Detecting dense gas tracers in the $z = 3.042$ gravitationally lensed star-forming galaxy SDP.81 through a matched filter in the uv-plane

THESIS

Submitted in partial fulfillment of the
requirements for the degree of

MASTER OF SCIENCE
in
ASTRONOMY

Author :	J. van Marrewijk
Student ID :	1644971
Supervisors :	M. Rybak & J. Hodge
2nd corrector :	M. Hogerheijde

Leiden, The Netherlands, July 31, 2020

Detecting dense gas tracers in the $z = 3.042$ gravitationally lensed star-forming galaxy SDP.81 through a matched filter in the uv-plane

J. van Marrewijk

Huygens-Kamerlingh Onnes Laboratory, Leiden University
P.O. Box 9500, 2300 RA Leiden, The Netherlands

July 31, 2020

Abstract

Submillimeter galaxies (SMGs) are extreme star-forming galaxies with large dust reservoirs. However, the link between these extreme star-forming conditions and the molecular gas of SMGs at high-redshift is still unknown. The line luminosities of the dense gas tracers HCN, HCO^+, and HNC are 1-2 orders of magnitude fainter than low-J CO-emissions, which leads to a lack of observational constraints on high-z dense gas tracers. In this work, we evaluate if a Matched Filter (MF) in the uv-plane, introduced by Loomis et al. (2018), can be used to detect the dense gas tracers HCO^+(4-3), HCN(4-3), and HNC(4-3) in high-redshift SMGs, to overcome the faintness problem of these transitions. This method is validated on the gravitationally lensed, high-z SMG SDP.81, and through extensive ALMA Band 3 simulations. Using the MF-method on new Band 3 Cycle 6 ALMA observations of the SDP.81, we obtained a 4.1s-detection of the HCO^+(4-3)-emission, while no detection is visible in the image-plane or via a spectral line extraction through aperture masking. This detection is confirmed with a spectral line extraction (6.3s) on a concatenated observation with roughly twice the on source time. We obtained upper limits on the HCN(4-3) and HNC(4-3) emission. The HCO^+(4-3) detection is the first high-redshift observation of the HCO^+(4-3)-emission in a SMG. We found that the HCO^+(4-3)/HCN(4-3) ratio is 2 than any other high-z observation. Furthermore, we found a low HCN/CO luminosity ratio, which indicates that, unlike Gao et al. (2007) and Oteo et al. (2017), not all SMGs have high dense gas fractions.

Contents

1 Introduction 7
1.1 The Critical Path of Stellar Evolution 7
1.2 Dense Gas Tracers 8
1.3 Star Formation Laws 10
1.4 The Empirical Kennicutt Schmidt-Relationship 11
1.4.1 The Kennicutt Schmidt-Relationship in the Local Universe 11
1.4.2 The Kennicutt Schmidt-Relationship at High-Redshift 15
1.5 The Matched Filter in the uv-Plane 16
1.6 The SDP.81, Target Description 17
1.7 Goals 18

2 Methods: The Matched Filter in the uv-Plane 19
2.1 Linear Filters 21
2.1.1 Matched Filter, Mathematical formalization 22
2.2 The Matched Filter: Line Detections in the uv-Plane 24
2.2.1 Implementation 25
2.2.2 Flux Estimates 28

3 Proof of Concept: The Matched Filter evaluated on the SDP.81 31
3.1 SDP.81 Cycle 4 & 5 ALMA Observations 31
3.2 Results of the Matched Filter Approach 33

4 Matched Filter Assessment through Simulated ALMA Observations 37
4.1 Sensitivity of the Filter Response 38
4.2 Testing the Performance of the MF on Simulated ALMA Observations 39
4.2.1 Simulation Setup and Results 39
4.2.2 Discussion on the Simulated Correlations 41
4.3 Comparison Between a Conventional Spectral Line Extraction through Aperture Masking and the Matched Filter Method 46

5 Detecting Dense Gas Tracers in the SDP.81: Uncharted Territory 51
5.1 Observational Details 51
5.2 Data processing, Analysis, and Results 53
5.2.1 Conventional Method: Spectral Line Extraction Through Aperture Masking 53
5.2.2 Additional Source Detected 57
5.2.3 The Matched Filter Approach 58
5.3 SDP.81 Compared to High-Redshift Observations 64

6 Future Directions & Possible Implementations of the Matched Filter in the uv-Plane 73
6.1 Further Assessments of the Matched Filter in the UV-Plane 73
6.2 Future Targets 74

7 Conclusion 77

A Mathematical Derivation of the Matched lter 85

B Additional Sensitivity Images. 89

1 | Introduction

1.1 The Critical Path of Stellar Evolution

In the Milky Way, most stars are formed in dense molecular clouds, while the bulk of star formation takes place in Giant Molecular Clouds (GMCs), where the gas density is highest. If we want to understand the physical processes inherent to star formation, we need to observe the critical path of stellar evolution (Kennicutt Jr & Evans, 2012) and with it the formation of these molecular clouds. The simplified version of this path starts when diffuse intergalactic medium falls into galaxies, increasing the mass of the molecular clouds, causing them to contract under their own gravity. The contracting clouds form denser structures such as clumps and cores. These clumps and cores further shrink to form stellar structures and singular (or binary) systems. These processes can be directly observed within our own Milky Way, but are impossible to detect for distant galaxies (Kennicutt Jr & Evans, 2012). While the individual contraction of clouds outside the Milky Way cannot be resolved, we can infer physical processes, like star formation rates (SFR) and star formation efficiencies (SFE), from the surrounding interstellar medium (ISM). The ISM is the collective of all matter (dust and gas) and radiation in between the stars. As abundances of molecules in the ISM change under higher pressures, we can track the evolution of the critical path by probing for different molecules in the ISM.

Because of the technological advancements of current telescopes like the Atacama Large Millimeter/submillimeter Array (ALMA) and the Very Large Array (VLA), we can obtain spatially resolved high-redshift ($z > 1$) observations on a sub-kpc scale (Lamarche et al., 2018; Hodge et al., 2019). This enabled studies on, for instance, resolved infrared (IR) (or far-infrared (FIR)) emission (Rybak et al., 2015a; Lamarche et al., 2018). Each kind of radiation is associated with different physical processes. For instance, hot young O/B stars heat the ISM, which therefore emits blackbody radiation in the IR. If we assume that the heating of the gas is only due to the stars within a GMC, then we can state that the IR is a direct tracer for star formation. By computing the luminosity in the IR (integrating a modified blackbody between 8 1000 μm, Carilli & Walter (2013)) we can determine the SFR of a specific galaxy.

Furthermore, the ALMA and the VLA can spatially resolve and identify the emission from molecules. By probing different molecular lines, we can trace the evolution of the critical path, as molecules converge to complex forms when the cold gas transforms into high dense star-forming regions. However, it is rather difficult to directly trace the bulk of the gas in regions within a galaxy, because GMCs are primarily composed of atomic Hydrogen (H_2), which is excited at temperatures of 500 K, while the averaged temperatures of GMCs are at the

order of 10K (Narayanan & Krumholz, 2014). Therefore, it is important to understand, what physical processes are inherent to the emissions of molecular line transitions and how we can convert these observed intensities to densities of the gas in which they are excited.

1.2 Dense Gas Tracers

Common molecular transitions in high-redshift sources, which are used to trace the density of the gas are, for instance, Carbon Monoxide (^{12}CO, from now on CO), ionized Carbon (C^+ or [CII]), Hydrogen cyanide (HCN), Formyl ion (HCO^+), and Hydrogen isocyanide (HNC) (Schöier et al., 2005).

Spectral lines are the absorption or emission of photons caused by changes in the rotational and/or vibrational states of a molecule (or atom/atomic nuclei), due to collisions with surrounding particles or excitation by high energy photons. Then, the observed emission corresponds to an energy difference from a molecule that goes from state J+1, to state J, with J de ned as the total angular momentum of the spin-orbit interaction between the electron and the core of the molecule. An example is the ground-state (J=1-0) rotational transition of Carbon Monoxide, which we write as CO(1-0).

The frequency of the photon that is released with such transitions, can be measured accurately in a laboratory. Since the environment can be controlled in a laboratory, we know which speci c temperature or density is necessary to excite a speci c transition of a molecule. Shirley (2015), explained that the critical densities of these low, optically-thin transition lines (J-lines) are proportional to:

$$n_{crit} \mu m^2 n^3_{J+1-J} \tag{1.1}$$

Where mis the dipole moment and $n_{J+1-J}$the rotational frequency corresponding to a J+1 to J transition.

The excitation temperature of the CO(1-0)-transition is roughly 5 K, with a low critical density of, n_{crit} 10^2 10^3 cm ^{3} (Narayanan et al., 2008). CO is the second most abundant molecule in GMCs after H_2 (Narayanan & Krumholz, 2014), and its ground-state excitation is excited at roughly the temperatures of GMCs. Therefore, it is common to convert CO luminosities to gas masses with a converting factor a_{CO}, as H_2 (which abundance dominates the GMCs) is not excited at those speci c temperatures (Casey et al., 2014).

The dipole moment of CO is roughly 30 times less than the dipole moment of more complex molecules, such as HCN, HCO^+, and HNC (Oteo et al., 2017), which leads to higher critical densities of the HCN, HCO $^+$, and HNC, via Eq.

1.2. Therefore, the HCN, HCO^+, and HNC are known as dense gas tracers, with critical densities, corresponding to ground-state transitions of, $n_{crit} \quad 10^5$ cm ^{3}.

When going up on the CO-excitation ladder to higher J-transitions, called spectral line energy distribution (SLED), there is an increase in the rotational frequency. Therefore, higher transitions of molecules correspond to larger critical densities via Eq. 1.2 and are assumed to trace denser regions. However, even critical densities traced by higher CO-transitions (CO(3-2), $n_{crit} \quad 10^4$ cm ^{3}) are still one order of magnitude lower than the critical densities of ground-state transitions of the dense gas tracers. This illustrates that CO is a bad tracer for dense gas.

There is still debate on which complex molecule is the best-unbiased tracer for dense gas regions. For instance, Papadopoulos (2007), argues that HCO^+, unlike HCN, is a molecular ion and therefore more sensitive to changes in its environment, as it is easily destroyed by recombination with free electrons. This illustrates that comparisons between different luminosities of the dense gas tracers can lead to further understanding of the environment in which they are excited.

Finally, we introduce the ionized Carbon line, [CII]. The (ne-structure) transition of single ionized carbon ($^2P_{3/2} \quad ^2P_{1/2}$) is one of the brightest emission lines in star-forming galaxies and is a cooling mechanism of the ISM (Narayanan & Krumholz, 2017). Also, this excitation is mainly caused by collisions with Hydrogen (H_1 or H_2) or electrons and is therefore used as a tracer for low-density gas. However, due to the low ionization potential of [CII], 11.3 eV (Narayanan & Krumholz, 2017), it can trace each phase of the critical path of the stellar evolution. For example, Kennicutt Jr & Evans (2012) state that it can be used as a proxy for the SFR, just like the FIR-Luminosity. However, resolved studies at high-redshift (Lamarche et al., 2018; Rybak et al., 2020), show that the emission of [CII] can be more extended than the FIR emission. These, and more, high-redshift studies deviate from local observations. This phenomenon called the [CII]-FIR de cit (Narayanan & Krumholz, 2017).

Ratios between the FIR and the gas tracers are especially interesting as they couple the physical processes (called mechanical heating processes) behind the molecular transitions with the SFR, for instance, probed by the FIR luminosity. These ratios have been computed for many different galaxies and correlate over at least 3 orders of magnitude in the IR, with a scatter less than 1 dex (Gao & Solomon, 2004a). These empirical correlations, in which different abundances of the ISM are correlated with the SFR, enabled a measurement to follow the critical path of stellar evolution, and link them with the mechanical heating processes inherent to the dense gas tracer used for the correlation. These correlations are called Star Formation Laws.

1.3 Star Formation Laws

Since the 1950s, researchers were trying to nd a physical explanation for the empirical relationship between the SFR and the local gas density (Schmidt, 1959; Kennicutt Jr, 1989). As a result of the early works of Kennicutt and Schmidt, is the name of this star formation law called the Kennicutt-Schmidt (KS) Law or the KS-relationship. Due to low surface brightnesses of the ISM in high-redshift galaxies, is the KS-relationship mainly based on local observations. From a historical point of view is the KS-law expressed in surface densities (Casey et al., 2014):

$$S_{SFR} = e^0 S_{gas}^b \tag{1.2}$$

The two main components are e^0 and b. b describes the power law of the relationship and is usually obtained by tting a power-law through the observed correlation. e^0 is the normalization factor. This factor depends on which dense gas tracer is used to investigate the correlation, but usually, e^0 represents the inverse of the gas-depletion and can be thought of how ef ciently stars are formed out of a clump of gas. Therefore, the physical processes behind star formation are translated to these two parameters, b, and e^0. The quantities S_{SFR} and S_{gas} are the observable surface densities.

As the KS-law is already over 60 years old, there are many different representations of this law in the literature. For instance, Gao & Solomon (2004a,b) illustrated this empirical relationship based solemnly on observational parameters. They plotted the IR luminosity (L_{IR}, in units [L]), against the apparent line luminosity (L'_{gas}, in units [K km/s pc ^{2}]) of CO(1-0) and HCN(1-0) (Figure 1.1). While Narayanan et al. (2008) transformed the observational quantities to physical quantities, like the mean density along the line of sight. In this section, we will continue to explore the physical implementations of the KS-law, while in the next section, we continue with the observational aspects of the KS relationship.

Narayanan et al. (2008), provides a physical explanation on the observational SFR-L_{gas} (or L_{IR}-L_{gas}) correlation:

$$SFR \mu L_{gas}^a \tag{1.3}$$

They argue that the exponent of the found correlation, a, does not truly resemble a physical property that describes the star formation ef ciency. For instance, a galaxy forms stars at a constant rate:

$$SFR \mu r^b \tag{1.4}$$

Then, the exponent of the found correlation, a in Eq. 1.3, is not necessarily equal to b, as we have to consider how much the line luminosity (proportional to the critical density) correlates with the local density:

$$L_{gas} \mu r^{N} \tag{1.5}$$

With N = b/ a. Therefore, the exponent N describes how the critical density (as described in section 1.2) translates to the local density of the gas in the GMCs. Thus, an understanding of how the luminosity is converted to a molecular gas density is necessary to interpret the KS-relationship. To explain this ef ciency we make two clear distinctions.

First, when the critical density is smaller than the local density, the gas will be in thermal equilibrium (thermalized), and the exponent (N) of Eq. 1.5, will be unity (Narayanan et al., 2008). Therefore, the measured correlation will have an exponent equal to the KS-exponent (a = b).

Secondly, if the critical density corresponding to the observed dense gas tracer is larger than the local density, then, the gas will only be partially thermalized. This would cause Eq. 1.5, to be super-linear, resulting in a sublinear observed correlation. Narayanan et al. (2008) went in great detail on how the local density relates to the critical density. They predict that: "The SFR- L_{mol} slope for tracers with a critical density higher than HCN (J = 1 0) or CO(J = 3 2) is directly predicted to be sublinear".

1.4 The Empirical Kennicutt Schmidt-Relationship

1.4.1 The Kennicutt Schmidt-Relationship in the Local Universe

Gao & Solomon (2004a,b) performed the rst large extragalactic survey of HCN(1-0) in nearby galaxies and found a tight correlation between the infrared luminosity (L_{IR}) and the HCN(1-0) line-luminosity (L^{0}_{HCN}). They compared the L_{IR}-L^{0}_{HCN} correlation with the L_{IR}-L^{0}_{CO} correlation (both shown in the left panels of Figure 1.1) and found that the correlation with the dense gas tracer (probed by HCN) is consistent over at least 3 orders of magnitude in the IR, with a scatter less than 1 dex (Gao & Solomon, 2004a), while the low-density gas tracer (probed by CO) exhibits an evolving trend when observing more luminous CO-emission.

This is especially clear in the panels shown on the right of Figure 1.1, as they illustrate that the $L_{IR}/L^{0}_{CO(1\ 0)}$ ratio increases with the IR luminosity, while no trend is found for the HCN(1-0) counterpart. These ndings indicate that the L_{IR}-L^{0}_{HCN} correlation is tighter than the L_{IR}-L^{0}_{CO} correlation, which suggests that the SFR in galaxies can be traced by the HCN(1-0) line luminosity. This is

Version of July 31, 2020– Created July 31, 2020 - 21:42

Figure 1.1: The the Kennicutt-Schmidt (KS) relationship (left) of Gao & Solomon (2004a,b) for HCN(1-0) (upper-left) and CO(1-0) (lower-left) on the same sample of galaxies. LIRGs and ULIRGs are represented with the circles filled with crosses, while less luminous spiral galaxies are represented by the open circles. Both KS-relationships are fitted with a power law. The slope matches the HCN data for both low and high IR luminosities, while the CO luminosities evolve with increasing IR luminosities. This is especially clear in the two figures on the right, which show on the upper-right, the L_{IR}/L^{0}_{HCN}-L_{IR} correlation and on the lower-right the L_{IR}/L^{0}_{CO}-L_{IR} correlation. These correlations suggest that the star formation depends on the amount of dense molecular gas (Gao et al., 2007). Figure is adopted from Gao & Solomon (2004a), Figure 1a,b and 2a,b.

in agreement with the description of the critical path of stellar evolution, as the correlation suggests that the star formation depends on the amount of dense molecular gas (Gao et al., 2007).

The ndings of Gao & Solomon (2004a,b) are supported by observations of GMCs within the Milky Way (Wu et al., 2010; Liu et al., 2016). However, the exponent of the correlation is inconsistent with the ndings of observations on higher J-lines, as Bussmann et al. (2008) used the same sample as Gao & Solomon, but probed HCN(3-2) and found a lower correlation exponent. Other, more recent, observations on high J-transitions of HCN and HCO^+ found a super-linear correlation for star-forming galaxies (Graciá-Carpio et al., 2008; Zhang et al., 2014; Imanishi et al., 2018).

Casey et al. (2014) stated that there is a tentative trend that higher-J transitions, which corresponds to higher critical densities, appear to have lower SFRs. However, recent studies on 23 detected (SNR > 5) local galaxies by Li et al. (2020), illustrate the uncertainty in comparing exponents between high and low-J transitions, as they found a large scatter between the HCN(1-0)/HCN(3-2) ratios, with the scatter ranging between a fraction of 0.5 1.7.

Finally, Tan et al. (2018) with their MALATANG survey, closed the gap in the KS-relationship, between resolved studies on clumps within the Milky Way and the integrated studies of local galaxies. They added observations on resolved local star-forming galaxies, by probing for the HCO^+(4-3) and HCN(4-3) lines. They mapped the inner 2^0 2^0-region, with 14" (FWHM) resolution (corresponds to a linear scale of 0.2 1.0 kpc), of each galaxy.

Jiang et al. (2020), performed a more detailed analysis on one of the targets of the MALATANG survey (NGC 253) by adding extra CO(3-2) and CO(1-0) observations. They found that the emission of HCO^+(4-3) and HCN(4-3) follow more concentrated morphologies than the CO(3-2), and are consistent with the morphologies obtained from the IR-emission. Therefore, they concluded that indeed the HCO^+(4-3) and HCN(4-3) are robust tracers of dense gas and ongoing star formation. Furthermore, they found the SFR-M_{dense}correlation, with constant factors a_{CO} and a_{dense} to be super-linear with an exponent of b(HCN) = 1.14 and b(HCO+) = 1.10, which are consistent with the most recent surveys of Zhang et al. (2014) and Imanishi et al. (2018). Note that these ndings contradict the predictions of Narayanan et al. (2008). This indicates that more star-forming galaxies have higher star formation ef ciencies than previously thought. Figure 1.2 shows how the MALATANG survey, together with the surveys from Zhang et al. (2014) and Imanishi et al. (2018) fall on the KS-relationship. This gure also includes high-redshift observations which are discussed in the next section.

Version of July 31, 2020– Created July 31, 2020 - 21:42

Figure 1.2: A summary of the Kennicutt-Schmidt relationship of the most recent HCN(4-3) (left) and HCO^+ (4-3) (right) surveys on local star-forming galaxies, combined with high-redshift observations. In red, the resolved observations on star-forming galaxies of Tan et al. (2018). In black and green, integrated observations on local star-forming galaxies by Zhang et al. (2014) and Imanishi et al. (2018), respectively. The high-redshift SMGs of Béthermin et al. (2018) in purple and Oteo et al. (2017) in yellow. Finally, we included two high-redshift quasars, namely, the APM quasar by Riechers et al. (2010a) and the Cloverleaf by Barvainis et al. (1997); Riechers et al. (2010b); Uzgil et al. (2016). Triangles indicate upper- or lower-limits at a 3s-level, squares AGNs or AGN contaminated sources, and circles star-forming galaxies. The solid line is the bet tted power-law of Zhang et al. (2014). The gray shaded region represents the error on the power-law exponent of their t.

Version of July 31, 2020– Created July 31, 2020 - 21:42

1.4.2 The Kennicutt Schmidt-Relationship at High-Redshift

To further examine the infrared-dense gas tracers correlation, we need to extend the eld to sources outside of the local group. However, observing rotational vibrations of dense molecular gas tracers is inherently dif cult, due to the low abundances of the dense gas tracers w.r.t. CO or [CII].

Typically, the spectral lines from dense gas tracers are one order of magnitude fainter than CO observations in LIRGs and ULIRGs, and two orders of magnitude fainter than in spiral galaxies (Oteo et al., 2017). Therefore, observations of these dense gasses are mostly biased to extreme conditions like Quasars and Active Galactic Nuclei (AGNs). For several years, these extreme sources were the only targets to study dense gas tracers at high-redshift. Two famous quasars are the APM 08279+5255 (from now on APM), z = 3.91 (Riechers et al., 2010a) and the Cloverleaf, z = 2.56 (Barvainis et al., 1997; Riechers et al., 2010b; Uzgil et al., 2016). For both sources, multiple dense gas tracers have been observed, which made it possible to constrain temperature, typical densities, and excitation conditions, based on CO and HCN ladders. Therefore, these two sources, in particular, are still used today as comparison material for general star formation laws.

Fortunately, due to ALMA's increased sensitivity and large bandwidth (Hodge & Da Cunha, 2020), there have been more studies on dense gas tracers which are less-biased to extremes. Two notable studies are Oteo et al. (2017) and Béthermin et al. (2018), in which they used strongly lensed Sub Millimeter Galaxies (SMGs) to probe for multiple transitions of multiple dense gas tracers. Most of their detections were tentatively and interpreted as upper limits, but both studies found two sources with multiple detections (SNR > 4).

The reason these detections were possible is due to the strong gravitational lensing effects, which magni es the surface brightness of the lensed sources. Furthermore, SMGs are de ned as galaxies with a large sub-millimeter (submm) rest-frame (> 1mJy at 850 mm, Hodge & Da Cunha (2020)), and therefore, are very luminous in the submm wavelengths (10^{12}L). In general, SMGs are very massive (10^{10} 10^{11}M), with large dust reservoirs (& 10^{8}M), and are extreme star-forming galaxies with a typical SFR of 10^{2} 10^{3}M yr ^{1} (Hodge & Da Cunha, 2020).

SMGs are popular sources for high-redshift observations, as the extreme star-forming conditions (in combination with gravitational lensing magni cations) overcome the faintness problems at those redshifts. As of today, most SMGs have only been studied in the FIR, [CII]-, and the low-J CO lines, not the line emissions from the dense gas tracers (Hodge & Da Cunha, 2020). Therefore, the actual link between the molecular gas and the extreme star-forming conditions in SMGs is still relatively unexplored (Rybak, 2019). Figure 1.2, compares

Version of July 31, 2020– Created July 31, 2020 - 21:42

the local surveys on star-forming galaxies (described in section 1.4.1) with the most recent high-redshift mid-J observations including, the SMGs of Spilker et al. (2014); Oteo et al. (2017); Béthermin et al. (2018), the Cloverleaf quasar (Barvainis et al., 1997; Riechers et al., 2010b; Uzgil et al., 2016), and the APM quasar (Riechers et al., 2010a), by placing them in the KS-relationship.

Carilli & Walter (2013) discussed the early results on how the high-redshift observations compare with local star-forming galaxies. They concluded that at a given L_{IR}, the found L^{0}_{dense} to be smaller than ratios found in the local universe. This would suggest a superlinear trend, however, these results are mostly based on observations of quasars and AGNs. The latest results from Béthermin et al. (2018) and Oteo et al. (2017) show that both observations on HCN(4-3) and HCO^{+} (4-3) are consistent with the best- tted power-law of Zhang et al. (2014), which are based on local star-forming galaxies.

Even though these high-z studies shine the rst light on how the SFE evolves w.r.t. redshift, the total amount of detections on high-redshift sources is still to thin to perform any statistical analysis. Even when considering sources with extreme conditions (Gao et al., 2007; Bigiel et al., 2015) or tentative detections of Oteo et al. (2017); Béthermin et al. (2018); Spilker et al. (2014), the total amount of detections is below ten unique sources. This raises the question: How to increase the sample size of high-redshift detections on dense gas tracers, to be able to perform a statistically signi cant analysis on the KS-law at those redshifts?

1.5 The Matched Filter in the uv-Plane

In this research, we evaluate if the Matched Filter (MF) technique of Loomis et al. (2018), can increase the signal to noise ratio (SNR) of emission lines from high redshift sources. If successful, this could lead to an increase in the sample size of high-redshift observations that are less-biased to extreme conditions.

A MF-method is a common technique to detect unresolved sources at high-redshift in deep surveys (Brinchmann et al., 2017; Vio & Andreani, 2016). However, Loomis et al. (2018) developed a technique for high-resolution observations that uses prior knowledge of the source's spatio-kinematic structure to increase the sensitivity of spectral line observations. In contrast with the more conventional MF-techniques, they used the MF in the uv-plane to simultaneously boost the SNR, while avoiding computational cost and ambiguities associated with traditional imaging (Loomis et al., 2018).

Loomis et al. (2018) tested the performance of the MF-method on Proto-Planetary Disks (PPDs) and found that this different representation of the data could boost the SNR by a factor of 60 400%. This method has been con- rmed in practice on PPDs, for which detections with aperture extractions were

unsuccessful (Carney et al., 2017; Booth et al., 2019; Loomis et al., 2020) (with Booth et al. (2019) a 3.5 -detection). In these studies, the MF method provided useful lower limits on the ux estimates of the spectral line emissions.

However, an equal amount of attempts, found in the literature, were unsuccessful when the MF was applied on PPDs (Notsu et al., 2019; Carney et al., 2019; Harsono et al., 2020). Furthermore, there is only one mention in the literature of this speci c MF-technique applied to high-redshift observations (French et al., 2018), which was also unsuccessful. Thus, illustrating that this technique is still relatively new and ready to be further explored.

1.6 The SDP.81, Target Description

We will evaluate the performance of the MF on simulated and real observations of the high-redshift galaxy, SDP.81 (H-ATLAS, J2000 09:03:11.6 +00:39:06, Eales et al., 2010; Bussmann et al., 2013). The SDP.81 is a strongly lensed (m_{FIR} = 18.2 1.2, Rybak et al., 2020) SMG at redshift z = 3.042, and was used as a science veri cation for the 2015 ALMA Long Baseline Campaign (Partnership et al., 2015). Therefore, this high-redshift galaxy is extensively studied with high-resolution (20 milliarcseconds) ALMA observations, enabling precise measurements on the spatial-kinematic details from continuum emission and the ISM (Partnership et al., 2015; Rybak et al., 2015a,b; Dye et al., 2015; Tamura et al., 2015; Hatsukade et al., 2015; Swinbank et al., 2015), making it an ideal target for an evaluation of the MF-method on high-z sources.

Furthermore, the SDP.81 is observed with low-resolution spectroscopy and imaging by the Herschel Telescope (Valtchanov et al., 2011), and followed up with high-resolution FIR spectroscopy by the same telescope (Valtchanov et al., 2011; Zhang et al., 2018). It is also observed in the near-infrared by the Hubble Space Telescope (Dye et al., 2014).

The most recent work on the SDP.81 is performed by Rybak et al. (2020). They brought together multiple CO observations of different J-lines to constrain estimates on the temperature, density, and local heating mechanisms that drive the excitation of the molecular lines in the SDP.81. All observations combined make the SDP.81 one of the most extensively studied SMGs. However, the dense gas tracers of the SDP.81 have never been detected.

In this work, we have a rst look at new ALMA, Cycle 6 observations of the SDP.81, which frequency set up covers the HCO^+ (4-3), HCN(4-3), and HNC(4-3) emission lines. This observation, combined with old Cycle 5 observations from M. Rybak and I. Oteo, creates a very deep measurement (225 minutes on source time) on which we can test the performance of the MF-method, and try to detect the dense gas tracers.

1.7 Goals

To summarize, in this work we will:

> Use simulated ALMA observations to measure the performance and limitations of the matched lter in the uv-plane to detect weak spectral lines from high-redshift galaxies, such that in future work, this method can be used to ll the underrepresented, high-redshift domain of the Kennicutt-Schmidt law.
>
> Detect the emission from of HCO^+ (4-3), HCN(4-3), and HNC(4-3) vibrational transitions, from a combination of new and old (but never published) ALMA observations of the lensed SMG SDP.81. To detect the dense gas tracers, we will use the MF-method, such that we can con rm, in practice, that this novel approach is applicable to high-redshift ALMA observations.
>
> With the ux estimates on the dense gas tracers, obtained with the MF or by conventional spectral extraction, determine mechanical heating processes in the SDP.81 to aim to explain the physical processes inherent to the extreme star-forming conditions in this SMG.

In Chapter 2 we provide in-depth instruction on how to implement the MF in the uv-plane, and how to perform a data analysis with the matched ltered data. This is followed up with the result chapters, which are split into three. First, in Chapter 3, we provide a proof of concept that the MF-method is applicable to high-z observations, by running the method on Cycle 4 and 5 ALMA observations of the SDP.81. Second, in Chapter 4, we performed a detailed analysis of the performance of the MF, with the use of simulated ALMA observations, to probe the limitations and the performance of the MF-method. Then, in the -nal result chapter (Chapter 5), we applied the MF-technique and conventional methods, to detect the dense gas tracers HCO^+ (4-3), HCN(4-3), and HNC(4-3) in the SDP.81. The nal two chapters, Chapters 6 and 7, of this thesis, will be a discussion on future directions and possible implementations of the MF-method and the conclusion of the thesis, respectively.

2 | Methods: The Matched Filter in the uv-Plane

In this chapter we describe how to process interferometric data sets to detect weak spectral lines at low Signal to Noise Ratio (SNR). These data sets are, in radio astronomy, referred to as visibilities.

Visibilities are samples of the Fourier transform of the distribution of emission intensities from an astrophysical source at a given spatial and spectral resolution (Loomis et al., 2018). A visibility is de ned as (Thompson et al. (2017), page 93):

$$V(u,v) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{A_N(l,m)\, I(l,m)}{\sqrt{1-l^2-m^2}}\, e^{-j2\pi(ul+vm)}\, dl\, dm \tag{2.1}$$

With $A_N(l,m)$ the effective normalized collecting area of each antenna, and $I(l,m)$ the source intensity distribution. Combined with the bandwidth of the antenna ($\Delta\nu$) and integrated over the solid angle ($d\Omega$), the effective collecting area with the intensity distribution provides a power to each antenna equal to $P = 1/2 \quad A_N(\vec{s})\, I(\vec{s})\, \Delta\nu d\Omega$, with $\vec{s}$ the coordinates in the sky, projected on a celestial sphere perpendicular to the line of sight of the antennas. $\vec{s}$ can be disbanded in the coordinates (l,m) (assuming the depth of the source is neglectable), such that the solid angle, $d\Omega$, is written as:

$$d\Omega = \frac{dl\, dm}{\sqrt{1-l^2-m^2}} \tag{2.2}$$

Thus, the combination of Eq. 2.1 and 2.2 shows that the visibility is indeed the Fourier transform of the emission intensities per given position (l,m) in the sky.

The coordinates of the visibilities (u,v), are the projected baseline distance between antennas in a plane normal to the direction of the phase reference position (Thompson et al. (2017), page 91). Considering that an observation is performed with several antennas, each visibility has a precise position in the uv-plane, corresponding to the absolute projected distance between two antennas.

We can Fourier inverse the visibilities, to go from the uv-plane to the image-plane. This allows us to observe the intensities per frequency channel. At rst hand, the intensities are contaminated with interference patterns, which arise from the incomplete uv-coverage. This is referred to as the *dirty image* and the interference patterns are called the *dirty beam* (Thompson et al. (2017), Page 552). Contamination means that every point source in the astronomical signal, in the image-plane, is convolved with the dirty beam. Thus, to recover the astronomical signal, a deconvolution of the dirty image with the dirty beam, needs to be

Figure 2.1: An illustration of different analysis applied to an interferometric data cube. Counter-clockwise from top-left: 1) Integrated channels weighted by their frequency, called Moment Maps; 2) Individual Channels; 3) Spectra originating from (top to bottom) a) a single-pixel extraction; b) obtained by integrating over an aperture, which is identical in each channel, and c) a spectral line pro le obtained using a matched spatio-kinematic mask (dashed red contours in the Channel Map). The synthesized beam is shown in the lower left of the Moment-0 and Channel maps. Figure is adopted from Loomis et al. (2018), Figure 1.

performed. The function C LEAN (Högbom, 1974; McMullin et al., 2007) Fourier inverts the visibilities and than numerically deconvolves the intensities. This results in an image cube with the Right Ascension (RA) and Declination (DEC) on the x- and y-axis and frequency on the z-axis. Such a cube is shown in Figure 2.1. The cube contains a series of emission intensities separated by a constant frequency spacing (channels). These channels can be projected to radial velocity bins.

Ideally, the emission is directly observed in the channel maps, however, when the emission is too weak we must apply operations to the image cube to increase the SNR. For instance, moment maps are images created by marginalizing the frequency axis. Noise is uncorrelated, while the signal is not, therefore marginalizing the frequency axis reduces the noise by a square-root of the number of channels marginalized and thus increases the SNR of the observation.

Another option is to extract a spectrum to investigate spectral lines, by collapsing the image plane. This could be achieved with a single-pixel extraction, when the source is spatially unresolved. However, when the emission is extended and shows more complex velocity structures, extracting the spectra, becomes more dif cult. Usually, a spatio-kinematic mask is applied to the bright-

est structures in the image-plane. With this operation, the brightest regions (or the regions where a signal is expected) are masked, to exclude noise when the image plane is collapsed (summed over the pixels within the aperture mask) into a spectral line pro le. The described operations on the image cube are also visualized in Figure 2.1.

The spatio-kinematic mask is often the chosen technique to detect spectral lines. After masking the brightest structures, one usually applies the C LEAN algorithm to correct for the limited spectral frequency coverage (Thompson et al. (2017), Page 551). CLEAN nds the peak value in the spatio-kinematic mask and than deconvolves the interference pattern of the incomplete uv-coverage from this position. C LEAN ing reduces the total ux of the image by mainly reducing noise outside of the masked region. However, this removal sacri ces meaningful spectral baselines, making weak detections more dif cult (Loomis et al., 2018). Furthermore, CLEAN ing tends to introduce artifacts, like stripes, clumps, or other erroneous details, due to the nature of the algorithm and by Fourier inverting the visibilities with a discrete Fourier sampler (Thompson et al. (2017), Page 559). Finally, imaging the visibilities might be a non-trivial cost for high-resolution observations or spectral surveys with large bandwidths, as it might be time-consuming. (Loomis et al., 2018).

We can overcome these limitations and remain the spatio-kinematic masking advantages, by applying a Matched Filter (MF), which is a linear lter, directly to the visibilities (Loomis et al., 2018). When prior information on the signal is available, we can create a linear lter that matches the signal, and cross-correlate the noisy signal with the lter to maximize the SNR. This approach overcomes the limitations of conventional methods and enables a fast unbiased approach for weak line detections (Loomis et al., 2018).

In this chapter, we provide more information on what linear lters (section 2.1) and matched lters (section 2.1.1) are, how to implement them in the uv-plane for weak spectral line detections (section 2.2), and how to obtain lower limits on ux-estimations with the use of matched ltering (section 2.2.2).

2.1 Linear Filters

Filters are functions that are used to nd signal; separate noise from a source; or compress data sets (Sellentin, 2020). Some of the most common lter methods are the Principle component Analysis (PCA) (Wold et al., 1987), Neural Networks (NN) (Géron, 2019), or more basic linear Filters, like Wavelet- or Matched Filters (MF) (Vio & Andreani, 2016; Sellentin, 2020). There are many examples in the eld of observational astronomy that apply lters to their data, for instance: Mary et al. (2020) used an iterative PCA technique to remove nuisance sources

in MUSE data cubes; or Morningstar et al. (2018) applied, rst a Recursive NN to deconvolve the dirty image, and then retrieved, with the use of Convolution NN, characteristics of lensed galaxies; while Brinchmann et al. (2017) used a MF to nd weak emission line sources in the MUSE Hubble Ultra Deep Field Survey.

2.1.1 Matched Filter, Mathematical formalization

In our work, we used a MF to increase the SNR of our data. A MF is a linear lter designed to maximize the ability to detect a signal of a known structure that is buried in additive Gaussian random noise (Vio & Andreani, 2016). Usually, prior knowledge is available on the source, which is desired to be detected. This prior knowledge can be transformed into an optimal linear lter.

When a MF is 'applied' to the data we speak about the following operation:

$$x_F(t) = \int_a^b F(t')x(t \quad t')dt' \tag{2.3}$$

With $x(t)$ the data stream, $F(t)$ the lter, and $x_F(t)$ the ltered data, also known as the lter output, the lter response, or the response function. Eq. 2.3 resembles a convolution, which can be interpreted as a sliding dot-product, between the lter and the data.

As integrals are linear operators and most data, like the image cube in Figure 2.1, have a discrete spectral and/or spatial spacing, we can rewrite Eq. 2.3 in terms of linear algebra:

$$\vec{x}_{MF} = \vec{f}^T \vec{x} \tag{2.4}$$

At some t in the data stream. Note that $\vec{x}_{MF}$, $\vec{f}$, and $\vec{x}$, can be multidimensional, like a 3D-array with declination, right ascension, and frequencies on its axis. Furthermore, the lter output, $\vec{x}_{MF}$, has no longer the physical units of Flux or Power, rather it denotes the degree of similarity between the lter, $\vec{f}$ and the data, $\vec{x}$. Figure 2.2 shows a simpli ed schematic of this interpretation.

To maximize the signal output of $\vec{x}_{MF}$, we need to nd an optimal linear lter, $\vec{f}$, such that $\vec{f}$ matches the signal, $\vec{s}$, for $\vec{s} \in \vec{x}$, as close as possible. In other words, the lter $\vec{f}$ that maximizes the SNR of the lter response (SNR_F), is the lter that matched the signal, $\vec{s}$ in data $\vec{x}$, optimally. When the optimal lter is found, the lter is called the matched lter (MF). There are several ways to analytically obtain a MF.

Vio & Andreani (2016); Vio et al. (2017, 2019) interpreted the maximization of the SNR as a least square problem and determined for which response function, $\vec{x}_{MF}$, the log-likelihood of detection was at a maximum. We derived the optimal

Figure 2.2: A two-dimensional schematic view on the interpretation of the response function of a linear filter, given by Eq. 2.4. For simplicity, the filter, $\vec{f}$ and the data, $\vec{x}$, are two-dimensional vectors, where the filter does not match the data on the left and resembles the data partially on the right. Thus, we can interpreter the output of the dot product in both panels, from left to right, as $\vec{f}$ not in $\vec{x}$; and $\vec{f}$ display similarity to $\vec{x}$.

MF with the use of Linear Algebra and Cauchy-Schwarz theorem. For a one-dimensional discrete signal with known structure, $\vec{s} = [s(0), s(1), ..., s(N)]^T$ of size N, the following assumptions are necessary to derive (and apply) the MF (Vio & Andreani, 2016):

1. The signal has form $\vec{s} = a\vec{g}$, with a a scalar and, g some smooth function.

2. The signal is embedded with additive noise $\vec{n}$, such that the observed data is in the form of $\vec{x} = \vec{s} + \vec{n}$, with $E[\vec{n}] = 0$ and $E[.]$ the expectation operator.

3. The noise $\vec{n}$ is stochastic noise, with an hermitian covariance matrix $\vec{C} = E[\vec{n}^T\vec{n}]$

We provided the full derivation of a generic (uv-plane and non-uv-plane) MF in the Appendix, section A. Here, we brie y summarize the relevant mathematical aspects of the MF. These aspects follow from the derivation performed in the appendix, which follows closely the derivations performed by Sellentin (2020). To understand the mathematical formulation of the MF we need the operation, described in Eq. 2.4, and the assumptions listed in the enumeration above.

The response function, given in Eq. 2.4, uses the filter $\vec{f}$, that maximizes the SNR_F of the filter response, which is de ned as:

$$\begin{aligned} SNR_F &= \left(\frac{S}{N}\right)_F \\ SNR_F &= \frac{\left(\tilde{f}^T \tilde{s}\right)^2}{\tilde{f}^T C \tilde{f}} \end{aligned} \tag{2.5}$$

The filter that maximizes this equation is given by:

$$\tilde{f} = a C^{-1} \tilde{s} \tag{2.6}$$

With a, the normalization factor:

$$a = \frac{1}{\sqrt{\tilde{s}^T C^{-1} \tilde{s}}} \tag{2.7}$$

Such that the filter response, following the definition of Eq. 2.4, is given by:

$$\begin{aligned} x_{MF} &= \tilde{f}^T \tilde{s} \\ x_{MF} &\simeq a \tilde{s}^T C^{-1} \tilde{s} \end{aligned} \tag{2.8}$$

Under the assumption that the data is dominated by the signal $\tilde{s}$ of the astronomical source, such that $\tilde{s} + \tilde{n} \simeq \tilde{s}$.

To summarize, the output of the MF, called the filter response, is some linear combination of the signal to noise of the input data. Due to the normalization of the filter response, the noise of the response function becomes normally distributed (A Gaussian with a standard deviation of one), as we assumed that the input data has Gaussian noise properties. Thus, the unit of x_{MF}, becomes σ, and is understood as a measurement of resembles between the filter and the data set.

2.2 The Matched Filter: Line Detections in the uv-Plane

We implemented the MF in the uv-plane, directly to the observed visibilities, in order to detect weak-spectral lines. There are several reasons to implement the MF in the uv-plane, instead of the conventional image-plane approach.

First, there are no restrictions to apply the MF in the uv-plane or the image-plane, as the MF operation is a cross-correlation with the data. Therefore, the mathematical formulation of the previous section is applicable for the uv-plane,

when the signal $\vec{s}$ and the covariance matrix $\mathbf{C}$ are also determined in the uv-plane.

Second, when the MF is applied in the uv-plane, artifacts caused by transforming the data to the image-plane, are bypassed. For instance, with CLEAN, regions outside of the mask where the signal might be buried beneath the noise are over subtracted, this phenomenon is called over-CLEANing. Usually, the dense gas tracers are not directly visible in the image-plane, and therefore are over-CLEANed, reducing the probability of detection.

Finally, directly applying the MF to the visibilities avoids computational tasks, such as fully imaging wide bandwidths (Loomis et al., 2018). Furthermore, it provides a straightforward detection interference. In the following section, we summarized the steps on how to implement the MF in the uv-plane, and how to perform the detection interference.

2.2.1 Implementation

The MF in the uv-plane was first introduced by Loomis et al. (2018). They piloted the method to detect weak spectral lines in protoplanetary disks at high-resolution (0.1 arcseconds). We used the same technique to probe for weak spectral lines in high-redshift sources, and therefore our implementation will closely follow that of Loomis et al. (2018) .
There are four steps to implement the MF in an incomplete uv-plane:

1. Preparation of Interferometric visibilities.
2. Generating a filter in the uv-plane, which approximates the true signal.
3. Cross-correlation of the filter with the visibilities.
4. Normalization of response function and the detection interference.

Steps 2,3, and 4 are summarized in the schematics shown in Figure 2.3.

Preparation on Interferometric Visibilities

Each visibility, $V(u,v)$, is associated with its own weight, based on the variance of $V(u,v)$ over time, which originates from temperature fluctuations of the antennas. Each visibility is measured at a series of spectral frequencies (channels), therefore the dimensions of the visibilities are $(u, v, \text{channel})$. The visibilities are resampled to a sparse representation, with the amount uv-points (n_{uv}) on the x-axis and number of channels (n_c) on the y-axis.

A Python-based open-source implementation can be found on: https://github.com/AstroChem/VISIBLE

It is recommended to recalculate the weights before running the MF-method with a task such as STATWT of CASA. Weights of measurement sets (MS- les) are often set to arbitrary values (e.g. 1). STATWT empirically measures the visibility scatter, as a function of time, antenna, and/or baseline (McMullin et al., 2007).

Filter Generation

The second step (the rst step in Figure 2.3), is to create a lter for the MF-method. This lter is called a kernel in the uv-plane, and a model in the image-plane. With a MF, prior information on the spatio-kinematic structure is used to lter the data. There are two approaches to obtain a model in the image-plane, before transforming it to a kernel, namely a data-driven and a model-driven approach.

A great example of a model-driven approach is when the MF is used to detect gravitational waves. There are mathematical descriptions on the shape of the signal of these waves, which can be used to create a template bank with different models corresponding to slight changes in the parameters that describe the gravitational waves. For galaxies, there are no detailed mathematical descriptions. Therefore, we approximate the desired signal -s. As it is unknown how closely the source resembles a model, any detection will be a lower limit (Loomis et al., 2018). Examples of model-driven approaches for the detection of high-redshift sources are, a basic rotating Keplerian disk (Loomis et al., 2018) or a detailed MAP sky-model of, for instance, the SDP.81 (Rybak et al., 2020).

A data-driven approach is when a model is created from prior observations on bright emission lines. The lter is most effective if the line used to create the kernel shows a matched spatial distribution with the weak spectral line. For instance, Carney et al. (2017) showed for protoplanetary disks that a data-driven approach, based on a strong H_2CO line emission, was able to detect fainter transitions of the same molecule. This, however, might be a bottleneck for using the MF to detect the dense gas content of high-redshift sources. HCN, HCO^+, and HNC do not have bright counterparts, as their ground state transition is often one or two orders of magnitude fainter than for instance, [CII]- or CO(3-2)-emissions (see Chapter 1, section 1.4.2). Furthermore, Rybak et al. (2020) showed that the [CII], CO(3-2), and the FIR-emission show spatial offsets, with respect to each other. Therefore, models based on data-driven approaches created from different molecular lines will be less effective in detecting weak spectral lines than molecular transitions which are known to be co-spatial.

When the prior knowledge on the spatio-kinematic structure is gathered into a model in the image-plane, the model is Fourier transformed and resampled to match the uv-coverage of the observations, such that the number of uv-points

of the kernel is identical to that of the data.

Loomis et al. (2018) incorporated their own visibility sampling routine, called VIS_SAMPLE, to obtain the proper kernel in the uv-plane. Other sampler routines, such as CASA-SIMOBSERVE, may also be used, however, tasks such as SIMOBSERVE are relatively slow, compared to Loomis et al. (2018) visibility sampler. Do note, that the VIS_SAMPLE-task breaks down when the image size and pixel size of the model do not ful ll the Nyquist sampling criteria that the pixel size $Dx < 1/2\, u_{max}$, $Dy < 1/2\, v_{max}$ and the primary beam is at least twice the eld of view (Thompson et al. (2017), page 46).

The weights of computed visibilities are then used as the approximated signal-s. To nish the generation of the kernel, the inverted noise covariance matrix, C^{1}, is determined directly from the observational data weights (Loomis et al., 2018).

Cross-correlation

The created kernel is convolved with the data, by the operation described in Eq. 2.4, for each channel in the observation. To perform a dot product the kernel and the data need an identical amount of visibilities (n_{uv}), while the kernel has fewer channels than the data. Therefore the sliding dot-product operates along the spectral axis.

Note that, the data in the uv-plane contains both an imaginary and a real part. Therefore, any phase misalignment between the sky locations of the lter and the source will result in a leak of power from the real to the imaginary part (Loomis et al., 2018). If the source and the lter are properly aligned, all the information in the response function will be contained in the real part of the impulse response spectrum. Therefore the resulting impulse response spectrum, x_{MF}, is computed by taking the real part of the complex inner product of the windowed data with the kernel (Loomis et al., 2018).

Detection interference

When the lter response spectrum is obtained, the nal step is to properly interpret the ltered data. As described in section 2.1.1, the data is transformed from units of mJy/Beam to a measure of resembles, between the lter and the data in the uv-plane. The schematic image of Figure 2.2, illustrates that the output of the lter response is zero when the lter does not resemble the data. However, due to temperature uctuations in the antenna, which are manifested as Gaussian random noise, the linear lter will output, via the convolution, Gaussian random noise as well. If the data weights are properly calibrated, with the STATWT-task, the noise in the lter response, will be properly normalized to a

normal distribution (mean of zero, and a standard deviation of unity). When the data weights are not correctly calibrated or when continuum emission is still present in the data, a manual rescale of the full lter response spectrum is required to obtain the desired noise properties (Loomis et al., 2018).

When normalized, it is common to set a certain detection threshold, with a known false positive rate. Then, lter responses that cross this threshold are considered to be a detection. Since the noise properties are in this stage normalized, the detection interference is rather easy. If the exact location of the spectral line is known, the probability density function (PDF), which sets the false positive rate, is then the normal distribution. Therefore, a common detection-threshold is 4 or 5 (as $s = 1$). However, we want to stress that this method does not hold when the exact location of the spectral line is unknown.

There are several studies that go into extreme detail on the detection interference of the MF-method (Vio & Andreani, 2016; Vio et al., 2017, 2019). The main point, which is most relevant in our case, is when the assumption is broken that the location of the spectral line is precisely known. For instance, when performing a blind search, the assumption is made that the position of the signal corresponds to a peak of the ltered data (Vio & Andreani, 2016). Then, the false positive rate is not measured from the PDF that originates from random uctuations of the Gaussian eld but is obtained from measurements of other peak values in the lter response spectrum. Therefore, the PDF originates from a maximized Gaussian random eld, instead of the normal distribution. If not accounted for the change in the PDF, you can underestimate a false detection by a factor of 30, when choosing a detection threshold of $4s$ (Vio & Andreani, 2016). Examples of scenarios in which this might occur, when probing for weal spectral lines with the use of the MF are, blind deep ALMA spectral surveys with extremely large bandwidths, or when probing for Lyman a emitters when the offset from the systematic redshift is unknown.

2.2.2 Flux Estimates

Finally, we want to discuss how the lter response spectrum can be used to obtain lower limits on ux estimates of observations. When a line is identi ed, the ratio between the lter response of this line and that of another re ects the ratio of the ux, if both observations have similar noise properties.

As described in the previous section, the inverse of the covariance matrix, in Eq. 2.8, is obtained directly from the weights of the observations. Therefore, when both lines are observed with identical observational properties like a similar total on source time, weather conditions, identical uv-coverage, and if identical kernels are used to run the MF-method (Loomis et al., 2020), the normalization factor a in both lters (Eq. 2.8) cancels out when the ratio is taken

Figure 2.3: A schematic on the implementation of the matched lter in the uv-plane. The implementation consists of three steps. 1) Create a model with prior information on the spatio-kinematic structure of the source in the image-plane, and Fourier transform it to obtain the kernel for the Matched ltering. The kernel is resampled to a two-dimensional plane with dimensions (n_{uv}, n_k), corresponding to the number of channels in the kernel horizontally and the number of visibilities vertically. The amplitude of the complex kernel has been binned and pixelated to be visually intuitive. 2) Cross-correlate the kernel with the data. The complex data shown in gray-scale is also binned and pixelated, with the number of visibilities identical to the kernel, and the number of channels in the data, n_c n_k. The cross-correlation is performed with a sliding dot product and is shown at several positions in the data. A stronger correlation is visualized with a stronger red color. 3) The real part of the response function is summed over the entire region to produce the impulse response spectrum, per channel. This Figure is adopted from Loomis et al. (2018), Figure 3.

between the lter responses of both observations. Thus, the ratio in the lter response is proportional to the ux ratio of both lines. When one of the two lines is also detected with a spectral extraction, the ratio of the lter responses can be used to obtain a lower limit on the ux ratio of both observations.

Do note that the main utility of this MF-technique is to obtain a rapid detection instead of detailed characterization (Loomis et al., 2018). When a line is identi ed it is common, if possible, to further identify characterizations with the use of the conventional methods. When a particular weak line is identi ed,

Version of July 31, 2020– Created July 31, 2020 - 21:42

which is not visible in the spectral extraction or the image-plane, it is recommended to go to deeper observations to further characterize the line. Here, the MF provides a powerful predictive tool, as it provides robust targets for future observations (Loomis et al., 2018).

3 | Proof of Concept: The Matched Filter evaluated on the SDP.81

We split the results sections into three different chapters. First, we discuss in this chapter, initial testing of the Matched Filter (MF) on the lensed galaxy SDP.81. In the literature, there are no successful results found on the use of this MF-technique on high-redshift (lensed) galaxies. Therefore, as a proof of concept, we rst validate the performance of the MF on bright spectral lines, before moving to fainter lines. By testing the MF on the bright lines, we can compare the results of the MF-approach to the ux estimates of Rybak et al. (2020).

The second part of the results, Chapter 4, expands on the performance of the MF-method, provided by Loomis et al. (2018). In that chapter, we go beyond the simulations and provided by Loomis et al. (2018), to understand how we could optimize a model to obtain higher lter responses, and be able to give predictions when the MF-method should be able to detect a source by investigating correlations and limitations, between the lter response and observational parameter such as the total observation time, surface brightness and, resolution of simulated ALMA observations of the SDP.81 .

Finally, in Chapter 5, we used ALMA Cycle 5 and 6 observations of the SDP.81, provided by M. Rybak and I. Oteo, to probe for dense gas tracers at this high-redshift lensed SMG. On this data set, we applied conventional spectral extractions and the MF-method, to probe for detections, upper limits, and lower limits on the dense gas tracers HCN(4-3), HCO^+ (4-3), and HNC(4-3).

3.1 SDP.81 Cycle 4 & 5 ALMA Observations

To validate the MF-method, we used the data provided by M. Rybak. The SDP.81, ALMA observations, are fully described in Rybak et al. (2020). In this section, we used the channels containing [CII] (Cycle 4, Project # 2016.1.01093.S, with n_{obs} = 470.02 GHz) and CO(3-2) (Cycle 5, Project # 2016.1.00633, with n_{obs} = 85.55 GHz), line-emissions. The lines are observed in Band 8 and Band 3, with a peak SNR of 11s and 5.6s in the image-plane, respectively. The resolution (Beam FWHM) of the [CII] and CO(3-2) are at 0.32 0.26 and 0.36 0.24 arcsec. Finally the lines are detected in between 85.509 and 85.571 GHz for CO(3-2), and in between 469.791 and 470.253 GHz for the [CII]-line, which give rise to a total integrated ux of 11.8 2.3 Jy km/s and 170 20 Jy km/s, respectively. The velocity integrated dirty-images of these two lines are shown in Figure 3.1.

Figure 3.1: ALMA velocity integrated dirty-images of the SDP.81. Left: [CII], Right: CO(3-2). Contours are drawn at 3s, raging between 3s up to 12s.

We tested the MF-method, with the use of a data-driven approach. Therefore, we transformed the bright [CII]-emission into a model to detect the fainter CO(3-2) transition, as the CO(3-2)-emission is roughly one order of magnitude fainter than the [CII]-emission.

To create a kernel in the uv-plane, we needed prior information on the velocity structure of the CO(3-2)-emission in the plane of the sky. We approximated the velocity structure of the CO(3-2)-emission, by assuming that the [CII] and CO(3-2) emissions are co-spacial. Therefore, the model for the MF is created by CLEAN ing the [CII] data cube. We did not directly use the velocity structure of the CO(3-2)-line in order to mimic a data-driven approach where the emission from a bright line is used to approximate the velocity structure of the faint spectral line.

The total bandwidth of the ALMA Band 8 observation is 8 GHz. We narrowed it down to a bandwidth of 1.4 GHz, with a central frequency of 470 GHz. We applied 40 km/s frequency averaging to enhance the SNR. The [CII]-line in the CLEAN ed (natural-weighted) cube is detected within a velocity width of 720 80 km/s.

To evaluate the assumption that the [CII] and CO(3-2) are co-spacial, we normalized the CO(3-2) peak surface brightness to the [CII]-emission and subtracted the velocity integrated maps (the right from the left panel of Figure 3.1) from each other. The results are shown in the left panel of Figure 3.2. The gure shows a clear off-set in the image-plane between the [CII] and CO(3-2) emissions. Therefore, we shifted the entire CLEAN ed [CII]-cube, to align with the CO(3-2)-emission. The cause of the misalignment is a difference in pointing of the two observations. The normalized intensity difference between the shifted

Figure 3.2: The difference between the velocity structure of the SDP.81 [CII] and CO(3-2) lines, where the velocity structure is misaligned (left and aligned (right). The intensity of the CO(3-2) w.r.t. the brightest pixel value of the [CII]-line. The contours are drawn from 6s up to 9s, with steps of 3s. s is determined by computing the standard deviation over the entire image, while masking out the regions where the line- ux of the panels in Figure 3.1 are present, with the use of an annulus mask.

[CII] and CO(3-2)-image are shown on the right of Figure 3.2. More information on model-optimization can be found in Chapter 4, section 4.1.

As a nal step, we applied 20s time-averaging to the CO(3-2) data, in order to reduce the size of the data- le. We choose 20s time-averaging, to optimize the trade-off between reducing the size of the data-set while minimizing the artifacts caused by time-averaging. Figure 3.3, shows these artifacts caused by 20s and 60s time-averaging of the CO(3-2)-data set, w.r.t. the original CO(3-2)-map.

3.2 Results of the Matched Filter Approach

We ran the MF with the shifted, CLEANed [CII]-cube, as a model on the CO(3-2) observations. We adjusted the model such that it only contained channels that showed signal. The result is shown in Figure 3.4. We observed a 19s-detection when we look at the real part of the response function. The imaginary part deviates around zero, as predicted in Chapter 2, section 2.1.1. From here on now we neglected the imaginary part of the response function.

We applied the same model to the [CII]-observations and found a lter response of 155s. This translates to a lter response ratio ([CII]/CO(3-2)) of 8.07. Section 2.2.2, describes that this ratio is identical to the relative emission strength, if the observational parameters of both spectral windows are identical. Table 1

Version of July 31, 2020– Created July 31, 2020 - 21:42

Figure 3.3: Residue images of time-averaged, dirty-imaged SDP.8,1 CO(3-2)-data. From left to right we obtain the difference between 0s, 20s, and 60s w.r.t the original CO(3-2)-map.

of Rybak et al. (2020), provides the ux ratio of the [CII]/CO(3-2) emissions, which corresponds to a ratio of 170/11.8 [mJy/Beam km/s] = 14.4. Here we assumed the noise of both observation to be identical, in order to illustrate the use of the MF-method.

Figure 3.4: A lter response of the SDP.81 CO(3-2) Cycle 5 ALMA observations, obtained with a data-driven approach, by ltering the observations with a CLEAN ed-[CII] cube. The orange-solid line represents the real part of the response functions, the blue-dashed line the imaginary, and the green-dotted line the absolute value. The vertical red-dotted line represents the CO(3-2) observed frequency. We obtained a 19 s-detection, con rming that the MF-method is applicable to high-redshift lensed galaxies.

When we look at the right panel of Figure 3.2, we noticed residue-signal, which indicates a mismatch in the velocity structure of the [CII] and the CO(3-2) emissions. Therefore, obtaining a lower limit on the estimate of the ux ratio that is within a factor of two w.r.t the observed ratio, can be explained with different velocity structures of the two lines.

Finally, we performed two additional tests to observe how the lter response reacts to resolution changes in the data. The results are shown in Figure 3.5. The rst tests, on the left panel, shows that the maximum lter response value decreases, with decreasing frequency resolution of the CO(3-2)-emission. The cause of this negative correlation is due to the interpolation that the MF-method performs on the kernel to match the different frequency spacings between the data and the kernel. This causes interpolation artifacts, resulting in a mis-match between the kernel and the data, which results in lower lter responses.

For the second test, on the right panel of Figure 3.5, we tapered the CO(3-2) data, by removing baselines larger than 1000, 500, and 250 k lambda. We ran three different kernels on this test. Each kernel contains a different amount of channels. The bottom green dots, represent the kernel that was obtained by CLEAN ing the [CII]-observations described above. Due to C LEAN ing-artifacts, the rst channel had a larger noise amplitude than all other channels. The orange (middle) dots, represent the kernel that originates from the C LEAN ed-[CII] observations, but without that rst noisy channel. Then nally, we tested a model that only contained channels that included signal, thus we removed channels that were outside of the frequency range, 469.791 and 470.253 GHz. The latter model is the model used to obtain the lter response spectrum given

Figure 3.5: Responses of the lter response to resolution changes of the ALMA Cycle 5 SDP.81 observations of the CO(3-2)-emission. Left: Frequency averaging the CO(3-2) observations. Right: Tapering of the CO(3-2) data. The tapering is performed by discarding baselines larger than 1000, 500, and 250 k lambda while testing different kind of models. Explanation on the different models can be found in the text.

Version of July 31, 2020– Created July 31, 2020 - 21:42

in Figure 3.4.

Since there is no trend per tested model on the right panel of Figure 3.5, we can apply a high-resolution model on low resolution data, when performing the MF-method. In the next chapter, Chapter 4 section 4.2, we go into more detail, with the use of ALMA simulations, on how the resolution of the data effects the lter response.

To summarize, we performed the MF-method on the high-redshift galaxy SDP.81, with the use of a data-driven approach in which we C LEAN ed the bright [CII]-line and applied it on ALMA observations, which contained CO(3-2)-emission. We altered the image- and frequency resolution to obtain an intuition on how the lter response reacts to changes in the resolution of the data. In the next chapter, Chapter 4, we further expand on testing the performance of the response function.

4 | Matched Filter Assessment through Simulated ALMA Observations

As described in the previous chapter, we further investigated the performance of the Matched Filter (MF) method on simulated ALMA observations in this chapter. Loomis et al. (2018) explored the use of three different models, on a simulated proto-planetary disk (PPD). In these three models, they deviated the complexity and type of each model, namely: a basic rotating disk, a parametric model, and a model obtained by a data-driven approach. They demonstrated the performance of each model on a single simulated data cube and compared it to a conventional spectral line extraction through aperture masking, see Figure 4 and 8 of Loomis et al. (2018).

However, Loomis et al. simulated only ideal scenarios (perfect Matched Filters). They ran simulations based on an input model and used the same model as a kernel for the MF. Therefore, the results they obtained illustrated the maximum performance the MF can achieve in that speci c scenario. These best-case results are unrealistic when the MF is applied to real data, where prior information on the velocity structure is limited, due to limitations in the sensitivity of ALMA measurements (Carney et al., 2019) or artifacts caused by imaging the observations, such as clumps, stripes or small-scale roughness (Thompson et al. (2017), page 559).

To test the performance when prior knowledge is limited, we illustrated in section 4.1, how the lter response changes w.r.t. small deviations in its size, velocity orientation, and misplacement in the sky-plane. These sensitivity images are important as they provide predictions on how the lter response should behave w.r.t these small changes. This illustrated the sensitivity of the MF-method, and it enabled us to optimize kernels without over tting noise patterns.

Then, in section 4.2, we used simulated observations to extend on the tests we performed in Chapter 3, Figure 3.5. In this chapter, we altered the surface brightness, resolution, and integration time of the simulated observations, to provide predictions and illustrate the limitations of the MF-method.

In the nal section of this chapter, we compared a conventional spectral line extraction through aperture masking with the MF-method, similar to Loomis et al. (2018). However, we aimed to provide a comparison that illustrates a more honest approach to how the MF-method should perform on real ALMA observations, as Loomis et al. (2018) only compared the spectral line pro le with an ideal MF.

4.1 Sensitivity of the Filter Response

We performed ten different simulations on the sensitivity of the lter response, w.r.t. small changes in the model, shown in Figure 4.1 and in the Appendix section B, Figure B.1. In this section we presented the four sensitivity curves we used to optimize our models in further sections of this work. The other six performance tests can be found in the Appendix, section B, as most of those tests are correlated with the results we already show in this section or show no response to changes at all.

To investigate the sensitivity of the response function, we used an ideal MF, as a baseline for each test. We simulated a noisy SDP.81 ALMA observation from

Figure 4.1: Sensitivity measurements of the lter response w.r.t. to small deviations in the kernel of an ideal matched lter. The performance are tested on a simulated SDP.81, lensed galaxy with a resolution of half an arcsecond. Explanation on what test are performed per panel can be found in section 4.1.

the MAP sky model of Rybak et al. (2020), shown in the third row of Figure 4.2, and used that noiseless model to create a kernel for the MF.

We simulated the SDP.81 ALMA observations to have a resolution of half an arcsecond, with a Flux of 2.4 Jy km/s. We set the channel-width (inwidth) at 9.766 MHz, with a total bandwidth of 18.750 GHz, at a central frequency of 97.730 GHz, identical to the simulations in the next section. We also evaluated the performance of the ten sensitivity tests on simulated data with a 0.1 arcsec resolution and on a proto-planetary disk, which was provided by Loomis et al. (2018). For each simulation, we found similar results.

The upper two tests in Figure 4.1 are created by rotating the model (left panel) and shifting the model in the image-plane (right panel), w.r.t. the data. Then for the lower panels, we obtained the curves by altering the header information on the frequency resolution (left) and pixel size (right).

First, we point out the difference between the sensitivity images in this chapter and the tests performed in Chapter 3, Figure 3.5. In the previous chapter we changed the resolution of the data, while with these sensitivity images, we keep the data constant and deviate only the model.

All curves show smooth structures when above the 5 s-threshold, except for the image in the lower-left panel. Here we note that at 100 MHz, the velocity width of each channel corresponds to 300 km/s. Therefore the most useful information can be found in the 0-100 MHz range, and we neglect the responses above the 100 MHz channel width.

4.2 Testing the Performance of the MF on Simulated ALMA Observations

4.2.1 Simulation Setup and Results

In this section, we extended the resolution tests performed in Chapter 3, Figure 3.5, by simulating over 300 different setups. With the use of the CASA-task SIMOBSERVE (CASA-version 5.6.0, SIMOBSERVE-version 0.1.118, McMullin et al. (2007)), we were able to transform a model, with a complex velocity structure in the sky-plane, to a noisy data-set in the uv-plane.

We used the MAP sky model of Rybak et al. (2020), to simulate their Cycle 5 ALMA Band 3 observations. The model is visualized in the third row of Figure 4.2. With the proper setup, the Band 3 observations should cover the spectral lines, HCO^+ (4-3), HCN(4-3), and HNC(4-3), when targeting a high-redshift (z = 3.042) galaxy, at the frequencies: 88.26, 87.71, and 89.72 GHz, respectively. Therefore, these simulations will provide us with predictions on how well the

Version of July 31, 2020– Created July 31, 2020 - 21:42

Figure 4.2: Each row represents one model used to obtain lter responses on simulated observations. From Top to bottom we have: 1) A data-driven model, obtained from CLEAN ing the [CII] observations from Chapter 3. 2) An optimized data-driven from the CLEAN ed [CII] model. It is optimized by aligning the [CII]-observations to the simulated observations in the image-plane and applying a SNR cut, by only selecting pixels which exceed a pixel count larger then 3s. 3) The MAP sky model of Rybak et al. (2020). 4) A NGC 5194 model, with ux masking (only using pixels, with counts larger than 3s. On the left, we show the ten most centered channel maps of each model, with a channel width of 40 km/s. On the right, we show the velocity integrated moment-0 map of each model. Each tick represents 1.5 arcsec.

MF should perform when tested on real data. We also simulated a very extended spiral galaxy NGC 5191, in order to test different spatial structures. We obtained the NGC 5194 from a galaxy catalogue, galsurvey.cat (MINTERFEROMETER, version 5.9). The NGC 5194 galaxy originates from the Berkeley Illinois Maryland Array, Hat Creek Radio Observatory data. The model we used to simulate the NGC 5194 galaxy as observed in Band 3 from ALMA, is shown in the bottom row of Figure 4.2.

For each simulation, we set the channel-width (inwidth) at 9.766 MHz, with a total bandwidth of 18.750 GHz, at a central frequency of 97.730 GHz, in order to simulate the entire band. Furthermore, we set the time in between observations (integration) at 20s. The noise parameters were set at default, and are determined by J. Pardo's ATM library (tsys-atm) Pardo et al. (2001).

With the simulations, we choose to deviate three parameters: The total integration time (minutes), the peak Surface brightness (mJy/pixel), and the resolution of the simulated observations (arcseconds). For each simulation, we kept 2 variables constant, while deviating the other. We set the range of the integration time between 5 and 60 minutes, to limit the data size of each simulation, such that the observation tted in local RAM. We varied the peak surface