorrelated Gaussian noise, the appropriate goodness-of-fit statistic for the spectra is

\[ \Delta \chi^2 = \sum_i \left( \frac{d_i - F(v_i; \theta)}{\tilde{\sigma}_i} \right)^2, \]

where the sum is taken over the frequency bins. This defines the likelihood \( L(\theta|d) \propto e^{-\Delta \chi^2/2} \). We systematically explore the likelihood surfaces of our simulated data using Markov Chain Monte Carlo (MCMC) and nonlinear optimization (fitting) methods in the next section. Since we have assumed that the noise rms \( \sigma_i \) (i.e., the statistical weight) \( \tilde{\sigma}_i = \sigma_i/v_i \) is constant and is independent of model parameters.

\(^3\) This column density \( \dot{N}_{\text{HI}} \gtrsim N_{\text{HI}} \) because scattering increases the total path a \( \text{Ly}\alpha \) photon traverses before it escapes from the shell.

\(^4\) A uniform emission pdf would achieve the same effect, but this would be inefficient, overpopulating the wings of the spectrum.

\(^5\) The online tool can be accessed at http://maxgronke.wordpress.com/tools/thac_web/ or http://bit.ly/man-alpha. On the website, it is possible to (i) plot up to four shell-model spectra, (ii) upload and display your own spectra, and, (iii) download the plotted data.

\(^6\) These were drawn from a uniform distribution with the bounds given in Table 1, except for \( \gamma_0 \), which was drawn from [0, 2] to save on computational resources.

\(^7\) While we expect this range to be sufficient for most observed spectra (i.e., wide enough to sample the \( \text{Ly}\alpha \) line and the adjacent continuum), it is possible to alter this range if needed since our method is not dependent on this choice.

\(^8\) http://subarutelescope.org/Observing/Instrument
the statistic

\[ \Delta^2 = \sum_i \left( d_i - F(v_i; \theta) \right)^2 \]  

(6)
can be used interchangeably with \( \Delta \chi^2 \) by optimization algorithms, a fact that we will also use in Section 3.

Note that there is also a “theoretical uncertainty” associated with the model spectrum \( F(v; \theta) \). Because each spectrum is calculated through an MC radiative transfer procedure with a finite number of photons, there is a Poisson error on the value of \( F \) in each bin, determined by the number of photons that ended up in that bin (and their respective weights). Since the number of photons per bin also varies as a function of the input parameters, the theoretical uncertainty will vary across the parameter space in a potentially complicated way. This uncertainty has been mitigated as much as possible by our use of a large number of photons to calculate each model on the grid of simulations, as described in Section 2.2. This helps to ensure that the assumed observational uncertainty, \( \delta_i \), dominates the Poisson uncertainty in each bin. Under these conditions, the theoretical uncertainty can safely be ignored, and Equation (5) remains valid.

### 3. RESULTS

#### 3.1. Intrinsic Degeneracies

To investigate whether the best-fit parameters recovered by the standard spectral fitting procedure could be misleading, we performed 640 local \( \Delta^2 \) minimizations on each of the 50 spectra in our fully simulated observational data set (see Section 2.2) without adding any additional noise \( (n_i = 0) \). We chose the number of local minimizations rather arbitrarily, but sufficient to show a few specific cases that highlight the dangers of blindly following this procedure. We started each minimization from a randomly chosen initial guess. We then discarded the fits where \( \Delta^2 \) was less than the \( \Delta^2 \) for the true model parameters. A more systematic study that includes observational uncertainties is presented in Section 3.2.

Figure 1 shows examples of degenerate model fits for each of the shell-model parameters. In each panel, we display the “observed” spectrum (in gray), the spectrum obtained for the true input model parameters (black), and an alternative best-fit model (blue). It can be seen that no shell-model parameter is protected from catastrophic recovery errors, as the magnitude of the difference in each of the example cases allows significantly different physical interpretations.

As a concrete example, the central panel in the bottom row of Figure 1 shows a spectrum that can be explained with a very
high dust content ($\tau_d = 5$), although it was actually produced by a model with very little dust ($\tau_d = 0.29$). In fact, the value of $\tau_d = 5$ here is the (arbitrarily chosen) upper limit of our parameter space (see Section 2.2), so an even higher value may be possible. In this model, the low value of $\sigma_i$ and the high outflow velocity combined with the low hydrogen column density results in essentially no interaction between the photons and the hydrogen. The path length through the shell (and thus the chance of absorption) is therefore approximately the same for each photon, and so $\tau_d$ has little or no effect on the shape of the resulting spectrum.\footnote{In the notation of Equation (1), this means that in this particular case, $N_{\rm H_\alpha} \sim N_{\rm H_\beta}$ for all photons, leading to no spectral shape change due to a change of $\tau_d$.} The same phenomenon also explains why a $\sim 1.5$ order of magnitude decrease in $\overline{H\alpha}$ column density barely affects the spectrum in the central panel of the top row.

Another case where a parameter hits its prior boundary is in the lower left panel of Figure 1, where $\sigma_i$ reaches its maximum permitted value of 800 km s$^{-1}$. The reason the intrinsic spectral width plays no role in the shape of this absorption feature is because the high hydrogen content causes each Ly$\alpha$ photon to be scattered many times. The relatively large value of $\tau_d$ leads to a high absorption probability, yielding this broad absorption feature. While in this case $\sigma_i$ plays only a minor role, with different values leading to qualitatively similar spectra, the same goodness of fit can only be reached by also changing the other parameters, in particular, $\tau_d$ and EW$i$. This can be explained as follows: while the increase in $\sigma_i$ means that there are initially more Ly$\alpha$ photons in the wing, which have a higher chance of not being absorbed, this is compensated somewhat by the higher dust content. Since this increase also (and more strongly) affects photons traveling longer distances (i.e., the ones closer to the core), a higher number of Ly$\alpha$ photons is also needed to return a similarly good fit as the true model.

The EW$i - \tau_d$ degeneracy is also observable in the bottom right panel, although the difference in EW$i$ is not as large. This is because for emission features, EW$i$ seems to be reasonably well constrained by the continuum level.

Finally, the expansion velocity is thought to be well constrained by the position of the spectral peaks and troughs. The situation shown in the top left panel is therefore less straightforward—the effects of changing of $v_{\text{exp}}$ can only be compensated by jointly changing EW$i$, $\sigma_i$, and $\tau_d$.

3.2. Parameter Uncertainty

We now turn our attention to the uncertainty associated with the estimated parameters obtained through shell-model fitting. First, we consider two example cases, each represented by a spectrum for which the input shell-model parameters were correctly recovered. Note that our simulated data set contains absorption, single-, and double-peak emission profiles—just as observed Ly$\alpha$ spectra do (e.g., Steidel et al. 2010; Rivera-Thorsen et al. 2015; Yang et al. 2015). Out of these, the two cases chosen feature a double-peaked emission and a broad absorption profile to show the extent of possible degeneracies. Moreover, in some cases (especially at higher redshift), the blue peak may be further suppressed by the intergalactic medium (Dijkstra et al. 2007; Laursen et al. 2011), in which case our double-peaked example is actually more representative of what has been observed.

We begin by constructing a simulated observation of each spectrum, as described in Section 2.3. The noise in each bin is chosen to have an rms of $\bar{\delta}_i = 0.5I$, where $I$ is the mean intensity of the spectrum. Note that while the noise properties have been chosen rather arbitrarily, the procedure does not depend on this choice and also works with more realistic data errors. This choice of $\bar{\delta}_i$ ensures that $\bar{\delta}_i > \bar{\delta}_i_{\text{Poisson}}$ (see Section 2.3) and can be thought of as representing random errors due to instrumental effects and so on.

This noise level corresponds to signal-to-noise ratios ($S/N$s) of $\sim15$–$50$, which is comparable with existing surveys (e.g., Adams et al. 2011). We estimated the $S/N$ by maximizing the quantity $\sum d_i/\sqrt{\sum \hat{s}_i^2}$, where the sums are taken over several adjacent bins. This corresponds to the standard procedure in observing pipelines (S. Wilkins 2015, private communication). For double-peaked profiles and absorption features, different measures are sometimes used—e.g., taking the difference between the continuum level and the absorption feature—that tend to result in higher $S/N$ estimates. We will not consider such measures here.

Next, we sample the likelihood of Equation (5) using the affine invariant MCMC ensemble sampler emcee (Goodman & Weare 2010; Foreman-Mackey et al. 2012). We use 900 walkers with 500 steps each (including 50 steps of burn-in). For the starting positions of the walkers, we used the $\Delta^2$ minima found in Section 3.1, weighted by the value of the likelihood at that point, plus a small random perturbation to avoid producing initial paths that are too similar.

Figure 2 shows the results of the MCMC parameter estimation for the first example case,\footnote{This and the other triangle plots were produced using a modified version of triangle.py (Foreman-Mackey et al. 2014).} an asymmetric, double-peaked profile with an estimated $S/N$ of $\sim32$. The true (input) shell-model parameters are well recovered, falling within the 68% credible interval for all but $\tau_d$, which is estimated to be slightly higher than its actual value. One can also see that the expansion velocity and column density are very well constrained (in fact, reaching our grid resolution limit), and that the $1\sigma$ uncertainty on the temperature is almost half an order of magnitude.

The second example, a spectrum with a broad absorption feature and an $S/N \sim 20$, is shown in Figure 3. The uncertainties on the estimated shell-model parameters are much larger than in the previous example, with all but $N_{\overline{H\alpha}}$ being relatively poorly constrained. Degeneracies between many of the parameters can be seen clearly; the values of $\sigma_i$, EW$i$, $N_{\overline{H\alpha}}$, and $\tau_d$ are all correlated with one another, for the reasons discussed in Section 3.1. Note that the distinct directions visible in the $\tau_d - \overline{EW}$ plane, and other “striping” features in the plots, are a result of the discrete parameterization of log $N_{\overline{H\alpha}}$, which is mostly localized to the three preferred grid values of [20.4, 20.6, 20.8]. This was confirmed to be the case by plotting the MCMC steps falling in these three column density bins individually—it is not an artifact of the sampling procedure. A higher-resolution gridding of the log $N_{\overline{H\alpha}}$ parameter would reduce this effect. Figure 4 shows an overview of the estimated parameters for all 50 spectra in our simulated data set after running exactly the same MCMC procedure as for the two example spectra. The data points are colored according to spectral type, which was assigned to each spectrum following visual inspection. The
parameter estimation procedure reliably recovers at least some of the shell-model parameters for all spectral types, particularly the expansion velocity \( v_{\text{exp}} \) and column density \( \log N_{\text{HI}}/\text{cm}^{-2} \) (although the uncertainty is larger for smaller column densities). The intrinsic source parameters \( \sigma_i \) and \( EW_i \) are also mostly well recovered, but with a bigger uncertainty. An exception is for spectra with absorption features, where \( \sigma_i \) is typically overestimated by \( \sim 200 \text{ km s}^{-1} \).

The worst constraints are obtained for \( T \) and \( \tau_d \), for which the scatter and uncertainty often reach the prior boundaries for those parameters.

4. DISCUSSION

Given the large parameter space spanned by the shell-model parameters and the consequent variety of Ly\( \alpha \) spectra (as is nicely illustrated in Figure 5 of Schaerer et al. 2011), it is...
difficult to make foolproof statements about parameter degeneracies and uncertainties. We generally recommend comparing individual spectra to the theoretical predictions on a case-by-case basis instead. In this section, we discuss how we can nevertheless reach more generic conclusions on parameter degeneracies and uncertainties by analyzing a sample of 50 mock spectra.

4.1. Parameter Uncertainties and Degeneracies

From the results of our likelihood analysis, we find the following.

1. Lyα spectra are very sensitive to the expansion velocity, \( v_{\text{exp}} \). In particular, double-peaked profiles allow the underlying velocity field to be recovered with great accuracy (limited by the simulation grid spacing to \( \sim 10 \text{ km s}^{-1} \) in this study). Absorption features and single peaks lead to greater uncertainties of up to \( \sim 50 \text{ km s}^{-1} \). This is consistent with the findings of Verhamme et al. (2008).

2. The intervening column density, \( N_{\text{H}_1} \), can also be well recovered—at least for \( N_{\text{H}_1} \gtrsim 10^{19} \text{ cm}^{-2} \). In this high column density regime, the (68% CL) uncertainty was limited by our grid spacing to \( \Delta \log N_{\text{H}_1}/\text{cm}^{-2} = 0.2 \),

Figure 3. Same as Figure 2, but for a simulated spectrum with a Lyα absorption feature.
while for lower column densities the uncertainty can be up to one order of magnitude.

3. The effective temperature (including turbulent motion as well as the true temperature) has a complex effect on the \( \text{Ly} \alpha \) spectrum, and in most cases this parameter cannot be usefully constrained (also see, e.g., Verhamme et al. 2008).

4. The width of the intrinsic spectrum, \( \sigma_i \), can be recovered for \( \text{Ly} \alpha \) emission features with very high accuracy (\( \Delta \sigma_i \sim 50 \text{ km s}^{-1} \)). For absorption features, on the other hand, this parameter is not constrained so well (\( \Delta \sigma_i \sim 200 \text{ km s}^{-1} \)).

5. We found that the dust content, \( \tau_d \), was essentially unconstrained by the shape of the \( \text{Ly} \alpha \) spectrum. Exceptions to this are for some double-peaked features with low dust content, where the dust content defines the ratio of the heights of the peaks. If, however, measurements of the \( \text{Ly} \alpha \) escape fraction \( f_{\text{esc}} \) are available, it is possible to use this extra information in our analysis. We then expect \( \tau_d \) to be better constrained in some cases.

6. The intrinsic equivalent width, \( \text{EW}_i \), can mostly be recovered with an uncertainty of \( \sim 20 \text{ Å} \), regardless of spectral shape and the value of \( \text{EW}_i \).

Note that these numbers depend on the spectral resolution and quality (S/N). We present the result of changing these quantities in the next section.

We also want to highlight that additional parameters can easily be included into our analysis, which might lead to further degeneracies. For example, the line center of the intrinsic spectrum can be unknown or afflicted with uncertainties when dealing with real data. We found that in some cases this “spectral shift” is degenerate with the outflow velocity \( v_{\text{exp}} \) and/or the column density \( N_{\text{HI}} \).

4.2. Impact of S/N and Frequency Binning

To test the sensitivity of our results to the assumed measurement uncertainties, we randomly selected 10 out of the 50 simulated spectra and repeated the analysis of Section 3.2 for five different noise levels, \( \hat{\sigma}/I = (0.25, 0.5, 1, 2, 4) \). We also include the two spectra analyzed in Section 3.2, for which the resulting S/Ns are \( \sim (64, 32, 17, 9, 4) \) and \( (39, 20, 10, 6, 3) \), respectively. Note that different noise realizations were drawn for each of the noise levels for each spectrum.

Figure 5 shows the resulting parameter uncertainties as a function of S/N for each of the \( 10 + 2 \) spectra. For \( v_{\text{exp}}, N_{\text{HI}}, \) and \( \sigma_i \), there is a flattening in the uncertainty beyond...
for all types of spectra. A similar behavior is found for EW_{\text{E}}, but at a slightly higher S/N of \sim 30, although in this case the curves do not become completely flat, even at the lowest noise levels we considered. For the remaining two parameters (\tau_d, T), the evolution of the uncertainty with increasing S/N is not so systematic, with different behaviors for different spectral types. For T, some of the spectra show the same flattening at high S/N as the other parameters, for example, while others are considerably more scattered. Note that because the noise realizations change between the different choices of noise level, it is not surprising that there should be some random variation in the goodness of fit and parameter uncertainties. For \tau_d, there is a split between spectra for which the uncertainty rapidly decreases with S/N and those for which it changes only slightly (presumably in cases where the spectra are relatively independent of \tau_d, so it remains poorly constrained).

In summary, for S/N \sim 30, four of the six shell-model parameters can be obtained up to an uncertainty of (\Delta v_{\text{exp}}, \Delta \log N_{\text{HI}}, \Delta \sigma_{\text{E}}, \Delta EW_{\text{E}}) \sim (70 \text{ km s}^{-1}, 0.5, 100 \text{ km s}^{-1}, 40 \text{ Å}) for the majority of spectra, and these limits can be further decreased by increasing the S/N.

Finally, we also varied the frequency binning (\Delta v_i = (25, 50, 100, 200, 250, 300, 500) \text{ km s}^{-1}) for several of the mock spectra in order to test the influence of the spectral resolution on the parameter estimates. Figure 6 in the Appendix shows that our constraints depend weakly on R provided that R \geq 10^3. For lower R, the constraints on several parameters (especially v_{\text{exp}}) increases rapidly for R < 10^3, but only for some models. For example, for the case presented in Figure 2, the characteristic double peak disappears for \Delta v_i = 250 \text{ km s}^{-1} (R \sim 10^3), which naturally leads to drastically increased uncertainties on many of the parameters. We therefore caution against conclusions that are too general on the precise impact of R, as this strongly depends on the spectrum that is analyzed.

5. CONCLUSION

The “shell model” for Ly\alpha transfer through galactic outflows has enabled a wide range of Ly\alpha spectra to be characterized in terms of six parameters. An important goal is to understand what physical information is actually encoded in these parameters. This is an important question: if the parameters of the shell model contain a connection to the underlying physical properties of outflows, then the shell model provides an extremely quick and useful way to capture information about radiative transfer processes on scales that are difficult to model from first principles.

As a first step toward addressing this question, we have constructed a large library of shell-model spectra, which are available through an interactive online tool. A similar library was presented by Schaerer et al. (2011), which was used in fitting observed Ly\alpha spectra (e.g., Hashimoto et al. 2015). Our
work differs in that our grid of spectra is sufficiently closely meshed\(^{11}\) to allow a systematic study of possible degeneracies between model parameters via a fully automated likelihood analysis. In order to make this computationally tractable, we used a post-processing technique to model three of the six shell-model parameters. We then applied an automated fitting routine to a small simulated data set of “noisy” shell-model spectra to see if a likelihood analysis can accurately recover the true (input) model parameters. This presents an important test of the reliability of shell-model fitting procedures that are being used in the literature and provides a simple estimate of the uncertainties on the recovered best-fit model parameters.

Our main findings include that from the spectral shape alone it was not possible to provide good constraints on the dust content, \(\tau_d\), and effective temperature, \(T_e\), in most models. In contrast, we were able to recover the outflow velocity \((v_{\text{exp}})\) and the hydrogen column density \((N_{\text{H I}})\) particularly well (especially when \(N_{\text{H I}} \gtrsim 10^{20} \text{ cm}^{-2}\)). These two results reflect the fact that \(\text{Ly}\alpha\) radiative transfer observables are most sensitive to the hydrogen distribution and kinematics. Dust affects these observables (emerging spectrum, total flux), but how much depends on other parameters such as \(N_{\text{H I}}, v_{\text{exp}}\), and \(\sigma_i\). This is consistent with observations that indicate that \(\text{Ly}\alpha\) escape is greatly affected by gas kinematics and that is likely responsible for the observed large scatter between \(f_{\text{esc}}\) and \(\tau_d\) (see, e.g., Kornei et al. 2010; Blanc et al. 2011; Hayes et al. 2011).

More quantitatively, for spectra with \(S/N_s \sim 30\) and spectral resolving power \(R = 6000\), four of the six shell-model parameters can be obtained up to an uncertainty of \((\Delta v_{\text{exp}}, \Delta \log N_{\text{H I}}/\text{cm}^{-2}, \Delta \sigma_i, \Delta \text{EW}_\alpha) \sim (70 \text{ km s}^{-1}, 0.5, 100 \text{ km s}^{-1}, 40 \text{ Å})\) for the majority of our spectra (see Figure 5 and Section 4.1). These constraints can be improved by increasing the \(S/N\) (Figure 5). We found a weak dependence of our results on \(R\) down to \(R \sim 1000\) (below which our constraints deteriorate faster). However, statements about the impact of the resolving power \(R\) depends in detail on the features in the spectrum (e.g., the presence of double peaks clearly can depend on \(R\)).

In general, precise quantitative statements on the magnitude uncertainties and/or the extent of degeneracies depends on the location in the parameter space. (For example, it was not possible to recover \(\sigma_i\) specifically for spectra with an absorption feature.) We therefore recommend a case-by-case analysis of observed spectra using a full likelihood analysis (similar to the one presented in Section 3.2).

The likelihood analysis allows us to characterize spectra in a systematic, automated way and to produce robust estimates of parameters, their uncertainty, and the degeneracies with other spectra. This procedure will be useful in the near future, when a larger sample of \(\text{Ly}\alpha\) spectra with sufficient \(S/N\) and spectral resolution becomes available. In a follow-up paper (M. G. Gronke et al. 2015, in preparation) we will generate spectra for more realistic models and fit shell models to these. This analysis will help us take the next and final step toward

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\(^{11}\) Quantitatively, we have sampled the \((v_{\text{exp}}, \log N_{\text{H I}}, \log T)\) space with 10,800 models, while Schaerer et al. (2011) have 780 models to cover this parameter space. In addition, we allowed the dust opacity to vary continuously, while Schaerer et al. (2011) ran 8 discrete dust opacities.
understanding what physical information is contained in the shell-model parameters.

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APPENDIX

VARYING THE RESOLVING POWER $R$

For the main results we presented in the paper, we assumed $R = 6000$. Here, we quantify the impact of varying the spectral resolution/resolving power while keeping the S/N fixed at $\sim 35$. Note that we generate a different noisy random realization of a given shell model for each $R$. This explains why our constraints do not vary monotonically with $R$ for a given model.

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