

Cover photograph The Rosette Nebula, as captured by PACS and SPIRE on the Herschel Space Observatory in false-colour composite at three wavelengths: 70 microns (blue), 160 microns (green) and 250 microns (red). (*Photo: ESA/PACS & SPIRE Consortium*).

Astronomical Submillimetre Fourier Transform Spectroscopy from the Herschel Space Observatory and the JCMT

SCOTT CURTIS JONES

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Department of Physics & Astronomy University of Lethbridge LETHBRIDGE, ALBERTA, CANADA

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Abstract

Fourier transform spectroscopy (FTS) is one of the premier ways to collect source information through emitted radiation. It is so named because the principal measurement technique involves the analysis of spectra determined from the Fourier transform of a time-domain interference pattern. Given options in the field, many space- and ground-based instruments have selected Fourier transform spectrometers for their measurements.

The Herschel Space Observatory, launched on May 14, 2009, has three on-board instruments. One, SPIRE, comprises a FTS paired with bolometer detector arrays.

SCUBA-2 (Submillimetre Common User Bolometer Array) and FTS-2 have recently been commissioned and will be mounted within the collecting dish of the James Clerk Maxwell Telescope by Fall, 2010.

The use of FTS in these two observatories will be examined. While work towards each project is independently useful, the thesis is bound by the commonality between the two, as each seeks similar answers from vastly different viewpoints.

Acknowledgements

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Contents

Ał	ostra	\mathbf{ct}	iii
Ac	knov	wledgements	iv
Ta	ble o	of Contents	vii
Lis	st of	Tables	x
Lis	st of	Figures	xi
Li	st of	Abbreviations	xiii
Lis	st of	Equations	xv
1	Intr 1.1	Thesis Overview	1 4 4 5
2	Fou 2.1 2.2	rier Transform Spectroscopy Fourier theory	8 8 11 11 17 19 19
	2.32.42.5	Michelson interferometer	21 24 25 26 26 27
3	Det 3.1 3.2	ector Nonlinearity Overview	29 30 33

	3.3	Correction of Nonlinearities	38	
		3.3.1 Temperature-Based Nonlinear Correction Approach	44	
	3.4	Conclusion	46	
4	4 Spectral Line Fitting			
	4.1	Interstellar Medium	48	
		4.1.1 Interstellar Grains	49	
	4.2	Continuum Fitting	51	
		4.2.1 Line Fitting	52	
	43	FTS-2 Simulation	53	
	1.0	4.3.1 The ILS of a FTS	54	
		4.3.2 Line Fitting	56	
		4.3.2 Addition of Noise	- 60 - 60	
	1 1	4.5.5 Addition of Noise	62	
	4.4		03	
5	Pre	paring for Observations with FTS-2	66	
	5.1	SCUBA-2	66	
		5.1.1 FTS-2 versus Herschel/SPIRE	68	
		5.1.2 Transition Edge Sensors	68	
		5.1.3 FTS-2	71	
	5.2	Atmospheric Cancellation	73	
	5.3	SCUBA Legacy Catalogue	77	
		5.3.1 Extended and Fundamental Datasets	79	
		5.3.2 Handling FITS Files	80	
	5.4	Conclusions	83	
6	SPI	RE Data Analysis	85	
	6.1	Herschel Space Observatory	86	
		6.1.1 Spectral and Photometric Imaging Receiver	87	
	6.2	SPIRE Line Shape	89	
	6.3	Line Fitting	90	
		6.3.1 Threshold Detection	91	
		6.3.2 User-Supplied Line List	95	
		6.3.3 Detection of the Methylidyne cation	98	
	64	Botation Diagrams	101	
	0.1	6.4.1 Emission Lines	101	
		6.4.2 Botation Diagram Method	101	
		6.4.3 DR91	103	
	65	Conclusions	104	
	0.0		100	
7	Con	nclusion	108	
Bi	Bibliography 1			
Aj	Appendices 1			

Α	Publications and Conferences Proceedings	121
	A.1 Conference Proceedings	121
	A.2 Publications	122

List of Tables

2.1	Symmetry properties of Fourier transform pairs	15 19
2.2	Commonly encountered rouner pairs	10
3.1	SLWC3 Detector values	39
4.1	Comparison of simulated FTS and raw heterodyne fit parameters	61
5.1	Comparison of Herschel/SPIRE and JCMT/FTS-2	69

List of Figures

2.1	FT of a cosine function 1	3
2.2	FT of a sine function	4
2.3	FT of a phase-shifted cosine function	.6
2.4	Analytic sinc function	8
2.5	The Michelson Interferometer	21
3.1	Modeled nonlinear spectrum as compared to TES data	33
3.2	SPIRE Bolometer 3	\$4
3.3	Bolometer load curves	57
3.4	SPIRE detector nonlinearity as observed during PFM4 ground testing 4	10
3.5	Inverse responsivity curve used to derive JPL "K" coefficients	1
3.6	PFM4 nonlinear spectra corrected for nonlinearity 4	12
3.7	Recovered spectral powers pre- and post-correction	13
4.1	IRAS 60 μ m intensity map of G34	j 4
4.2	Measured line shape as captured by FTS-2 5	6
4.3	HARP G34.3 spectrum convolved to the resolution of FTS-2 5	57
4.4	Individual sinc fits to the convolved heterodyne spectrum 5	;9
4.5	Assembled fit to FTS-2 simulated spectrum	50
4.6	Line centre comparison between retrieved fit parameters and raw HARP data 6	;3
4.7	Integrated line area comparison between retrieved fit parameters and raw	
	HARP data 6	5 4
5.1	Superconducting transition of a Mo/Cu bilayer	70
5.2	Schematic illustration of Mach-Zehnder Fourier transform spectrometer 7	2
5.3	Rotation of FTS-2 ports with changes in elevation	'4
5.4	Simulated atmospheric emission above Mauna Kea	6
5.5	Atmospheric emission as viewed by each of the FTS-2 input ports 7	77
5.6	Difference in atmospheric emission between two input ports	'8
5.7	Orion KL emission map with predicted FTS-2 port positions	30
5.8	W3 (OH) emission map with predicted FTS-2 port positions 8	31
5.9	M17 emission map with predicted FTS-2 port positions	32
5.10	Sgr B2 emission map with predicted FTS-2 port positions	33
6.1	The Herschel Space Observatory	37
6.2	The SPIRE instrument	38

6.3	SPIRE ILS	90
6.4	Baseline fit to Orion spectrum	92
6.5	Orion spectral line identification	93
6.6	Orion spectral fit given detection threshold	94
6.7	Text file output from detection threshold fitting method	95
6.8	Orion spectral fit given input line list	96
6.9	Three emission lines from carbon-bearing species in Orion	97
6.10	Text output given input line list fitting method	98
6.11	CH doublet in Orion Bar spectrum	100
6.12	Model of emission and absorption within two-level atom	101
6.13	DR21 spectrum	105
6.14	DR21 rotation diagram	106

List of Abbreviations

AIG	Astronomical Instrumentation Group		
	Blue Sky Spectroscopy Transmission and Radiance Atmospheric Model		
	Blue Sky Spectroscopy Transmission and Radiance Atmospheric Model		
DEC	declination		
ESA	European Space Agency		
FITS	flexible image transport system		
FMOC	Fundamental Map Object Catalogue		
FOV	field-of-view		
\mathbf{FP}	Fabry-Perot Interferometer		
\mathbf{FTS}	Fourier transform spectrometer/spectroscopy		
FWHM	full width at half maximum		
HARP	Heterodyne Array Receiver Programme		
HIFI	Heterodyne Instrument for the Far-Infrared		
HIPE	Herschel Interactive Processing Environment		
IDL	Interactive Data Language		
IFTS	imaging Fourier transform spectrometer/spectroscopy		
ILS	instrumental line-shape		
\mathbf{IR}	infrared		
IRAS	Infrared Astronomical Satellite		
ISM	interstellar medium		
ISO	Infrared Space Observatory		
JCMT	James Clerk Maxwell Telescope		
\mathbf{LTE}	local thermodynamic equilibrium		
MCT	mercury-cadmium telluride		
NEP	noise-equivalent power		
NTD	neutron-transmutation doped		
OMC	Orion molecular cloud		
OPD	optical path difference		

LIST OF FIGURES

Photoconductor Array Camera and Spectrometer
photo-dissociation region
proto-flight model
performance verification
precipitable water vapour
right ascension
specialist astronomy group
Submillimetre Common User Bolometer Array
spectral energy distribution
SCUBA Legacy Catalogue
Spectral Legacy Survey
spectrometer long wavelength
signal-to-noise ratio
Spectral and Photometric Imaging Receiver
Superconducting Quantum Interference Device
spectrometer short wavelength
Transition-Edge Sensor
University of Lethbridge
zero path difference

List of Equations

2.1	Fourier series	9
2.2	Fourier coefficients	9
2.3	Infinite Fourier series	10
2.4	Inverse cosine Fourier transform	10
2.5	Inverse sine Fourier transform	10
2.6	Euler Fourier series	10
2.7	Forward Fourier transform	11
2.8	Cosinusoid	11
2.9	Fourier transform of a cosinusoid	11
2.10	Dirac delta function	12
2.11	Dirac delta function corollary	12
2.12	Sinusoid	12
2.13	Fourier transform of a sinusoid	12
2.14	Phase shifted cosinusoid	15
2.15	Magnitude of a complex-valued function	17
2.16	Phase of a complex-valued function	17
2.17	Boxcar function	17
2.18	Fourier transform of a boxcar function	18
2.19	Integral of a sinc function	18
2.20	Superposition theorem	19
2.21	Convolution	20
2.22	Integral of a theoretical ILS	20
2.23	Detector output given polychromatic input	20
2.24	Convolution theorem	21
2.25	Interferogram produced from monochromatic input	22
2.26	Interferogram without constant offset	23
2.27	Interferogram produced from polychromatic input	23
2.28	Interferogram produced from polychromatic input integrated over all wavenumbers	23
2.29	Spectrum produced from polychromatic input	23
2.30	Interferogram produced from polychromatic input without odd components .	23
2.31	Interferogram given limited OPD	24
2.32	Spectrum given limited OPD	24
2.33	Sinc function	24
2.34	Sinc FWHM	24
2.35	Resolving power of a FTS	25

$2.36 \\ 2.37$	Optical throughput of a FTS 25 Signal-to-noise ratio of a FT-IR instrument 27
$3.1 \\ 3.2$	Interferogram produced by a polychromatic source30Detector nonlinear voltage30
3.3	Theoretical nonlinear spectrum
3.4	Total bolometer power
3.5	Detector resistance
3.6	Temperature coefficient of resistance, α
3.7	Static thermal conductance
3.8	Bolometer heat capacity 36
3.9	Bolometer energy balance
3.10	Dynamic thermal conductance
3.11	Effective thermal conductance
3.12	Bolometer dynamic impedance
3.13	Electrical power dissipated in bolometer
3.14	Bias current through detector circuit
3.15	Input bolometer power
3.16	Output bolometer power
3.17	Nonlinear voltage correction equation
3.18	Integrated nonlinear voltage correction equation
3.19	Bath temperature drift correction equation
3.20	Final, temperature-drift correction detector timeline 44
3.21	Experimentally computed detector resistance
3.22	Bolometer temperature
3.23	Experimentally determined bolometer electrical power
3.24	Bolometer current from Ohm's law 45
3.25	Optical power incident on the bolometer
3.26	Total optical plus electrical power, from energy balance considerations 45
4.1	Spectral energy distribution of interstellar dust 49
4.2	Source intensity reduction resulting from intercepting dust
4.3	Planck blackbody function
4.4	Priddey greybody approximation
4.5	Colbert baseline function
4.6	Sinc line shape
4.7	Sinc FWHM
4.8	Sinc integrated area
5.1	Transition edge sensor coefficient of resistance
6.1	FWHM of SPIRE line shape
6.2	CH ⁺ formation scheme
6.3	Alternate CH^+ formation scheme with vibrationally excited H_2
6.4	Total intensity detected from a molecular transition
6.5	SPIRE beam-size conversion
6.6	Amplitude of a rotational transition line
	-

LIST OF EQUATIONS

6.7	Upper energy state emitter population	102
6.8	Upper state energy	102
6.9	Frequencies of rotational transitions	103
6.10	Rotational partition function	103
6.11	Fractional representation of upper state energy population	103
6.12	Rotation diagram equation	103
6.13	Line intensity ratio	104
6.14	Rotation temperature from rotation diagram	104
6.15	Column abundance from rotation diagram	104
6.16	Einstein A coefficient	105
6.17	Rotation diagram line strength quantity	105

Chapter 1

Introduction

Sir William Herschel, perhaps the most prominent astronomer of the late 18th and early 19th centuries, is credited with the discovery of infrared radiation. Herschel studied the energy distribution of sunlight passed through a prism [1], and by placing thermometers either side of the visible color spectrum, was able to detect additional heat above background levels. Born in Germany in 1738, he emigrated to Britain at age 19 as an accomplished musician skilled in both performance and composition. His musical aptitude for pattern recognition he found easily transferable to astronomy and soon Herschel was sight-reading the night skies with the same vigour as a cello score. During his most fruitful scientific years, he was accompanied by his sister Caroline, herself a recognized concert singer, in all sweeps and scans of the starry canvas. Together and individually, they made many celebrated breakthroughs and celestial catalogues; Caroline towards the understanding of comets and their motion, and William of nebulous formations. In addition to publishing his paper on infrared light, Herschel is also known for finding the planet Uranus in 1781, along with two of its moons.

The space between stars is typically thought of as just that, "space", an empty vacuum to the unaided eye. At the same time, one can make the obvious assumption that the Universe as it persists today is not as it was just after the Big Bang. For one, we know that it is expanding due to the observed red-shift of distant galaxies. For another, momentous events such as supernova explosions have been witnessed, the violent destruction of stars resulting in the expulsion of gas and dust, which go on to congregate in stellar nurseries, and ultimately power a nascent star. This recycling process between stars and the interstellar medium (ISM) continues indefinitely, with the caveat that some of the dust will endure in the ISM as a site of molecule formation.

The study of the physics and chemistry of the ISM continues to mature, particularly as infrared and submillimeter observatories start to become commonplace. These breakthroughs began with the launch of the Infrared Astronomical Satellite (IRAS) [2] in 1983, followed closely thereafter by the Diffuse Infrared Background Experiment (DIRBE) on-board the Cosmic Background Explorer (COBE) [3], launched in 1989. Whereas the former performed a broad sampling of the entire sky, DIRBE was designed to focus on the quantification of dust emission from the ISM. Both instruments acquired data sets that represented a wide range of physical conditions, from the cold temperatures encountered at the centre of dense molecular clouds to the highly excited photo-dissociated regions found near a young, hot star. As missions multiplied over the last two decades, progress was made on a host of scientific fronts, meaning that some division of responsibility needed to occur to limit the number of science-based questions that each instrument sought to answer. These data, benefacting from improved technology, begin to accumulate, we can now hope to synthesize them with the dated discoveries of IRAS, the Infrared Space Observatory (ISO) [4] and COBE, towards the betterment of our theoretical understanding.

Today, the Herschel Space Observatory is in orbit, measuring infrared radiation in the 55-672 μ m region, hoping to answer many fundamental astronomical questions, largely concerned with how and why the Universe evolves as it does. The three on-board instruments: the Heterodyne Instrument for the Far Infrared (HIFI), the Photodetector Array Camera and Spectrometer (PACS) and the Spectral and Photometric Imaging Receiver (SPIRE), will uniquely enable Herschel to do so. At its current orbital position roughly 1.5 million km from Earth, Herschel is beyond Earth's obscuring atmosphere and exposed to the entire sky opposite the Sun.

At the same time, many successful ground-based observatories are in operation, among them the James Clerk Maxwell Telescope (JCMT) on the summit of Mauna Kea, Hawaii. The JCMT used to house the Submillimetre Common User Bolometer Array (SCUBA) instrument, but will soon be replaced by its successor, SCUBA-2, commissioned in 2010. Both take advantage of narrow regions of the atmospheric electromagnetic spectrum that are relatively transparent to incident radiation, namely the 450 μ m and 850 μ m bands. While Herschel enjoys a much broader spectral coverage, SCUBA-2 will benefit from much greater angular resolution owing to the 15 m diameter collecting dish of the JCMT.

1.1 Thesis Overview

This thesis will consider infrared observations from Herschel as well as anticipated results from SCUBA-2. The two telescopes, one on the ground and one in space, provide two complementary methods to achieve many of the same scientific goals and each will be approached with an appreciation for its strengths and weaknesses. Data from each observatory will supplement current understanding of a series of concepts common to modern observatories. This introductory chapter presented the history of infrared measurements as a way of probing how future measurements will fit into the existing repertoire.

1.1.1 My Thesis

When I first began my study in the Masters program in May 2008, this thesis was to take a vastly different direction. At this time, it was decided that I would be involved in the FTS-2 project, which was to be tested in a laboratory and eventually deployed at the JCMT. Included in this work would have been the responsibility to predict and plan for observations with FTS-2, before ultimately collecting data on-site for a set of pre-defined targets. However, due to circumstances beyond my control, which caused a significant delay in the manufacture of SCUBA-2 detector wafers, such a course of action was no longer possible.

Fortunately, my research group, the Astronomical Instrumentation Group (AIG) at the University of Lethbridge (UL), led by Dr. David Naylor, is involved in several largescale projects. One of these, the Herschel Space Observatory, was successfully launched into orbit on May 14, 2009. At this time I had already begun work into observation preparation with SCUBA-2, based upon a comprehensive catalogue of past SCUBA measurements, but I had also been involved in the pre-flight analysis of spectroscopic data from the Spectral and Photometric Imaging REceiver (SPIRE), to be launched on-board Herschel. Being half-way through my Masters program, but given the opportunities that real data from Herschel would reward both myself and the group, it was here that the scope of the thesis took a different focus. Instead of a limited focus on SCUBA-2, work in the chapters that follow examines topics in Fourier transform spectroscopy from two perspectives, that of a space-based telescope in Herschel/SPIRE, and that of a ground-based telescope in SCUBA-2/FTS-2.

While these two observational platforms may appear disparate and unrelated, they actually strive towards many of the same science goals. Both use instrumentation in which the AIG is well-versed, in Fourier transform spectrometers (FTS) of largely similar designs. However, due to their different locales, the challenges faced by each FTS are unique. While FTS-2 at the JCMT has to contend with the atmosphere of the Earth, the SPIRE FTS has to function much more independently at its location roughly 1.5 million km from Earth, over a time range limited by the boil-off rate of the cooling cryogens. What follows is a survey of some of the common issues faced by each instrument, where all possible attempts will be made to draw parallels between both their operation and subsequent data analysis.

1.1.2 Thesis Outline

Chapter 2 introduces Fourier transform spectroscopy along with associated Fourier theory. Both SPIRE, mounted on Herschel, and SCUBA-2 make use of a FTS, and this chapter will additionally provide some background on the FTS instrument and its practical applications.

Chapter 3 goes on to examine one of the main concerns for sensitive detecting elements found on both Herschel and SCUBA-2, namely their nonlinear response to incident radiation. Each instrument is served by a type of detector called a bolometer and the theory and associated correction methods will benefit both. Data from Herschel, currently in operation, will be the focus, but initial laboratory tests have already shown the FTS-2 detectors to be susceptible to the effect as well.

Chapter 4 will introduce the concept of spectral line fitting, in the context of simulated FTS-2 data derived from HARP, a heterodyne receiver also at the JCMT. This particular area of work, while initially well-contained towards predicting the look of spectra to be received from FTS-2, has found use with SPIRE data also. Out of the line fitting software developed in this chapter came a much more functional rendition of the code that will eventually be distributed to the entire Herschel/SPIRE science team.

Chapter 5 more closely characterizes SCUBA-2 and FTS-2 and specifically, presents means for accounting for the atmosphere in upcoming observations. As perhaps the most necessary and important step in the observation planning process, the AIG must use the results from this work towards determining which sources are the most viable observing targets and whether or not they are viewable on any given night.

Chapter 6 was the last chapter to take shape, as it includes recent flight data from the SPIRE spectrometer, available to the AIG because of Dr. Naylor's position on many of the Specialist Astronomy Groups (SAG) within SPIRE. Much of the data presented there has only recently been gathered and processed, and provides an ideal test of many of the concepts developed to this point in the thesis.

Chapter 2

Fourier Transform Spectroscopy

This chapter will examine the theory behind Fourier transform spectroscopy (FTS), as these concepts are required to understand the remainder of the thesis.

Section 2.1 introduces Fourier theory, including Fourier transforms and how they are defined in terms of Fourier integrals, leading to the important concept of Fourier decomposition. These ideas are applied to a study of the Michelson interferometer, the earliest type of Fourier transform spectrometer in Section 2.3. Section 2.4 concludes with some of the practical considerations in the design of a Fourier spectrometer.

2.1 Fourier theory

The pioneer behind the mathematical analysis of periodic waveforms is Jean Baptiste Joseph, Baron de Fourier [5] [6] (1768 - 1830). Fourier was born in Auxerre, France, where, orphaned at an early age, he managed to enter a military school that ultimately fostered his interest in mathematics. Discouraged there by the restraints imposed by a low social ranking, he transferred to a Benedictine school in hopes of becoming a priest. Soon however, he was overcome by his interest in math and was subsequently appointed to a teaching post at his former school. While in and out of instructional positions, Fourier continued to hold strong nationalist sentiments that culminated with an association with Napoleon's Egyptian campaign. He remained in Napoleon's favour, carrying out diplomatic and administrative duties, up until France's defeat at Waterloo and the emperor's exile to Saint Helena.

Fourier's theory states that any periodic function f(x) can be expressed as an infinite sum of sinusoidal components,

$$f(x) = \sum_{m=0}^{\infty} \left[A_m \cos\left(mkx\right) + B_m \sin\left(mkx\right) \right]$$
(2.1)

where x is the position, $k = 2\pi/\lambda = 2\pi\sigma$ is the angular wavenumber and A_m and B_m are amplitude coefficients, the determination of which is the central problem in Fourier analysis. The amplitude coefficients can be computed via [7]

$$A_{m} = \frac{1}{L} \int_{-L}^{L} f(x) \cos mkx \, dx \quad m = 1, 2, 3, ...,$$

$$B_{m} = \frac{1}{L} \int_{-L}^{L} f(x) \sin mkx \, dx \quad m = 1, 2, 3, ...$$
(2.2)

where the interval [-L,L] represents one period $(L = \frac{\lambda}{2})$.

Aperiodic functions, which can be thought of as having an infinite period, can also be expressed as a Fourier series of infinitesimally small frequency segments summed together with a *Fourier integral*. The discrete summation in Equation 2.1 can be expressed in continuous form as [8]

$$f(x) = \int_{-\infty}^{\infty} A(\sigma) \cos(2\pi\sigma x) \, d\sigma + \int_{-\infty}^{\infty} B(\sigma) \sin(2\pi\sigma x) \, d\sigma \tag{2.3}$$

where the limits $\pm L$ have been extended to infinity to represent a function of infinite period. Here, $A(\sigma)$ contains only even terms and $B(\sigma)$ only odd terms. Equation 2.3 defines the *inverse Fourier transform*, where

$$f_c(x) = \int_{-\infty}^{\infty} A(\sigma) \cos(2\pi\sigma x) \, d\sigma \tag{2.4}$$

is the inverse *cosine* Fourier transform and

$$f_s(x) = \int_{-\infty}^{\infty} B(\sigma) \sin(2\pi\sigma x) \, d\sigma \tag{2.5}$$

the inverse *sine* Fourier transform.

Equation 2.3 is generally expressed as

$$f(x) = \int_{-\infty}^{\infty} \Phi(\sigma) e^{2\pi i \sigma x} \, d\sigma \tag{2.6}$$

where $i = \sqrt{-1}$ and for an asymmetrical function f(x), $\Phi(\sigma)$ is complex-valued and therefore contains both sine and cosine terms. The *Fourier pair*, or *forward Fourier transform*, is obtained as

$$\Phi(\sigma) = \int_{-\infty}^{\infty} f(x)e^{-2\pi i\sigma x} dx$$
(2.7)

where x and σ are known as *conjugate variables*, while $\Phi(\sigma)$ and f(x) are called *Fourier* pairs. These formulae are equally valid with time, t, and frequency, ν , and $\Phi(\nu)$ and f(t)as conjugate variables and Fourier pairs, respectively.

2.2 Theorems of Fourier Analysis

Fourier transforms have some basic properties that lead to more useful theorems that guide efforts in the field, collectively known as *Fourier analysis*. Topics to be covered in this section include symmetry, transform pairs and the superposition and convolution theorems, each of which are used in the remainder of this thesis.

2.2.1 Symmetry

The Fourier transform of an even cosinusoid of unit amplitude and spatial frequency $\sigma_0 \ (\mathrm{cm}^{-1})$ given by

$$f(x) = A\cos\left(2\pi\sigma_0 x\right) \tag{2.8}$$

is expressed as

$$F(\sigma) = \frac{1}{2}\delta(\sigma - \sigma_0) + \frac{1}{2}\delta(\sigma + \sigma_0)$$
(2.9)

where $\delta(\sigma')$ is the Dirac delta function [9] [10]. The Dirac delta function is defined by

$$\delta(\sigma') = \begin{cases} \infty & \text{for } \sigma' = 0 \\ 0 & \text{for } \sigma' \neq 0 \end{cases}$$
(2.10)

and

$$\int_{-\infty}^{+\infty} \delta(\sigma') \, d\sigma' = 1, \tag{2.11}$$

where $\sigma' = \sigma \pm \sigma_0$. As seen in Figure 2.1, two spectral features of identical magnitude positioned at $\pm \sigma_0$ have resulted from the Fourier transform of an even cosine, of spatial frequency $\sigma_0 = 2 \text{ cm}^{-1}$. Together, the amplitudes combine to yield that of the original function - that is, each function has height $\frac{1}{2}$. Both the $+\sigma_0$ feature and the $-\sigma_0$ feature are real-valued, with even symmetry about $\sigma = 0$.

Similar symmetry arguments apply to an odd function

$$f(x) = \sin\left(2\pi\sigma_0 x\right) \tag{2.12}$$

with a Fourier transform of

$$F(\sigma) = \frac{-i}{2}\delta(\sigma - \sigma_0) + \frac{i}{2}\delta(\sigma + \sigma_0).$$
(2.13)

This time, $F(\sigma)$ is imaginary-valued and of odd symmetry, with the positive and negative frequency components of opposite sign, as illustrated in Figure 2.2 for a sine function of spatial frequency $\sigma_0 = 2 \text{ cm}^{-1}$. Again, however, the amplitude of f(x) is evenly split between the two functions such that the negative frequency component has height $+\frac{1}{2}$ and the positive frequency component $-\frac{1}{2}$.

More generally, an arbitrary function will be asymmetric as a result of an additional



Figure 2.1: The Fourier transform of a cosine function (top) of spatial frequency $\sigma_0 = 2 \text{ cm}^{-1}$.



Figure 2.2: Fourier transform of a sine function of spatial frequency $\sigma_0 = 2 \text{ cm}^{-1}$.

f($\frac{1}{x}$	F($F(\sigma)$		
Real	Imaginary	Real	Imaginary		
even	0	even	0		
odd	0	0	odd		
0	even	0	even		
0	odd	odd	0		
asymmetric	0	even	odd		
0	asymmetric	odd	even		
even	odd	asymmetric	0		
odd	even	0	$\operatorname{asymmetric}$		
even	even	even	even		
odd	odd	odd	odd		
$\operatorname{asymmetric}$	$\operatorname{asymmetric}$	asymmetric	asymmetric		

Table 2.1: Symmetry properties of a Fourier pair

phase term. From Equation 2.8, if instead we now have

$$f(x) = \cos\left(2\pi\sigma_0 x + \phi\right) \tag{2.14}$$

where ϕ is the phase of the wavefunction, then the Fourier series now contains even and odd components, real and imaginary, respectively [9]. Correspondingly, upon Fourier transformation of Equation 2.14 there are now real and imaginary terms, where the real parts are symmetric about $\sigma = 0$ and the imaginary parts anti-symmetric, as shown in Figure 2.3 for $\phi = \frac{\pi}{3}$. These symmetry properties are summarized in Table 2.1.

In Figure 2.3, the magnitudes of the real functions are determined from the cosine of the phase, while the components of the imaginary parts come from the sine of the phase. This is equivalent to placing the total, unit magnitude as a complex vector on an Argand diagram [11], where the x and y components are the real and imaginary components, respectively. In that case, each function in the real domain has height $\frac{1}{4}$ and $\frac{\sqrt{3}}{4}$ in the



Figure 2.3: Fourier transform of a cosine function of spatial frequency $\sigma_0 = 2 \text{ cm}^{-1}$ phaseshifted by $\frac{\pi}{3}$ radians.

imaginary domain, and we have

$$1 = \sqrt{\operatorname{Re}_{\sigma}^2 + \operatorname{Im}_{\sigma}^2}.$$
(2.15)

where Re_{σ} is the real component of the spectrum, and Im_{σ} is the imaginary component. The Argand diagram is also imbued with information about the phase, which, via trigonometry, is given by

$$\phi = \arctan\left(\frac{\mathrm{Im}_{\sigma}}{\mathrm{Re}_{\sigma}}\right). \tag{2.16}$$

Out of this comes a process termed *phase correction* [10], used to correct asymmetric interferograms (see $\S2.3$).

2.2.2 Fourier Pairs

There are a set of functions and their Fourier transforms that are fundamental to Fourier transform spectroscopy [10]. In particular, one of these will be essential to the furthering of this thesis. The so-called box car (also top hat or rect), function, defined by

$$\Pi(x) = \begin{cases} 1 & \text{for } |x| < L \\ 0 & \text{for } |x| > L \end{cases}$$

$$(2.17)$$

has a Fourier pair [8]

$$\Phi(p) = \int_{-\infty}^{\infty} \Pi(x) e^{-i2\pi\sigma x} \, dx = \int_{-L}^{L} e^{-i2\pi\sigma x} \, dx = 2L \frac{\sin(2\pi\sigma L)}{2\pi\sigma L}$$
(2.18)



Figure 2.4: A sinc function

where $\frac{\sin(2\pi\sigma L)}{2\pi\sigma L}$ is usually written as $\operatorname{sinc}(2\pi\sigma L)$, known as the cardinal sine, or sinc function. Therefore, the boxcar and the sinc form a Fourier pair. The sinc function appears throughout mathematics and science, with $\operatorname{sinc}(x) = 1$ at x = 0 and $\operatorname{sinc}(x) = 0$ for $x = n\pi$, such that

$$\int_{-\infty}^{\infty} \operatorname{sinc} x \, dx = 1. \tag{2.19}$$

In the above example, the sinc function has zeros at $\sigma = \frac{n}{2L}$, where n = 0, 1, 2, ... It has a full width at half maximum (FWHM) of $\frac{1.207}{2L}$ and a secondary minimum at $\frac{1.43}{2L}$ (see Figure 2.4). Other Fourier transform pairs that have found broad usage are listed in Table 2.2 [10].
f(x)	$ $ $F(\sigma)$
$\Pi(x)$ (Boxcar)	$2L \mathrm{sinc}(2\pi\sigma L)$
$\Lambda(x) \text{ (Triangle)} = \begin{cases} 1 - \frac{ x }{2L} & \text{for } x < 2L\\ 0 & \text{for } x > 2L \end{cases}$	$4L^2 \mathrm{sinc}^2(2\pi\sigma L)$
$e^{-\pi x^2}$ (Gaussian)	$e^{-\pi\sigma^2}$ (Gaussian)
$e^{-2 x }$	$\frac{1}{1+\pi^2\sigma^2}$ (Lorentzian)
$\cos\left(2\pi\sigma_0 x ight)$	$\left \frac{1}{2} [\delta(\sigma - \sigma_0) + \delta(\sigma + \sigma_0)] \right $
III(ax) (Dirac comb)	$III(\sigma/a)$ (Dirac comb)

Table 2.2: Commonly encountered Fourier pairs.

2.2.3 Superposition Theorem

If two functions f(x) and g(x) have Fourier transforms $F(\sigma)$ and $G(\sigma)$ respectively, then their sum has a Fourier transform

$$f(x) + g(x) \Longleftrightarrow F(\sigma) + G(\sigma) \tag{2.20}$$

where \iff is used to indicate a Fourier transformation. This is known as the superposition, or addition theorem [10] [9] and holds true for both forward and reverse Fourier operations.

2.2.4 Convolution Theorem

Also known by its German name *Faltung*, or "folding", the convolution theorem is arguably the most important theorem in scientific data-processing. In fact, in Fourier transform spectroscopy, it is indeed unavoidable as any measurement made by a detector represents a convolution of the desired quantity with a weighting function, known as the Instrumental Line Shape (ILS). The ILS of a FTS is the sinc function. A convolution of two functions, f(x) and g(x) is a mathematical operation given by [9]

$$f(x) * g(x) = \int_{-\infty}^{\infty} f(u)g(x-u) \, du$$
 (2.21)

where the "*" represents the convolution operation. An ideal spectrometer exposed to a monochromatic source should produce as a spectrum a function, δ , of infinitesimal width at the wavelength of the source, or $kS\delta(\lambda - \lambda_0)$, where S is the intensity of the radiation and k depends on the instrumental throughput, geometry and detector sensitivity [8]. In actuality what is observed is a spectrum of some structure, namely $kSI(\lambda - \lambda_0)$, where I is the ILS and

$$\int_{-\infty}^{\infty} I(\lambda) \, d\lambda = 1. \tag{2.22}$$

Should the source intensity be continuous, or polychromatic, the spectrum becomes wavelength dependent, $S(\lambda)$, and the output at the detector, $O(\lambda)$, is

$$O(\lambda) = k \int_{-\infty}^{\infty} S(\lambda') I(\lambda - \lambda') \, d\lambda'$$
(2.23)

where $O(\lambda)$ is a convolution of the spectrum, $S(\lambda)$ and the line shape function, $I(\lambda)$ [8]. If both the source spectrum and the ILS of a particular spectrometer are known, then it is in principle possible using the convolution theorem to model what is seen by any spectrometer. These ideas are expanded upon in Chapter 4.

The convolution theorem states that

$$\int f(u)g(x-u)\,du \equiv f(x) * g(x) \Leftrightarrow F(\sigma) \cdot G(\sigma)$$
(2.24)

2.3. MICHELSON INTERFEROMETER



Figure 2.5: The Michelson Interferometer

where \Leftrightarrow has been used to indicate both a forward and reverse Fourier transform. In other words, the Fourier transform of a convolution is the product of the individual transforms of the two functions [10].

2.3 Michelson interferometer

The Michelson interferometer, shown in Figure 2.5, is the simplest type of Fourier spectrometer.

Electromagnetic radiation emitted by the source passes through the collimating mirror towards an ideal beamsplitter, which evenly divides the energy along two separate paths. One such path terminates at a fixed mirror, while the other ends at a moving mirror. Light from each is then reflected back towards the beamsplitter, where the two rays recombine.

At this point, half the radiation is lost as it returns toward the source, while the other half continues on to the detector. In this way a Michelson interferometer can be thought of as having two output ports, a scenario which will be compared with the Mach-Zehnder design in Chapter 5. Interferometers work on the principle of interference between the two electromagnetic waves, out of phase by an amount dependent on the optical path difference (OPD) between the two recombined beams. At one particular position of the moving mirror, the path lengths will be equal, a position known as zero path difference (ZPD). Here, either maximal constructive or destructive interference will occur, resulting in either a signal of greatest amplitude and greatest modulation or a dark spot, respectively. The goal is to achieve the highest possible signal at the detector.

Consider a monochromatic input beam of wavenumber σ_0 , and amplitude $B(\sigma_0)$ supplied to an interferometer like that in Figure 2.5. At the detector, a modulated signal known as an interferogram is produced, with intensity

$$I_0(x) = B(\sigma_0)[1 + \cos(2\pi\sigma_0 x)] \quad [W]$$
(2.25)

where x is the optical path difference. At the position of ZPD, x = 0, and the function is maximized. Customarily, the constant offset term is neglected, such that the interferogram is given only by the modulated part,

$$I_0(x) = B(\sigma_0) \cos(2\pi\sigma_0 x) \quad [W].$$
(2.26)

The extension to polychromatic light follows as expected. Now, at the wavenumber σ , $B(\sigma)d\sigma$ is the energy in the interval $d\sigma$, creating an interferogram component dI(x):

$$dI(x) = B(\sigma)\cos\left(2\pi\sigma x\right)d\sigma \quad [W].$$
(2.27)

Integrating over all wavenumbers,

$$I(x) = \int_{-\infty}^{\infty} B(\sigma) \cos(2\pi\sigma x) \, d\sigma \quad [W]$$
(2.28)

which is related to the spectrum, $B(\sigma)$ by a Fourier transform

$$B(\sigma) = \int_{-\infty}^{\infty} I(x) \cos(2\pi\sigma x) \, dx \quad [W].$$
(2.29)

As already discussed, in performing the transform in Equation 2.29, because $\cos(2\pi\sigma x) = \cos(-2\pi\sigma x)$, a spectral mirror image to $B(\sigma)$ will be created at negative frequencies, $B(-\sigma)$. Physically meaningless, this component is often ignored, but is in fact very important when attempting to retrieve the initial interferogram. The interferogram can be expressed in terms of the input spectrum $B_e(\sigma)$ as follows

$$I(x) = \int_{-\infty}^{\infty} B_e(\sigma) \cos(2\pi\sigma x) \, d\sigma \quad [W].$$
(2.30)

2.4 Practical Considerations in FTS

The material presented in §2.3 makes a number of mathematical assumptions. For example, an optical path difference of $\pm \infty$ is clearly unattainable. In reality, spectrometers are limited by the length of travel of the moving mirror, where $-L \leq x \leq +L$, for L as the maximum path difference. The effect of a finite x is to multiply the interferogram by a rectangular function

$$I_{obs}(x) = I(x) \cdot \Pi\left(\frac{x}{2L}\right).$$
(2.31)

In the spectral domain, this corresponds to a convolution with a sinc function,

$$B_{obs}(\sigma) = B(\sigma) * 2L\operatorname{sinc}(2L\sigma)$$
(2.32)

where the sinc function is the ILS of a Fourier transform spectrometer

$$I(\sigma) = 2L\operatorname{sinc}(2L\pi\sigma). \tag{2.33}$$

Instead of the infinitesimally small line width, which would result if the interferogram extended out to infinity, the ILS has FWHM given by

$$FWHM = 1.207\delta\sigma = 1.207\left(\frac{1}{2L}\right)$$
(2.34)

where $\delta\sigma$ is called the *resolution width*, or the distance between independent sampled points in the spectrum [10]. The resolution width is maintained throughout the spectrum in spite of the variations in noise with wavelength that might be observed. This is one of the main advantages of using a FTS.

Correspondingly, the resolving power is then

$$R \equiv \frac{\sigma}{\delta\sigma} = 2L\sigma. \tag{2.35}$$

In spite of the mathematical complexity, a FTS can be simple in its design and still finds frequent use due to some unique advantages.

2.4.1 Jacquinot's Advantage

All types of spectrometers may be judged on their throughput (also étendue or light-grasp), or the amount of light allowed to pass through the entrance aperture. Jacquinot was the first to recognize the throughput advantage from the circular symmetry of the input beam of a FTS when compared to the narrow area of the entrance slit of a diffraction grating spectrometer [12]. Quantitatively, the optical throughput may be defined as

Optical Throughput =
$$A\Omega\eta_0$$
 (2.36)

where A (m²) is the area of the entrance aperture presented to the source, Ω (sr) is the solid angle subtended by the collimating mirror or lens, and η_0 is the optical efficiency of the spectrometer [10]. In a FTS, light enters the instrument at an angle perpendicular to the initial optics, which permits a larger circular entrance aperture (typically on the order of centimeters) as compared to dispersive devices such as grating spectrometers. Natural apodization, which is a result of divergence within the interferometer, places a limit on the maximum attainable resolution and is therefore to be approached with caution for many applications [13].

2.4.2 Finite Entrance Aperture/Field-of-View

Due to the finite size of the entrance aperture of the interferometer, the incoming beam will be divergent. The path differences will therefore cover a range of values dependent upon the angle that radiation enters the instrument with respect to on-axis light. For the centre pixel, the effect of a finite aperture, known as natural apodization, is to multiply the interferogram by a sinc function [10]. This will both change the ILS and the frequency scale of the spectrum. Whereas for an on-axis signal, a spectral line would appear at σ_0 , for oblique rays entering at a relatively large angle, the line will be shifted to $\sigma_0[1 - \Omega/(4\pi)]$, where Ω is the solid angle of a circular aperture at the focus of the collimating mirror [10]. In addition, each of the spectral features will be broadened by $\Omega \sigma_0/(2\pi)$ [13]. However, in the case of the SPIRE FTS, the internal divergence is such that it does not, to first order, require correction and the sinc function is expected to be an accurate representation of the ILS.

2.4.3 Fellgett's Advantage

A second key advantage that a FTS has on other spectrometers is the so-called multiplex, or Fellgett [14] advantage. Fourier transform spectrometers are able to record data at all frequencies simultaneously, again, as opposed to grating spectrometers, which must measure each frequency separately in a time-consuming manner.

Both the multiplex and throughput advantages seek to maximize the signal-to-

noise ratio (SNR) of the FTS. The signal to noise in a FTS may be defined as

$$S/N = \frac{B(\sigma)\delta\sigma\Theta\eta t^{1/2}}{NEP}$$
(2.37)

where $B(\sigma)$ is the brightness, $\delta\sigma$ is the resolution, Θ is the optical throughput, η is the optical efficiency, t is the measurement time, and NEP is the noise-equivalent power, or the amount of power needed to yield a signal-to-noise ratio of unity [15]. In the case of the Fellgett advantage, the multiplex gain is typically proportional to the square root of the number of spectral elements. Thus, greater coverage of the range of frequencies included in the source spectrum can lead to a higher SNR, but only when the detector is the primary source of noise. If the FTS is photon-noise limited, then it may be more beneficial to reduce the number of sampled frequencies. This is known as a multiplex disadvantage. The connection to Jacquinot's advantage is more obvious, as a higher throughput means a larger signal which ultimately implies a sizeable SNR. Typically, these two combine to produce a SNR much greater than that for a dispersive, grating spectrometer.

2.5 Conclusions

This chapter has explored some theoretical *and* practical implications of using a Fourier transform spectrometer, which will be important in the remaining chapters. Reasons for selecting a FTS for spectrometry were touched upon in Sections 2.4.1 and 2.4.3. The Michelson interferometer was selected in Section 2.3 as an introduction to interferometers, however it is the Mach-Zehnder design employed by SPIRE and FTS-2, which will be examined more closely in Chapters 5 and 6. The application of most of the Fourier theory

2.5. CONCLUSIONS

to the remainder of the thesis will be more indirect, although Chapter 4 makes direct use of the convolution operation as a tool in simulating FTS-2 data.

Chapter 3

Detector Nonlinearity

This chapter will examine the behaviour of ultra-sensitive bolometers when exposed to a high photon background, a set of conditions that lead to a nonlinear relationship between the optical loading and the detector response. Section 3.1 will introduce this concept, explaining the manner in which nonlinearity impacts the derived spectrum. A summary of existing nonlinear correction techniques in the literature as they apply to photoconductive and photovoltaic mercury-cadmium-telluride detectors is presented. Section 3.2 goes on to illustrate a textbook example of nonlinearity, as seen in data from a cuttingedge type of detector intentionally driven nonlinear. Finally, Section 3.3 details advantages and disadvantages of the nonlinear correction method employed by the Herschel/SPIRE spectrometer.

3.1 Overview

The nonlinear response of astronomical detectors can significantly impact the retrieval of accurate spectral fluxes. This is especially true given the advent of detector technologies capable of providing optical noise equivalent powers (NEPs) approaching 10^{-19} W/\sqrt{Hz} [16]. At this remarkable sensitivity, observations of galactic sources with a Fourier Transform spectrometer (FTS) will produce such large modulations around the position of zero path difference (ZPD) in the measured interferogram that nonlinear effects in the derived spectrum will occur if left uncorrected. The effect will be manifested as a series of non-physical harmonic spectral features that effectively steal energy from the fundamental band(s).

The measured signal produced by a FTS is known as an interferogram. For a polychromatic source, the interferogram can be represented as

$$I(x) = \int_{\sigma_{min}}^{\sigma_{max}} B(\sigma) \exp\left(2\pi i \sigma x\right) d\sigma \quad [W]$$
(3.1)

where I is the power on the detector as a function of the optical path difference, x, for a source emitting over a wavenumber range from σ_{min} to σ_{max} and of intensity $B(\sigma)$.

For a nonlinear detector response, the resulting detector voltage V_d is related to the interferogram signal I(x) by

$$V_d(x) = \alpha + \beta I(x) + \gamma I^2(x) + \delta I^3(x) + \dots$$
(3.2)

where the coefficients α , β , γ and δ are dependent on the specific detector being used and

its operating characteristics. This in turn leads to a spectrum of the form

$$S(\sigma) = \alpha' + \beta' B(\sigma) + \gamma' [B(\sigma) * B(\sigma)] + \delta' [B(\sigma) * B(\sigma) * B(\sigma)] + \dots$$
(3.3)

The β' term represents the spectral radiance, $B(\sigma)$, centred at σ_0 and of width σ_w . The quadratic term, γ' , results in two spectral features of width $2\sigma_w$, centred at 0 cm⁻¹ and $2\sigma_0$. The cubic term, δ' also contributes two spectral features to the spectrum, and these occur at σ_0 and $3\sigma_0$, respectively, both of width $3\sigma_w$.

The subject of detector nonlinearity and its correction has been extensively studied in the literature for mercury-cadmium-telluride (MCT) detectors [17] [18] [19]. These detectors are commonly used in mid-infrared (2 - 20μ m) spectroscopic measurements and belong to two different subtypes: photoconductors and photovoltaics. In the photoconductive case, the detector shows a sharp change in electrical resistance with changes in incident infrared radiation, while in the photovoltaic case all current is provided by the electrons liberated by the photoelectric effect. Fourier transform spectrometers, because of the étendue advantage, first noted by Fellgett [14] and Jacquinot [12] (see Chapter 2), are the most efficient of spectrometers, but confers a disadvantage that the increased power on the detector can drive the device nonlinear. The easiest solution to this problem is to either reduce the source intensity or limit the spectral range, both of which negate the two main advantages of Fourier transform spectroscopy. Although nonlinearities can be induced by the detector readout electronics, by careful design such effects can be minimized. Here we focus on nonlinearity due to the detector itself.

In practice, both hardware and software solutions to the correction of nonlinearity

in MCT detectors have been proposed. For example, Guelachvili [20] used a two-output Connes-type interferometer to devise a mathematical relationship between the total gain at the two output ports, the zeroth through second order nonlinear coefficients, and the intensities at each of the two outputs, to provide a first-order correction to the nonlinear terms. Software methods have been created by Keens and Simon [21], who used the uncorrected spectrum to find two correction constants. This method relies on a fit to the low-frequency spectrum to determine the signal at zero frequency and an integral of the square of the high-frequency portion. Each of the two correction coefficients are functionally dependent on both these quantities. Carter et al. [22] found that by biasing the detector with a constant voltage, as opposed to a constant current as is typical, nonlinear effects could be lessened. Similarly, Carangelo [23] customized a preamplifier that could be adjusted to minimize the low frequency nonlinear behaviour. Finally, Abrams et al. [17] proposed a solution based on the physical principles of the MCT detector. They identified correction coefficients using a functional relationship between the detector and the input photon flux.

While the effects of nonlinearity in MCT detectors have been extensively studied, the same cannot be said about bolometer detectors, despite the fact that these effects are expected to be as, if not more, significant. Since the Fourier transform is a linear transform, it is essential that the measured bolometer signal be linear in its response to incident radiation while retaining sufficient sensitivity and stability. If it is not linear, the application of the Fourier relations discussed in Chapter 2 will lead to erroneous results because they rely on the principle of linearity. In the rest of this chapter I will discuss the theory behind the nonlinear response of bolometer detectors.



Figure 3.1: Examples of two FTS spectra exhibiting first- through third-order nonlinearity: a TES detector intentionally driven nonlinear and a theoretical bolometer model

3.2 Modeling of Nonlinear Behaviour

The SCUBA-2 camera project [24], currently being commissioned at the James Clerk Maxwell Telescope, contains superconducting Transition Edge Sensor (TES) bolometer arrays. A TES is an intrinsically linear device when operated at the center of the transition, but is susceptible to nonlinearities when used closer to the normal state of the metal film [25]. These effects manifest themselves in the spectrum as shown in Figure 3.1, where the green data represent nonlinearity as seen in the SCUBA-2 TES array intentionally forced nonlinear, and the red is a theoretical model of the effect. As a consequence of the over-exposure of the detector, first through third-order spectral features are observed, which alternate in sign. Two spectral features are contributed by each of the quadratic and cubic terms, with the quadratic term impacting the 0 and 23.2 cm⁻¹ regions, and the cubic term the centre of the fundamental band and the area around 34.8 cm^{-1} . The widths of the harmonics are as stated in §3.1 and are described mathematically by Equation 3.3. The model and measured spectra are seen to be in good agreement.



Figure 3.2: Diagram of a SPIRE bolometer (left) with associated electrical circuit (right). The bolometer voltage changes as a function of temperature, which in turn changes with the incident optical loadings, *Q. Inset Photos: SPIRE Consortium*

A bolometer is essentially a very sensitive thermometer, which consists of an absorbing substrate with a temperature-sensitive detecting element (shown schematically in Figure 3.2). The SPIRE (Figure 3.2) instrument on the Herschel space observatory is made from a silicon-nitride spider web substrate, onto which is glued a neutron-transmutation doped (NTD) detector. Submillimetre radiation is absorbed by the substrate which produces a change in the temperature of the bolometer and thus in its electrical resistance. This change in resistance produces a change in voltage (Figure 3.2), which, if the detector is operating in the linear regime, is proportional to the amount of incident radiation.

The theory that follows derives from papers by Griffin and Holland [26] and Sudi-

wala et al. [27]. In practice, a bolometer of temperature T is thermally coupled to a heat sink, or bath, at temperature T_0 , through a thermal link of length L and static thermal conductance G_s . A bias voltage V_b is applied across the circuit, which contains the bolometer in series with a load resistor R_L (as shown in Figure 3.2). The total power dissipated in the bolometer is

$$W = P + Q \quad [W] \tag{3.4}$$

where P = IV is the electrical power dissipated in the device, and Q is the absorbed radiant power.

The temperature-dependent detector resistance may be expressed as

$$R = R^* \exp\left(T_g/T\right)^n \quad [\Omega],\tag{3.5}$$

where R^* is a constant specific to the bolometer, T_g , is the band-gap temperature and n is a material-dependent constant.

The temperature coefficient of resistance, α , can be determined by differentiating Equation 3.5

$$\alpha = \frac{1}{R} \cdot \frac{dR}{dT} = -\frac{nT_g^n}{T^{n+1}} \quad [\mathrm{K}^{-1}].$$
(3.6)

Two other important parameters: the static thermal conductance, G_s , and the bolometer heat capacity, C, both carry a temperature dependence [27], with

$$G_s(T, T_0) = \frac{G_{s0}}{(\beta + 1)T_0^{\beta}} \frac{(T^{\beta + 1} - T_0^{\beta + 1})}{(T - T_0)} \quad [W/K]$$
(3.7)

and

$$C(T) = C_0 \left(\frac{T}{T_0}\right)^{\rho} \quad [J/K]$$
(3.8)

where G_{s0} and C_0 are the static conductance and heat capacity, respectively, for a temperature T_0 , and β and ρ (the heat capacity index) are both material-dependent constants. With these relations, the energy balance becomes

$$W = P + Q = G_s(T, T_0)(T - T_0) \quad [W].$$
(3.9)

Additionally, the dynamic thermal conductance, G_d , is given by

$$G_d = \frac{dW}{dT} = \left(\frac{A}{L}\right) k_0 \left(\frac{T}{T_0}\right)^{\beta} \quad [W/K]$$
(3.10)

where $G_{d0} = G_d(T_0) = (A/L)k_0$, A is the cross-sectional area of the thermal link, and k_0 is the thermal conductivity of the link at $T = T_0$. It should be noted that $G_{s0} = G_{d0}$ at the bath temperature T_0 . Meanwhile, the effective thermal conductance, G_e , includes electrothermal feedback effects [27]

$$G_e = G_d - \alpha P \left[\frac{R_L - R}{R_L + R} \right] \quad [W/K].$$
(3.11)

From this, one can derive the dynamic impedance, Z, which is a useful term in analyzing bolometer load curves

$$Z = \frac{dV}{dI} = R \left[\frac{G_d + \alpha P}{G_d - \alpha P} \right] \quad [\Omega].$$
(3.12)

The voltage-current characteristic, also known as the load curve, is the method by which



Figure 3.3: An example of the model fits (solid line), based upon the Equations presented in §3.2 to experimental data (dots) obtained for a single bolometer detector operating at five different temperatures [28].

several operating parameters of the device are deduced [28]. Load curves are synthesized experimentally by measuring the voltage across the bolometer for a range of bias currents and stage temperatures. Immediately from this, the resistance may be evaluated as a function of the temperature according to Equation 3.5, leading to determination of the material-dependent parameters R^* , T_g , and n from appropriate fits. At this point, models are fit to the load curve in order to calculate the remainder of the suite of detector parameters [27], as shown in Figure 3.2 for a bolometer exposed to zero external power loading.

The equations developed in this section form the basis for investigating nonlinear behaviour in bolometer detectors under the modulated signal produced by a FTS.

3.3 Correction of Nonlinearities

The goal of any detector used with a FTS is to determine the amount of optical power incident as a function of the optical path difference. In the case of a bolometer, the temperature of the device is the key variable as it constrains all other quantities of interest. In order to determine the operating temperature of a bolometer, thermal equilibrium is assumed - that is, the power entering the detector in the form of optical loading and electrical heating must match the power exiting the detector through the thermal link, towards the heat sink. The electrical power P is given by Ohm's law

$$P = IV_D = \frac{V_b}{(R_L + R_D)} \frac{R_D V_b}{(R_L + R_D)} \quad [W]$$
(3.13)

where

$$I = V_b / R \quad [A] \tag{3.14}$$

is the bias current through the circuit provided by a bias voltage V_b and $R = (R_L + R_D)$, where R_L and R_D are the load and detector resistances respectively.

The total power measured at the bolometer, P_{in} , is

$$P_{in} = P + Q \quad [W]. \tag{3.15}$$

The power leaving the detector depends solely on the thermal conductivity of the link to the bath and is given by

$$P_{out} = G_s (T - T_0) (3.16)$$

where G_s is defined as in Equation 3.7.

During the pre-flight test campaign, each of the two ports of the SPIRE Mach-Zehnder interferometer were exposed to calibration sources of different temperatures: two blackbodies, one held constant at 4.6 K and another whose temperature varied between 6.7 and 9 K. The effects of nonlinearity can clearly be seen in Figure 3.4, with larger amplitude distortions corresponding to larger luminosities from the second port. The central plot in this figure shows the effects of nonlinearity obtained with the SPIRE instrument over 0 to 60 cm^{-1} . The left part of the figure shows the effects of nonlinearity from 0 to 14 cm⁻¹ while the right part of the figure shows the second harmonic of twice the width and half the amplitude. These two features lie at the expected positions of 0 cm⁻¹ and $2\sigma_0$, twice the wavenumber of the centre of the fundamental band. Since the nonlinear response prevents the signal from reaching its true value, the spectral manifestations must be negative. In addition, as the signal of the spectrum in-band increases, the nonlinear signal in the spectral harmonic features also increases. In this particular example, the incident powers were not large enough to produce a third-order harmonic feature. Table 3.1 lists the associated detector parameters for the central pixel in the long wavelength band, SLWC3 (N. Lu (personal communication, March 17, 2009)).

Currently, the Herschel nonlinearity correction algorithm, based upon the bolometer model developed in Section 3.2, accounts for the nonlinear response between the input

Table 3.1: Detector values used towards the correction of nonlinearities in central detector SLWC3



Figure 3.4: Nonlinear behaviour as exhibited by the SPIRE FTS during PFM4 ground testing. Data were taken from the central pixel of the detector array in the long wavelength band, as one input port viewed a blackbody source at 4.6 K and the other whose temperature varied between 6.7 and 9 K. Figures (a) and (c) are extreme close-ups of the boxed harmonics in Figure (b), at 0 cm⁻¹ and $2\sigma_0$, respectively.

optical load, Q, and the voltage across the detector, V_D , with three parameters provided in calibration files for two different source brightness ranges. The conversion from the measured nonlinear signal, V_{nonlin} , to the corrected signal, V_{lin} , is expressed as

$$\frac{dV_{lin}}{dV_{nonlin}} = K_1 + \frac{K_2}{V_{nonlin} - K_3} \tag{3.17}$$

where the nonlinear coefficients are represented as K_1 , K_2 and K_3 and upon integration

$$V_{lin} = K_1(V - V_0) + K_2 \ln\left[\frac{V - K_3}{V_0 - K_3}\right].$$
(3.18)

Here, the integration constant V_0 represents the voltage at the detector when subject to



Figure 3.5: Inverse, normalized responsivity curve as generated from the bolometer model (black), with both the fit to the data (red) and the JPL curve (green) also shown. The K_{1-3} terms are derived from the fitted data. The residual differences with the model are shown for both the fit (red) and the JPL data (green), magnified by a factor of 10.

no radiant loading. The coefficients K_1 , K_2 , and K_3 are determined by fitting Equation 3.17 to the model-derived inverse responsivity over a range of optical loadings chosen to be much larger than expected during flight measurements. An example of such a fit is shown in Figure 3.5, where the inverse responsivity dQ/dV is plotted for a range of detector voltages resulting from optical loads between 0 and 20 pW. The green curve, which shows the inverse responsivity produced from the K_i values found in the calibration tables of the Jet Propulsion Laboratory (JPL), agrees well with both the modeled data in black, and the fit to the modeled data, in red.

3.3. CORRECTION OF NONLINEARITIES

The K_i parameters obtained from the fit in Figure 3.5 were used in Equation 3.18 to implement a nonlinear correction of the data shown in Figure 3.4. The results of this process are shown in Figure 3.6. It can be clearly seen that the non-physical harmonic spectral features have been significantly reduced and missing energy has been restored to the spectrum. Although the out-of-band harmonics represent only a small fraction of the total in-band power, upon correction, because this effect is nonlinear, a disproportionate change occurs in the integrated in-band power. Figure 3.7 shows this effect, which shows the recovered spectral power as a function of the known input power, determined by integrating the powers received by the SPIRE detectors as a function of the temperature of the blackbody shown in the middle panel of Figure 3.4. Not only is there a significant energy enhancement post-correction, but also a return to linearity, as shown by the best fit line of near unity slope. Each blue square corresponds to a spectrum of different temperature



Figure 3.6: Spectra for each of the cases from Figure 3.4 after having now been corrected for nonlinearity using Equation 3.18



Figure 3.7: Recovered spectral powers before (red diamonds) and after (blue squares) nonlinear correction for each temperature spectrum shown in Figures 3.4 and 3.6. A line of best fit is also shown.

(Figure 3.6). The red diamonds represent the equivalent pre-correction values. Although this method of correction using SPIRE calibration tables of derived K_i coefficients remains in use in the Herschel software pipeline, a more precise method is presented in §3.3.1, which relies on determining the operating temperature of the detector at each optical path difference position. In order to correct for variations in the bath temperature, the current pipeline applies a second correction after the nonlinear correction described above, which accounts for changes in bath temperature. In order to do this, a spline is fit to smooth the bath thermistor timeline, whereafter correction coefficients aT, bT and v_0T are applied as

$$CT(t) = aT \cdot \text{SplineInterp}(t) - v_0T + 0.5 \cdot bT \cdot \text{SplineInterp}(t) - v_0T^2$$
(3.19)

for each time-sampled voltage point. The final corrected timeline is computed from the input detector timeline D(t) as

$$S(t) = D(t) - CT(t).$$
 (3.20)

However, since the value T_0 is found throughout the bolometer model leading to the K_i coefficients, this step would do better if incorporated into the nonlinear correction algorithm.

3.3.1 Temperature-Based Nonlinear Correction Approach

As previously mentioned, the primary goal of a bolometer is to measure the amount of optical power striking its sensitive detecting element from the observed astronomical source. The directly measurable quantity however is the voltage across said detector. By inverse application of many of the same formulae outlined in §3.2, it is possible to compute directly the optical power loading as a function of optical path difference from the detector voltage. With knowledge of the load resistance R_L and the bias voltage V_b , the detector resistance is given by

$$R(x) = \frac{V(x)R_L}{V_b - V(x)} \quad [\Omega], \tag{3.21}$$

which can be converted to temperature using Equation 3.5 as follows

$$T(x) = \frac{T_g}{\left[\ln\left(\frac{R(x)}{R^*}\right)\right]^{1/n}} \quad [K],$$
(3.22)

where all constants are defined as before.

In addition to the optical power one must also take account of the dissipated electrical power, expressed as

$$P(x) = V(x)I(x) \quad [W] \tag{3.23}$$

where the current, I(x), is related to the resistance R(x) via

$$I(x) = \frac{V(x)}{R(x)}$$
 [A]. (3.24)

Finally, from Equation 3.9, one arrives at the incident optical power Q(x) as the difference of the total power W(x) and the electrical power P(x)

$$Q(x) = W(x) - P(x)$$
 [W] (3.25)

where the total power W(x) was stated in Equation 3.9 as

$$W(x) = G_s(T(x), T_0)(T(x) - T_0) \quad [W].$$
(3.26)

In this way, the nonlinear correction is achieved directly and without use of any error-

introducing, curve fitting steps. Results are arrived at quickly, and more importantly, can be summoned for each and every point of the interferogram. Temperature is the key variable which permits the determination of many desired detector parameters, and with previous knowledge of the bath temperature T_0 for all sampled points, nonlinear correction can be performed to a much higher degree of accuracy. The determination of the operating temperature of the detector is the principal method by which nonlinear correction will soon be implemented in Herschel/SPIRE data.

3.4 Conclusion

This chapter discussed the phenomenon of nonlinearity in bolometric detectors, considering its mathematical description as a means of modeling its spectral manifestations, through to methods for its correction in pre- and post-launch SPIRE data. The importance of such corrections was shown, as they affect the in-band spectral energy. The fact that the nonlinear correction routine is executed first in the Herschel/SPIRE software processing pipeline gives yet another indication of its central role, as modifications made here propagate through the remainder of the pipeline.

Chapter 4

Spectral Line Fitting

This chapter will consider the retrieval of physical parameters from astronomical spectra recorded by a Fourier transform spectrometer (FTS). The analysis involves fitting two components to the measured spectrum: a continuum component resulting from the emission of interstellar grains and a line component representing either emission or absorption from molecules, atoms or ions. Section 4.1 will present the methods and theory behind the separation of these two components, along with an introduction to the information provided by such analysis. Section 4.3 introduces the sinc line shape and its impact on a FTS spectrum and discusses how, with a knowledge of the line profile, it can be deconvolved from galactic spectra to yield a set of spectral parameters. All of this is considered in the context of data from the molecular cloud core G34.3 in §4.3.2.

4.1 Interstellar Medium

The region between stars located in the spiral arms of our Milky Way Galaxy is collectively known as the interstellar medium (ISM). There are two principal components: interstellar dust (grains) and gas, each of which may be probed by spectroscopy. The emission signature of dust is broad - continuous across a large range of frequencies, while gaseous regions either emit or absorb in discrete, narrow frequency segments manifested as spectral lines and determined from the quantized nature of the allowed atomic, ionic and molecular energy levels. The electromagnetic spectrum will convey information about both and it is one of the goals of this chapter to separate the two.

The continuum component provides information on the nature of the solid particulates including their physical properties, while line emission gives an insight to the ionic, atomic and molecular column abundances and other physical conditions. Lines observed in emission are most common, resulting from collisional excitation between atoms, molecules or ions, which is followed by a radiative decay to a lower energy state. Particularly dense gaseous regions contain a complex collection of molecules, each with their own set of emission lines, making the task of distinguishing individual spectral lines challenging. Similarly, when cold gas appears in the foreground of a hotter continuum source, then absorption lines, characteristic of the gas, are observed. The Astronomical Instrumentation Group (AIG) at the University of Lethbridge (UL) is interested in the conditions necessary for star formation in the ISM, known to take place at colder temperatures. In particular, molecular clouds in the ISM, conglomerations of molecular gas and dust, are known to be birth sites of new stars. From such clouds, emission due to cold dust and molecular transitions dominate the observed spectra, and both are needed to derive a thorough understanding of the physical conditions of the region. The following sections investigate facets of each in turn, beginning with a series of experimental claims that prove the existence of interstellar dust.

4.1.1 Interstellar Grains

Interstellar dust has a spectral energy distribution, S_{ν} , given by

$$S_{\nu} = (N_g M_g) \kappa_0 \left(\frac{\nu}{\nu_0}\right)^{\beta} B_{\nu}(T_d) \Omega \quad \text{[Jansky]}$$
(4.1)

where 1 Jansky = 10^{-26} Wm⁻²Hz⁻¹, κ_0 (m²/kg) is the dust emissivity at a reference frequency ν_0 (Hz), β is the dust emissivity index, Ω the solid angle, N_g the dust column density (m⁻²), M_g the mass of the dust grains (kg) and $B_{\nu}(T_d)$ (Wm⁻²str⁻¹Hz⁻¹) the Planck blackbody function for a dust temperature T_d (K) and a frequency ν (Hz) [29]. Most often, β ranges between 1 and 2, with a value of 2 significant for long wavelengths and metallic materials, whilst a value of 1 describes graphitic grains [30]. These two values constrain a range of estimates in the literature that depend upon grain type.

The most fundamental indication that grains comprise a large portion of the ISM is the signal degradation that occurs due to foreground absorbers as

$$I = I_0 \exp\left(\int_0^l \alpha \, dl\right) \tag{4.2}$$

where α is the extinction coefficient, I_0 the stellar intensity and l the path length of travel. It has been determined [31] that the coefficient α , rather than being constant, in fact varies with the density of the gas. Extinction can also be measured by direct comparison of two different stars of similar size and composition; one with little intervening material and one behind a cloud. To this end, intensity discrepancies are accounted for with the concept of brightness magnitudes [31] such that a factor of 100 change in intensity equates to a five-fold change in magnitude.

There are further indications that dust must comprise a substantial portion of the interstellar medium (ISM). Astronomers frequently use the solar elemental abundance as a reference for conditions elsewhere in space. For example, solar elemental abundances, while consistent with some other areas of the ISM, are not reflective of conditions in a molecular cloud. Certain of these elements are capable of, with increased distance from a stellar source, cooling enough to form refractory solids (grains), which are thus crystallized out of the gas phase. They may do this on their own, as in the case of iron, or in combination with other elements (i.e. silicates). What results is a noticeable reduction in certain elemental abundances to values that are incomparable to anything seen within our Sun [31].

Astronomers have also been pointed to the existence of interstellar grains by the optical polarization of starlight, found to be correlated with the amount of optical extinction. Should grains be taken as elongated, rather than spherical, there is a greater chance of an electric field vector passing unhindered perpendicular to the grains' long axes. This is especially true if there is some commonality in orientation, as provided by, for example, an external magnetic field [31].

4.2 Continuum Fitting

There are various ways of fitting a continuum spectral baseline, most of which seek to optimize a fit for two parameters: the dust temperature T_d , and the dust emissivity, ϵ . For example, the Planck function, as expressed in terms of frequency, ν ,

$$B_{\nu}(T_d) = \epsilon \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT_d} - 1} \quad [W \text{ m}^{-2} \text{sr}^{-1} \text{Hz}^{-1}]$$
(4.3)

is very often used as a fitting function, where h, c and k are Planck's constant, the speed of light in a vacuum and Boltzmann's constant, respectively, and ϵ and T_d are floating parameters.

In a theoretical model of dust emission, as described by a modified blackbody spectrum such as that in Equation 4.1, many of the variables are specific to the grain type being observed, and therefore largely unknown. As a result, authors have made simplifying assumptions leading to models that often bear resemblance to both Equation 4.1 and the Planck function. Priddey et al. [32], assuming grains in thermal equilibrium with the background radiation, and an optically thin molecular cloud, performed a χ^2 -minimization procedure with a function

$$S_{\nu Priddey} \alpha \frac{\nu^{3+\beta}}{e^{\frac{h\nu}{kT_d}} - 1} \quad [\mathrm{W} \ \mathrm{m}^{-2} \mathrm{sr}^{-1} \mathrm{Hz}^{-1}]$$
(4.4)

for free parameters β , the dust emissivity index (see Equation 4.1) and T_d . This method finds the best *isothermal* description of the dust, although it is more likely in practice that a range of temperatures prevails. Others, such as Colbert et al. [33] have directly incorporated the Planck blackbody equation, $B_{\nu}(T)$. They arrived at

$$S_{\nu Colbert} \alpha B_{\nu}(T_d)(1 - e^{-\tau_{Dust}}) \quad [W \text{ m}^{-2} \text{sr}^{-1} \text{Hz}^{-1}]$$
 (4.5)

having assumed $\tau_{Dust} \alpha \nu$. Again, such an optimization will only result in one temperature, although there remains a large amount of flexibility in the parameter τ_{Dust} , which can also be approximated as $\tau_{Dust} \alpha \nu^{1.5}$ or $\tau_{Dust} \alpha \nu^2$. It is more common to multiply each of Equations 4.3, 4.4 and 4.5 by Ω , the solid angle of the source, and so express the result in the astronomical unit of flux, the Janskies $(10^{-26} \text{ W m}^{-2} \text{ Hz}^{-1})$ [34].

4.2.1 Line Fitting

Fitting to spectral lines requires knowledge of the instrumental line shape (ILS), to be discussed in §4.3, and is designed to return a spectral line intensity, line position (centre) and full width at half maximum (FWHM). From this information, such parameters as the atomic and molecular column abundances, and their rotation temperatures can be gathered. By isolation of the line position (in units of frequency (Hz), wavelength (μ m), or wavenumber (cm⁻¹)), one can identify the atomic or molecular species through comparison with their equivalent values at rest. With sufficient spectral resolution, and a knowledge of the rest-frame wavelength, it is possible to determine the source's relative velocity, through the Doppler effect. The strength (intensity) of the source will be determined from the column abundance, the Einstein A coefficient, the temperature and the energy level of the transition, while the FWHM is related to the source environment, in particular its temperature and pressure. How the column abundance and temperature can be determined is explained in Chapter 6 where the rotation diagram method is applied to data obtained from Herschel/SPIRE. The following section utilizes line fitting techniques on a simulated FTS-2 source spectrum created from high-resolution heterodyne data from the JCMT.

4.3 FTS-2 Simulation

The Astronomical Instrumentation Group at the University of Lethbridge has been involved in the development of an imaging FTS (IFTS, FTS-2 [35]) for use in combination with the next-generation bolometer detector array (SCUBA-2), situated at the James Clerk Maxwell Telescope [36]. In order to predict the spectra that will be recorded by FTS-2, highresolution heterodyne data from the recently commissioned HARP imaging spectrometer [37], which also operates at the JCMT, have been used.

Heterodyne spectrometers are known for their extremely high resolving power. As an example, HARP [37] achieves a resolution of 1 MHz at a frequency of 325-375 GHz, for a resolving power of 325 000 - 375 000. While heterodyne spectrometers have extremely high resolving power they only operate over narrow bandwidths and therefore have difficulty establishing a reliable continuum. Thus, unlike a FTS, HARP is not well suited to the measurement of dust emission. Since HARP is operating in the same wavelength region, at the same telescope, through the same atmosphere that FTS-2 will be, it actually provides the most realistic spectral line measurement on which to model the performance of FTS-2.

In the following simulation, a complete spectral scan of the galactic source G34.3 by HARP forms the data for producing the realistic simulation of FTS-2. The data were made available by the JCMT's Spectral Legacy Survey (SLS) [38] team. The source is a





Figure 4.1: IRAS 60 $\mu \rm m$ intensity map of G34. Colorbar units are in MJy beam^{-1}

well-studied, ultracompact HII region with a hot molecular cloud core [39] (Figure 4.1). It can be divided into three separate sub-regions, two of which are ultracompact and one compact. Additionally, G34.3 has a cometary morphology and is found at a distance of 3.7 kpc.

4.3.1 The ILS of a FTS

In the ideal case, the Fourier transform spectrometer (FTS) has a well-defined line-shape (see Chapter 2) [10] given by the cardinal sine (sinc) function

$$F(\sigma) = 2L \frac{\sin\left(2\pi\sigma L\right)}{2\pi\sigma L} \tag{4.6}$$
where σ is the wavenumber (cm⁻¹) and L is the maximum optical path difference (OPD) between the two interfering beams in the interferometer. The sinc function has a FWHM of

$$\Delta \sigma_{FTS-FWHM} \simeq \frac{1.207}{2L} \quad [\rm cm^{-1}]. \tag{4.7}$$

First light has recently been captured with FTS-2 in the laboratory at the University of Lethbridge, prior to its shipment to the JCMT in Hawaii. The measured line shape of the instrument matches an ideal sinc function well, as shown in Figure 4.2. The absence of any sizeable ghosts in the power spectra shown, recorded in the time domain, suggest a remarkable stability in the moving mirror velocity.

In this simulation, a $\Delta\sigma$ of 0.01 cm⁻¹ was chosen so as to match the expected performance of FTS-2, and was achieved by convolving a sinc function of the appropriate width with the raw HARP data. Figure 4.3 illustrates measured HARP data (top) of source G34.3, with the eleven strongest emission lines identified by the blue vertical lines. The middle trace shows the result of convolving the upper data with a sinc function sampled at the same spectral resolution of 1 MHz. The sinc line shape features are clearly evident at each of the eleven lines of interest, and could easily be interpreted as adding noise to the data. These features are, however, a result of the sidelobes of the convolution kernel summing constructively and destructively at the different frequencies depending on the line content of the original spectrum. Finally, the bottom trace in Figure 4.3 sub-samples the centre plot to the resolution of 0.01 cm⁻¹, and therefore represents the most realistic simulation of FTS-2 measurements of G34.3.



Figure 4.2: The measured ILS of FTS-2 (black), without phase correction, plotted overtop a sinc function (orange) of the theoretical resolution of the FTS. The interferogram was sampled at regular time intervals.

4.3.2 Line Fitting

In order to fit to experimental data, some form of minimization routine is necessary. Several are available, of which the most common are the IDL routines Amoeba[®], based upon the downhill simplex method developed by Nelder and Mead [40], Powell[®], which makes use of the powell routine described in *Numerical Recipes in C: The Art of Scientific Computing* [41] and mpfitfun[®], which employs a Levenberg-Marquardt [42] nonlinear leastsquares algorithm. The latter option was chosen for the fitting presented here, as it allows the greatest control over the optimized parameters: line centre, width and amplitude. While



Figure 4.3: Raw HARP G34.3 spectrum (top) with each of the eleven strongest emission lines denoted by the blue lines. The middle trace shows the raw data convolved with the sinc ILS of the FTS to a fine spectral resolution of 1 MHz. The bottom plot further sub-samples the spectrum to a new resolution of 0.01 cm^{-1} , expected for FTS-2.

each of the other choices may settle in to a *local* minimum, mpfitfun[®] can constrain each of the three floating values so as to only find the absolute minimum.

The first step was to make an estimate of the noise threshold in the spectrum, arbitrarily set at three times the standard deviation. Should any sampled points lie above this threshold, then they are identified as emission lines and stored for fitting. After the initial fit, a residual difference between initial spectrum and fitted spectrum is calculated, which is then treated as a new spectrum and the process repeats. This continues until the reduced chi-squared differs by less than a user-supplied threshold on successive iterations $(10^{-10} \text{ in this case})$. All lines detected above the noise threshold are simultaneously fitted to yield values for the position and intensity of each line. A FWHM is required in the fitting process but in general is fixed based upon the resolution of the FTS. Since the heterodyne data have been baseline corrected, there is no requirement to fit an underlying continuum, although this is relatively straightforward to include. A summary of the fit is shown in Figure 4.4, separated by line, where the overlapping sidelobes of neighbouring lines contribute to the perceived noisiness of the final, convolved spectrum. The eleven components are synthesized into a single spectrum in the middle trace of Figure 4.5, with the filled circles showing the sampled points at the lower, 0.01 cm^{-1} resolution. The integrated flux (mK $\rm cm^{-1}$), was determined directly from the returned fit parameters according to the theoretical sinc integral

$$\int_{-\infty}^{\infty} A \frac{\sin\left(2\pi(\sigma - \sigma_0)L\right)}{2\pi(\sigma - \sigma_0)L} \, d\sigma = \frac{A}{2L},\tag{4.8}$$

where A is the amplitude of the line, σ_0 is the line centre, and L and σ are defined as in Equation 4.6. The flux, combined with the line centre and amplitude, yield a set of three



Figure 4.4: The convolved spectrum shown at centre in Figure 4.3 with each of the eleven sinc fits, offset for clarity. The blue lines show, as before, the positions of the initial guesses supplied to the line-fitting routine.



Figure 4.5: Cumulative fit to raw heterodyne data. The top curve shows the sub-sampled spectrum, at a resolution of 0.01 cm^{-1} (300 MHz). The middle curve shows the recovered FTS-2 spectrum plotted at high resolution (1 MHz), with the filled circles marking sampled points at the 0.01 cm⁻¹ resolution. At bottom is the residual difference. All spectra are offset for clarity.

spectral parameters that can be compared directly with similar data from the heterodyne spectrum.

Prior to convolution, the spectral line areas were determined from a numerical integration of the heterodyne data over a small wavenumber range. The final results of this analysis are summarized in Table 4.1. Both the line centres and areas show strong

	Ι	Line Centre	(cm^{-1})		Integrated Line A			rea (mK $\rm cm^{-1}$)	
Line	Het.	FTS	Difference	Difference $(\% \text{ of } \Delta \sigma)$	Het.	FTS	Difference	Error (%)	
1	11.02489	11.02390	0.00099	9.9	3.10	3.20	0.10	3.23	
2	11.19061	11.18947	0.00114	11.4	1.15	1.26	0.11	9.57	
3	11.24069	11.23861	0.00208	20.8	1.07	1.22	0.15	14.02	
4	11.28716	11.28781	0.00065	6.5	1.60	1.46	0.14	8.75	
5	11.34269	11.34243	0.00026	2.6	1.73	1.52	0.21	12.14	
6	11.38587	11.38831	0.00244	24.4	0.68	0.70	0.02	2.94	
7	11.43485	11.43656	0.00171	17.1	1.27	1.39	0.12	9.45	
8	11.53191	11.53203	0.00012	1.2	5.04	5.08	0.04	0.79	
9	11.65190	11.65057	0.00133	13.3	1.06	1.03	0.03	2.83	
10	11.73115	11.72896	0.00219	21.9	0.69	0.87	0.18	26.09	
11	11.82237	11.82168	0.00069	6.9	1.92	1.94	0.02	1.04	

Table 4.1: Comparison of line centres and integrated areas from the raw heterodyne spectrum and the simulated FTS spectrum. Associated differences are also shown.

agreement. The positions, measured to an accuracy of $1 \text{ MHz} (3.36 \times 10^{-5} \text{ cm}^{-1})$, typically differ by less than ten percent of a resolution element of the FTS for lines of significant signal-to-noise. All of the secondary maxima/minima of the sinc functions surrounding any given line act to constrain the fit at the centre, leading to the tremendous accuracies noted in Table 4.1. Additionally, the percentage errors in integrated areas (where the heterodyne data were taken as the reference) are inversely proportional to the strength of the line.

This is to be expected as the lines of higher amplitude are easier to fit. For instance, the line at $\sigma_0 = 11.532 \text{ cm}^{-1}$, a $J = 3 \rightarrow 2$ CO transition and by far the most intense of the eleven, produces the smallest error, while the weakest line, a methanol emission signature at $\sigma_0 = 11.731 \text{ cm}^{-1}$, produces the largest error.

As a test of the line fitting procedure, the same analysis was performed upon the introduction of random noise into the spectrum.

4.3.3 Addition of Noise

Normally-distributed white noise with a mean of zero was generated in IDL with the Box-Muller method [43] and added to the 0.01 cm⁻¹ resolution spectrum, shown at the top of Figure 4.5. A noise amplitude of ten percent of the largest peak (the CO $3 \rightarrow 2$ line at 11.53 cm⁻¹) was chosen. Random deviates were merged into the spectrum one hundred times and then averaged, so as to eliminate any spurious data values. Line centre and amplitude were returned by the fitting routine as before, for each of the same eleven lines, allowing comparison with the FTS spectral simulation. Analysis sought to verify the concept already mentioned in §4.3.2, that the fitting improves with the strength of the line. Figure 4.6 examines the line centre error with respect to the heterodyne reference for each of the chosen eleven lines. There is a clear inverse relationship born out by the over-plotted curve, a theoretical reciprocal function derived from a spectral signal to noise argument [10]. The errors were calculated as the absolute value of the difference between the retrieved line parameters for the FTS-modeled data with and without noise added. The same trend was observed for the errors in line areas, as shown in Figure 4.7. Having verified the decrease in precision of the line fitting method with decreased line area, all that remains is to attempt



Figure 4.6: Errors in line centres for each of the eleven fitted lines, as a percentage of a resolution element. The errors clearly follow an inverse relationship with integrated spectral line area.

to lessen the error across all integrated areas. The data presented here identified the eleven strongest lines and fitted them each based on a fixed FWHM. While the HARP spectrum was provided without any underlying continuum, as will be seen in Chapter 6, its removal is often a key determinant in the quality of the achieved line fits.

4.4 Conclusion

A detailed knowledge of the instrumental line shape function is key to maximizing the information that can be extracted from a spectrum, for example the column abundances, ionization state and physical conditions of the region under study. A particular advantage



Figure 4.7: Errors in integrated line areas for the eleven fitted lines, expressed as a percentage. The same inverse relationship with integrated heterodyne line area is noted.

of observing at submillimetre wavelengths, is that, except under extreme conditions, sources are optically thin, allowing one to peer into the cores of star-forming regions. Fortunately the line shape for both SPIRE and FTS-2 is well-known. Spectra can provide two types of information: that related to the icy dust often obscuring light sources beyond, and that on the emitting region in particular. A Levenberg-Marquardt least squares optimization technique was introduced, which will find use in Chapter 6 when the method is applied to flight data from the SPIRE spectrometer, complete with a non-zero baseline. The utility of the IDL-fitting script was proven through a comparison of the actual spectral parameters (line centre, amplitude and FWHM) from HARP's G34.3 spectrum to the numbers recovered from the FTS simulation, both with and without noise. It therefore exists now as a robust, stand-alone routine.

Chapter 5

Preparing for Observations with FTS-2

This chapter will summarize the observation planning relevant to FTS-2, a second generation Fourier transform spectrometer being built at the University of Lethbridge for use with the Submillimetre Common User Bolometer Array (SCUBA-2) at the James Clerk Maxwell Telescope (JCMT) atop Mauna Kea, Hawaii, USA. FTS-2 is the first of two Fourier transform spectrometers that will be discussed in the thesis, the other associated with SPIRE on the Herschel Space Observatory (see Chapter 6).

5.1 SCUBA-2

SCUBA-2 is a staggering upgrade of the highly successful SCUBA camera, which was operational at the JCMT from July 1996 until 2005 [36]. An international team with partners from Canada, the United States and Europe undertook the development of the new generation camera, which is currently approaching scientific readiness. The consortium agreed to develop two instruments to increase the capabilities of the camera: one, a polarimeter to allow polarization mapping, has been realized as POL-2 [44]; the other, a FTS, has been built by the AIG to provide imaging spectroscopic functionality.

The JCMT is a 15-m diameter telescope situated atop Mauna Kea in Hawaii, a site known for its extremely dry conditions, ideal for astronomy. Where SCUBA had 128 detectors subdivided between two wavelength arrays accessible with a dual input filter wheel, SCUBA-2 has ~10,000 detectors, resulting in mapping speeds potentially a thousand times faster to reach the same signal-to-noise [45]. By coupling the SCUBA-2 camera with a Fourier transform spectrometer (FTS), the following investigations can be conducted

- the interstellar medium FTS-2 will uniquely image the dust continuum and line emission simultaneously.
- infrared galaxies the spectral energy distribution (SED) of dust.
- planetary atmospheres provide insight into their dynamical evolution, driven by the interaction of molecular species.
- supernovae remnants including how they interact with the interstellar medium.

within each of two relatively narrow wavebands, centred at 450 and 850 μ m. Spectroscopy will occur in these windows concurrently, which will address a number of scientific goals at the forefront of submillimetre astronomy.

5.1.1 FTS-2 versus Herschel/SPIRE

The parallel observing goals of Herschel and the JCMT are to observe the cold submillimetre universe where stars are formed. Spectroscopic imaging conditions are drastically different on the ground versus in space. Table 5.1 compares a series of aspects involved in observing with each telescope. While affected by emission from the surrounding optics, Herschel, free from the Earth's atmosphere, is most sensitive to radiation from the sources towards which it points. Nevertheless, Herschel must employ older, space-proven technology, which includes a primary mirror of diameter 3.5 m, of which only the central \sim 3.29 m is used to avoid diffraction effects. At this size, the telescope is limited by the maximum resolution that can be attained. On the other hand, the complementary aims of the JCMT are benefited by a telescope of diameter 15 m (\sim 20 times greater collecting area), with a spectrometer, in FTS-2, of ten times the spectral resolving power. At the same time, the spectrometer on-board Herschel, SPIRE, has 56 pixels split between two wavelength arrays, with unfettered access to the wavelength range shown in Table 5.1. On the other hand, FTS-2 enjoys \sim 10,000 exquisitely sensitive TES (see §5.1.2) detectors which can only observe in the two atmospheric windows shown in Table 5.1.

The AIG at the University of Lethbridge is privileged to be involved in both projects, and thus both are described in this thesis.

5.1.2 Transition Edge Sensors

The theory behind bolometric detectors was presented in Chapter 3. The transitionedge sensor (TES) is a type of bolometer that measures input radiant flux according to the

	FTS-2	SPIRE FTS
dominant noise source	atmosphere	telescope
collecting area (diameter)	15 m	3.29 m
angular resolution	7" & 14"	19-35"
spectral resolution	$0.006 \ {\rm cm^{-1}}$	$0.04 \ {\rm cm}^{-1}$
spectral range	$11-12.5 \& 21-24 \text{ cm}^{-1}$	$14.9-51.5 \text{ cm}^{-1}$
number of pixels	10,000	56

Table 5.1: Comparison of Herschel/SPIRE and JCMT/FTS-2

change in resistance of a superconducting film [25]. As mentioned, SCUBA-2 has ~10,000 TES detectors equally split between two wavelength arrays. The sensitive detectors are designed for conditions of high background loading, which are slightly worse than might be expected on a typical observing day at Mauna Kea. A TES is voltage-biased to operate at select temperatures between the normal and superconducting states, a narrow region where the electrical resistance lies between zero and its normal value. The TES sensors must be designed in anticipation of the worst conditions they could observe. The remarkable sensitivity of a TES is due to the width of this transition, such that a temperature change of ~0.02 mK can alter the resistance by ~20 m Ω [25] (see Figure 5.1). The temperature coefficient of resistance, α , that determines the slope of this transition is given by

$$\alpha = \frac{1}{R} \frac{dR}{dT} \quad [\mathrm{K}^{-1}] \tag{5.1}$$

where R is the resistance. This sensitivity can be up to two orders of magnitude better than a semiconductor thermometer [25]. One of the recent advances that has given the TES more widespread appeal is the development of superconducting quantum interference device (SQUID) current amplifiers, which can multiplex the readout of a large array of



Figure 5.1: An example of a superconducting transition [25].

detectors [46]. This greatly reduces the number of wires needed for this purpose.

5.1.3 FTS-2

The choice of spectrometer to use in conjunction with the SCUBA-2 camera was narrowed to three types: a grating spectrometer, a Fabry-Perot interferometer, and a FTS. The decision to employ a FTS over these other types was based upon extensive research and a careful critique of how each would fit into the pre-existing SCUBA-2 design limitations [45].

Both grating spectrometers and Fabry-Perot interferometers (FP) suffer from a low throughput and poor instrumental line shape function. Additionally, they are not well suited to the bolometric detectors, which are optimally operated at large radiant exposures at both 450 and 850 μ m. Although other types of spectrometers were considered to provide an imaging spectroscopic capability with SCUBA-2, it was quickly realized that a FTS was the optimal solution. As noted in Chapter 2, Fourier transform spectrometers are known for their high throughput, extending over a wide spectral range that allows simultaneous observing in both SCUBA-2 bands. Moreover, the FTS is well matched to the radiant loading design of the SCUBA-2 detectors, as it introduces no extra radiant loading. Finally, as shown in Chapter 4, the FTS has the best instrumental line shape of any spectrometer, and in the case of a well designed system has been shown to be the classical sinc. Therefore the FTS was chosen to provide SCUBA-2 with imaging spectroscopic capabilities.

Built by the AIG at the University of Lethbridge, FTS-2 is of the Mach-Zehnder design [47], and identical to the SPIRE FTS. As shown in Figure 5.2, the MZ-FTS differs from the Michelson interferometer introduced in Chapter 2 in a number of ways. Firstly, the design separates the two input ports (A and B) and two output ports (1 and 2), each of



Figure 5.2: Schematic illustration of Mach-Zehnder Fourier transform spectrometer.

which are accessible to the user. Different from the Michelson design, all radiation (excluding that absorbed by imperfections in any of the mirrors or the two beamsplitters) that passes through the spectrometer is measured. One input is reserved for the astronomical target of interest plus the background sky, while the other is exposed solely to the background sky, which is then removed from the observation in real-time.

5.2 Atmospheric Cancellation

The two input ports of FTS-2 are at a fixed angular separation, such that one port views the astronomical object of interest and the other a nearby region of the background sky [48]. As observing proceeds, the second (background) port rotates around the central pixel of the companion port, as a result of the alt-az telescope mount. Such port rotation simulations have been performed for a number of possible astronomical targets and atmospheres. Figure 5.3 shows possible pixel positions during the time that the Orion molecular cloud (OMC) is visible. As port 2 circles the brightest regions of the source, the source changes elevations according to the sketch on the left of Figure 5.3, such that the start and the end altitudes are identical, and the point of maximum elevation corresponds to the greatest atmospheric transmission and least emission.

As the pixels from each of the two ports make their way around the center, they experience slightly different amounts of flux through the Earth's atmosphere. The dualport nature of FTS-2 is able to isolate the source signal in real-time using measurements of the dark sky from port 2. Proper calculation requires knowledge of the exact rotation characteristics of the ports, as well as a comprehensive model of atmospheric fluxes across



Figure 5.3: Image of the Orion molecular cloud from the SCUBA Legacy Catalogue with possible port positions superimposed. Port 1 remains centred on the target, while Port 2 arcs around, experiencing differing flux amounts. The recorded interferogram is a difference of the signals from the two ports. At left, the two red lines indicate the start and end positions of the rotation.

a range of elevations.

To this end we used BTRAM, the Blue Sky Spectroscopy transmission and radiance atmospheric model [49], at both the 450 and 850 μ m bands, across elevations from zenith to 70°, in steps of 10°. These simulations are shown in Figure 5.4. Conversion to Janskys (Jy) was achieved using beam sizes of ~7 arcsec for the 450 μ m band, and ~14 arcsec for the 850 μ m band, according to

$$Flux = \overline{Radiance} \cdot \frac{1}{3^{10}} \cdot \frac{\pi}{4} \cdot \left(\frac{beamsize}{3600} \cdot \frac{\pi}{180}\right)^2 \cdot 10^{26} \quad [Jy]$$
(5.2)

where $\overline{Radiance}$ is the BTRAM spectral radiance averaged across the bands as defined by the filters [50]. Due to the symmetric design of FTS-2, the resulting difference between the two input ports (Figure 5.5) is always a horizontal gradient across the arrays (Figure 5.6). They are symmetrically located about their center, meaning that there is an imbalance which is always most pronounced at one edge of the field-of-view (FOV) [48]. The amplitude of the residual varies with elevation. It is therefore necessary to model the gradient for a range of elevations and precipitable water vapour amounts in order to remove the residual atmospheric contribution from the spectrum. Nevertheless, the magnitude of the difference is extremely small in comparison to the scales plotted in Figure 5.4. While the emission from the atmosphere is on the order of 10^3 Jy, the corresponding flux difference is seen to near 10^{-2} Jy, which speaks to the quality of atmospheric cancellation being performed.



Figure 5.4: Atmospheric emission for a simulated atmosphere above Mauna Kea at each of the two wavelength bands observed with SCUBA. At left, the BTRAM [49] results for the 450 μ m band for precipitable water vapour (pwv) amounts of 0.5 mm (top) and 1 mm (bottom). Traces represent 10 degree steps in elevation from zenith, with decreasing transmission. The same plots are repeated from the 850 μ m band on the right.

5.3. SCUBA LEGACY CATALOGUE



Figure 5.5: Atmospheric emission viewed from each of the two input ports at 850 μ m and 40° elevation. Port 1, at left, is stationary on the target while port 2, right, rotates around the optical axis of the telescope, indicated by the small 'o'. The fields of view (FOV) of the respective detector arrays are given as the larger, outlining rectangles.

5.3 SCUBA Legacy Catalogue

To assist in the preparation of the observations of SCUBA-2, use has been made of the SCUBA Legacy Catalogue (SLC) [51] as a tool for observation planning. The SLC is a complete collection of 35455 data files, including continuum maps comprising data from 450 and 850 μ m of all astronomical sources observed with SCUBA. In all, it describes the time of measurement, the location observed in the sky and the measured difference between the "on-target" voltage and a specific background position. After removal of Solar System objects, whose positions are time-varying and therefore cannot be traced over the short timescales of SCUBA, as well as a small amount of unrecognized source names, 28534 data files remained [51]. Of these, regions of the sky such as the Galactic Plane and nearby molecular clouds such as Orion and Ophiuchus were particularly well sampled.

All maps and objects located therein found in the SLC are downloadable from the website of the Canadian astronomy data centre (CADC) [52]. In addition to the raw spectral data, there are preview images for individual targets, which permits quick dataquality checks or source identification opportunities. The data are archived as flexible image transport system (fits) files [53], a standard format for astronomical images and data. They



Figure 5.6: Difference in atmospheric emission between the two input ports shown in Figure 5.5 above. The horizontal gradient as shown varies in amplitude with changes in elevation.

are named such that they may be identified by the galactic coordinates of their center pixel. For example, the file "scuba_E_178d6_-19d8_850um.emi.fits" is a SCUBA-processed 850 μ m emission map (emi) from the Extended Dataset (E), with coordinate center (178.6, -19.8) [51]. The following section provides the details as to the difference between the two types of data: extended and fundamental.

5.3.1 Extended and Fundamental Datasets

The catalogue has been further subdivided into two categories of maps. The "Fundamental Map Dataset" contains only data with superior atmospheric opacity calibration, while the "Extended Map Dataset" comprises all data, irrespective of the quality of the opacity calibration [51]. The Fundamental Map Dataset contains the most accurate fluxes while the Extended Map Dataset is useful when seeking an expanded areal coverage. To this end, the 450 μ m wavelength band is excluded by the Extended Map Dataset, because of the low quality of the 450 μ m data under poorer observing conditions. In total, 1423 850 μ m Fundamental maps contain $\sim 7.06 \times 10^6$ pixels spanning 19.6 square degrees. The Extended maps at 850 μ m comprise 10.6×10^6 pixels across 29.3 square degrees, 1.5 times more than the corresponding Fundamental Map Dataset. All data are summarized in the Fundamental Map Object Catalogue (FMOC) and the Extended Map Object Catalogue (EMOC). Along with the SLC are provided two text files, "scuba_fmoc.txt" and "scuba_emoc.txt", each containing an expansive table that functions primarily as a look-up chart relating right ascension (RA) and declination (DEC) coordinates of a particular astronomical object to the galactic coordinates of the center pixel when observed by SCUBA. In this manner, one may separate their fits file of interest from the entire SLC.



Figure 5.7: Emission map of Orion KL with superimposed port positions. Port 1 remains fixed on the target while port 2 rotates around.

For each of the two wavelengths, three maps were created: an emission map with intensity values in Jy beam⁻¹, an error map including standard deviations for each pixel, and a coverage map indicating the number of times a position was observed by SCUBA for each pixel.

5.3.2 Handling FITS Files

Once downloaded using the CADC's JAVA interface, the user then requires a separate application to ingest the fits file. Of the most commonly encountered are NASA's fits viewer [54] and the Smithsonian Astrophysical Observatory's (SAO) SAOImage ds9 [55]. Work in this chapter typically employed fv, for purposes of previewing the source and its brightness, before the data itself were incorporated into IDL[®] using the "mrdfits" function. What follows are a series of examples of emission maps from the SLC, for four well-known sources that will be studied by FTS-2. Figure 5.7 shows the Orion molecular cloud, the closest high-mass star-forming molecular cloud to Earth, along with the superimposed port positions. While the port alignment for this source, as shown, must navigate the varying intensities of the dark filament, other targets have less strenuous constraints. For example,



W 3(OH)

Figure 5.8: Emission map of molecular cloud W3 (OH) with superimposed port positions.

Figure 5.8 shows W3 (OH), another major star-forming cloud in the W 3 complex of Perseus [56], characterized by an OH maser, where the positioning of port 2 is largely free to be set. Meanwhile, Figures 5.9 and 5.10 are both sites of star formation in Sagittarius. M17



Figure 5.9: Emission map of nebulous region M17 with superimposed port positions.

(NGC 6618) (Figure 5.9), the Swan or Horseshoe nebula, is a star-forming emission region nebula, while Sgr B2(M) (Figure 5.10) is the middle region of a dense molecular cloud near the centre of the Milky Way. In each of these two regions, it is crucial to correctly register the port 1 centres so as to capture the brightest parts of the source, while the second port is again, mostly unconstrained. In the case of Sgr B2 however, one would be careful to avoid



Figure 5.10: Emission map of molecular cloud Sgr B2 with superimposed port positions.

the darker spots in the lower left of the Figure. In each plot, the color scales are in units of $Jy \text{ beam}^{-1}$.

5.4 Conclusions

Fourier transform spectrometers have become the spectrometers of choice for both space-based and ground-based telescopes. Their broad spectral coverage, variable resolution and high throughput are well-matched to the demands of submillimetre astronomy. The Mach-Zehnder design of FTS-2 has been presented, whose advantages include access to all four ports: two input and two output. The new species of detectors to be used at these outputs are the Transition Edge Sensors, that if biased accurately at the midpoint of the superconducting transition, provide sensitivities at least two order of magnitude greater than achievable with SCUBA.

FTS-2 was shipped early in July 2010, to be commissioned later this year. As such, it will become ever more instructive to look back at the methods used in the analysis of SCUBA data. The techniques of atmospheric cancellation will be just as relevant as FTS-2 sets out to reproduce the entire SCUBA Legacy Catalogue. The tools presented in this Chapter will be key to planning observations with FTS-2 during the commissioning and performance verification stages.

Chapter 6

SPIRE Data Analysis

The goal of this chapter is to discuss Fourier transform spectroscopy from the SPIRE instrument, on-board the Herschel Space Observatory (Herschel), which faces its own unique challenges quite distinct from those encountered by ground-based instruments such as SCUBA-2/FTS-2 (see Chapter 5). As Herschel/SPIRE has recently entered the routine science operations phase of its lifetime, SPIRE has already produced pre-flight and performance verification (PV) data which will be reviewed in the context of concepts already introduced. These include an application of a comprehensive line-fitting program to measured spectra. This will be followed by analysis of resulting rotation diagrams [57] [58], highly useful tools toward the physical understanding of molecular clouds and other such sources. Finally, the FTS line shape will be briefly revisited in order to validate the line-fitting methods.

6.1 Herschel Space Observatory

The Herschel space observatory is a flagship mission of the European Space Agency (ESA) [59]. The 3.5 metre diameter mirror is the largest such space-borne telescope to date and indeed the largest monolithic instrument capable of surviving launch conditions [59]. Herschel is shown during its final ground-based testing phases in Figure 6.1. The payload comprises three instruments: SPIRE [60], which will be the focus of this chapter, the Photoconductor Array Camera and Spectrometer (PACS) [61], and the Heterodyne Instrument for the Far-Infrared (HIFI) [62]. While each has its own unique objectives, Herschel works best as a collective space facility devoted to the study of far infrared and submillimetre astronomy, a window which can only be accessed from space or high-altitude aircraft and balloons.

The science data produced by Herschel will complement that of other observatories, such as IRAS [2], ISO [4], Spitzer [63] and AKARI [64]. However, the wavelength spectral range, 55 - 672 μ m (14.8 - 182 cm⁻¹), is much wider than any of these and therefore enables an assortment of aims [59]. Among them, Herschel will be ideally positioned to perform photometric and spectroscopic surveys of star-forming regions and stellar environments. On a more distant scale, the evolution of entire galaxies will be probed, as will the space between galaxies and stars, the interstellar medium, whose dust emission peaks at wavelengths accessible to Herschel.

Herschel was launched on May 14, 2009, and reached its operational orbit at the second Lagrangian point [65] (L2) of the Sun-Earth system approximately three months later. Here, at a distance of about 1.5 million km from Earth, Herschel is always stationed

6.1. HERSCHEL SPACE OBSERVATORY



Figure 6.1: ESA photo of the Herschel space observatory

on a line with the Earth and the Sun, allowing unfettered access to the entire FIR/submm spectrum. Additionally, this orbit is known for thermal stability at low temperatures, which, combined with the low emissivity of the telescope, provide the background necessary for photometry and spectroscopy. Present and future missions are making use of L2 for these reasons, including Planck, and the yet to be launched James Webb Space Telescope [66].

6.1.1 Spectral and Photometric Imaging Receiver

SPIRE is composed of a three-band camera centred at 250, 350 and 500 μ m, and an imaging Mach-Zehnder Fourier transform spectrometer spanning 194-672 μ m [67]. The field-of-view of the spectometer is circular, 2.6 arcmin across, whilst the spectral resolution

6.1. HERSCHEL SPACE OBSERVATORY



Figure 6.2: The SPIRE instrument. Photo: SPIRE Consortium, RAL

is tunable to three spectral resolutions between 0.04 and 0.83 cm⁻¹ [60]. Among its scientific goals, SPIRE seeks to explain the statistics and physics of galactic formation and analyze the early epochs of star formation. Similar to FTS-2, SPIRE uses two bolometer arrays, one covering 194-313 μ m (31.9-51.5 cm⁻¹) (spectrometer short wavelength (SSW)) and the other 303-671 μ m (14.9-33.0 cm⁻¹) (spectrometer long wavelength (SLW)). The SPIRE instrument is shown in Figure 6.2, before integration with the rest of the Herschel payload. Part of the requisite verification and calibration of the SPIRE instrument prior to launch included pre-vibration and post-vibration tests. Together, these were termed the cryogenic qualification model (CQM) and proto-flight model (PFM) test campaigns. The vibration testing was meant to simulate launch conditions; pre- and post-vibration tests were geared towards ensuring all components would survive launch. Finally, the performance verification (PV) phase allowed the Herschel team to test all systems in flight. Data in this chapter will largely come from the PV phase.

6.2 SPIRE Line Shape

In Chapter 2, the instrumental line shape of a FTS was discussed in terms of the cardinal sine, or sinc function. As part of the performance verification phase of Herschel, studies were undertaken to assess the validity of this assumption in flight data. The nature of this is critical to the spectral line-fitting algorithm, as already observed in Chapter 4.

To this end, all ¹²CO lines from the centre detectors for three observations of NGC 7027 and two of AFGL 2688 were collected. Having first removed the baseline from the entire scan using a second order polynomial, a one wavenumber segment centred on each line was then isolated and interpolated onto a common grid. All lines were normalized by their respective maxima and then averaged with a weighting determined by their amplitudes. The results are shown in Figure 6.3, where forward and reverse SPIRE spectrometer scans have been processed independently.

Immediately obvious are small deviations to the first negative high frequency lobe. Future renditions of the line fitting code will need to account for this discrepancy when performing fits. This analysis shows that the SPIRE line shape is not a classical sinc function as defined analytically but in fact some variation that will need to be studied further. Forward and reverse scans continue to be analysed independently, with modest



Figure 6.3: Normalized ILS from over 1000 individual ¹²CO lines. The lower trace shows the difference of the forward and reverse averages, to the same scale, but shifted for clarity. In black, a classical sinc function has been fitted to the average of the green and blue.

variations observed with frequency, especially for lines of greater signal-to-noise.

6.3 Line Fitting

In chapter 4, a program was developed to perform spectral line fits on a simulated FTS-2 spectrum, derived from initial HARP data, as a means of retrieving the spectral line parameters, both before and after the addition of noise. This program was modified to ingest SPIRE flight data. The code was created with the intent that either spectral *.fits files as provided by the Herschel Interactive Processing Environment (HIPE) for the specialist astronomy group (SAG) teams, or IDL[®] save files could be accepted as input
data formats. From this point, the program then proceeds in one of two ways: automatic detection of a set of spectral lines based on their relative amplitudes or ingestion of a userdefined line list. Both methods then deliver their initial line centre guesses to the iterative fitting routine.

6.3.1 Threshold Detection

The first step in any line fitting algorithm is the subtraction of the baseline, which may be approximated in a number of ways. The underlying continuum represents emission from interstellar dust located in the spiral arms of galaxies (see Chapter 4). As a result, the fitting function chosen often constrains the fit so as to deduce physical information about the dust grains, such as temperature and emissivity. Examples of fitting functions were detailed in Chapter 4 and include the Planck blackbody function, and the Priddey [32] and Colbert [33] functions. If one is interested solely in information derived from the spectral lines, a second- or higher-order polynomial can also serve as an adequate baseline. Such a fit is illustrated in Figure 6.4 to spectral data from the central SLW pixel from scans of the Orion Bar [68].

Once the continuum has been removed, all the remaining information to be gleaned from the spectrum comes from the individual lines. The user is asked to specify a threshold, or number of standard deviations, above which all data points are flagged in the case of emission lines. Should fitting also be required for absorption lines, then all points below the negative of the threshold are also noted. Using the same data as in Figure 6.4, each of the detected lines are shown in Figure 6.5. In the figure, the chosen threshold was three standard deviations for both absorption and emission lines (red horizontal lines). Upon inspection,



Figure 6.4: Polynomial fit (top) to Orion Bar spectrum. In the lower plot the fit has been subtracted in order to isolate the spectral lines

seven lines were found outside these limits and are marked in red. Subsequently, all of the "red" lines were fitted with sinc functions of fixed width (as dictated by the resolution of the SPIRE instrument),

$$\frac{1.207}{2L} = 0.0481 \quad [\text{cm}^{-1}] \tag{6.1}$$

a residual calculated, and a new standard deviation determined (blue horizontal lines). On the second check of the threshold against this residual, five additional lines were found, shown in blue. This repeats until there are no longer any data points above the threshold in the residual or until the user-specified maximum number of passes has been reached. The final pass was adjudicating the lines against the threshold shown in orange, however all new



Figure 6.5: Orion baseline-subtracted SLW spectrum, with each of the lines that have been selected for fitting. The orange lines indicate the threshold above or below which lines are deemed legitimate in the final pass through line identification.

lines detected here were too close to previously identified features.

While line identification in this manner is automated and largely user-independent, occasionally non-physical lines may be identified. For example, most of the features selected in Figure 6.5 are legitimate, as shown in Figure 6.6, with the exception of the two large sidelobes either side of the line at 30.74 cm^{-1} . In this case, the strength of the emission line leads to relatively high amplitude ringing surrounding the line, resulting in false positive identifications. The same check that prevented any lines from entering the fitting stage in the third iteration (those beyond the orange lines in Figure 6.5) did not catch these particular outliers as they were found in the first pass and thus accepted by the program



Figure 6.6: Fit of each of the selected lines to the entire SLW spectrum. Underneath, in blue, is the residual difference between raw spectral data and fitted spectral data

by default. In a similar fashion some real lines may be neglected, if they fall below the threshold. This happens in the case of the neutral carbon emission line at 26.99 cm⁻¹, due to its proximity to the neighbouring CO J=7-6 emission line.

Figure 6.6 shows the cumulative fit to the long wavelength (SLW) part of the spectrum, with each of the identified lines indicated. The fitting is done by a nonlinear least-squares iterative IDL[®] algorithm called mpfitfun that proceeds until the reduced chi-squared value is less than 1×10^{-10} over successive iterations, or until 200 iterations have been performed. The residual, shown in blue underneath, speaks to the quality of the fit.

The line centre, line amplitude and ILS FWHM are returned to the user in a set of

Soldware Version: SPIRE_lineFit_V0_5_4D, input FileNAME: 2:(Jones(merschei/SAG34(Orion(Conswidth(OrionBar_SODD))	98b_finalSpec							
DATE: Thu Jun 03 15:25:24 2010,								
Array: SLW,								
Detector: SLWC3,								
Low Frequency cut-off (cm-1): 15.000000,								
High Frequency cut-off (cm-1): 31.500000,								
Line FWHM used in fitting (1.207/2L): 0.048107000,								
Varying/floating linewidth: 0 (0: fixed, 1:floating),								
The Threshold used was: 3.00000 standard deviations,								
Input error from fits file was used in MPFIT function: 1.0000000 (0:yes, 1:no),								
Fixed line width was determined from input fits file: 1 (0:yes, 1:no),								
Line parameter errors reported have been weighted using Chi-squared from MPFIT: 1 (0:no, 1:yes),								
Convergence tolerance used in MPFIT routine: 1.0000000e-010,								
Maximum iterations allowed in MPFIT routine: 200,								
Number of MPFIT Iterations in Final fit: 13,								
Standard Deviation of Residual [input - (baseline + line fit)]: 9.8201029e-019,								
Continuum coefficients are (*x^0,*x^1,*x^2): ,								
4.033214e+000, -4.923349e-001, 1.630084e-002,								
Center (cm-1), Center Error (cm-1), Amplitude, Amplitude Error, FWHM (cm-1), FWHM Error (cm-1), Integrated Area, Int. Are	ea Error							
15.374493, 1.725697e-003, 1.396471e-017, 1.100631e-018, 0.048107, 0.000000e+000, 5.565869e-019, 4.386	747e-020							
18.373353, 2.582519e-003, 9.270639e-018, 1.091060e-018, 0.048107, 0.000000e+000, 3.694968e-019, 4.3480	502e-020							
19.219155, 7.616404e-004, 3.143028e-017, 1.090615e-018, 0.048107, 0.000000e+000, 1.252706e-018, 4.3460	328e-020							
22.045125, 1.680591e-003, 1.424234e-017, 1.090932e-018, 0.048107, 0.000000e+000, 5.676521e-019, 4.3480	093e-020							
23.058958, 4.120508e-004, 5.809309e-017, 1.090989e-018, 0.048107, 0.0000000e+000, 2.315397e-018, 4.3483	818e-020							
25.715400, 9.558382e-004, 2.504236e-017, 1.090627e-018, 0.048107, 0.000000e+000, 9.981050e-019, 4.3460	377e-020							
26.899350, 2.403285e-004, 9.964471e-017, 1.090721e-018, 0.048107, 0.000000e+000, 3.971506e-018, 4.3472	250e-020							
27.850547, 3.900503e-003, 6.140468e-018, 1.090948e-018, 0.048107, 0.000000e+000, 2.447386e-019, 4.348	155e-020							
29.388728, 6.938829e-004, 3.455775e-017, 1.093018e-018, 0.048107, 0.000000e+000, 1.377357e-018, 4.3564	104e-020							
30.700407, 1.305509e-002, 5.371920e-018, 2.239331e-018, 0.048107, 0.000000e+000, 2.141069e-019, 8.925	229e-020							
30.739737, 4.526492e-004, 1.543220e-016, 2.320193e-018, 0.048107, 0.000000e+000, 6.150762e-018, 9.247	517e-020							
30.819171, 2.412552e-002, 1.207533e-018, 1.183068e-018, 0.048107, 0.000000e+000, 4.812826e-020, 4.715	316e-020							

Figure 6.7: Text file output from the final stage of the line fitting routine in which the line width was held fixed.

two text files. The first is populated by the fitting parameters as determined during the line identification stage of the fitting process, along with the pass number each line was found in. The second text file contains, for each of the lines listed in the first file, parameters deduced from the final fit of all lines to the whole data set (Figure 6.6). Associated errors are included for the line centres, amplitudes and widths (provided they are allowed to vary), alongside an integrated area (see Figure 6.7).

6.3.2 User-Supplied Line List

In section 6.3.1, inconsistencies were encountered in the line detection method, resulting in two adverse scenarios: lines being flagged that are not physical, and lines being omitted that are physical. Both situations may be avoided by side-stepping the entire line identification procedure and simply inputting starting guesses for each line of concern. In this way, if it is suspected that a particular molecular species will be seen in



Figure 6.8: Final fit to all known physical lines in the Orion KL spectrum

a given spectrum, then all rotational emission lines in the SPIRE wavelength range can be included.

The input line list must retain a form very similar to that shown in Figure 6.7. Thereafter, the remainder of the fitting procedure occurs as before. The same Orion spectrum was fitted with a pre-selected list of lines, the results of which are shown in Figure 6.8. Again, all known lines have been labeled, with the exception of the boxed area, which is magnified in Figure 6.9. To be noted is the improvement in the residual difference, of significantly lower magnitude. Fitting of these extra features constrains the residual, as more of the spectrum surrounding lines is fitted.

Figure 6.9 plots separate fits for three different carbon-containing species; the



Figure 6.9: Zoomed-in subplot of a segment of the *Herschel*/SPIRE Orion SLW spectrum, illustrating emission lines from three different carbon-bearing species. The blue line, offset for clarity, is the residual difference between the data and the sum of the three fits, each also offset for clarity.

molecular rotation transition CO 7-6, the neutral carbon emission line ([CI]), and an ionic emission signature from CH⁺ [68]. Vertical lines give the known positions of each of the lines, which align well with both the data and the fits, after correction for obliquity effects. The slight shifts observed in the sinc fits for each of the [CI] and CH⁺ lines are explained by interference from neighbouring side-lobes, as the best fit to the entire region is sought. The resulting text output file lists all lines that were fitted, and is given in Figure 6.10.

Software version	: SPIRE_lineFit_v0_5_4b, Input FIL	ENAME :	Z:\jones\H	erschel\SAG34\Orion\	consWidth\OrionBa	ar_5000198b_final:
DATE:	Fri Mar 19 09:48:16 2	010,				
Array:	SLW,					
Detector:	SLWC3,					
Low Frequency cu	ut-off (cm-1):	15.000000,				
High Frequency o	ut-off (cm-1):	31.500000,				
Line FWHM used i	n fitting (1.207/2L):	0.0481070	DO,			
Varying/floating	<pre>s linewidth: 0 (0: fixed, 1:</pre>	floating),				
A user supplied	text file was used to identify lin-	es to fit.				
Input error from	a fits file was used in MPFIT funct	ion: 1.000	0000 (O:yes,	1:no),		
Fixed line width	was determined from input fits fi	le: 1 (0:y	es, 1:no),			
Line parameter e	rrors reported have been weighted	using Chi-squared	from MPFIT:	1 (O:no, 1:ye	es),	
Convergence tole	rance used in MPFIT routine: 1.0	000000e-006,				
Maximum iteratio	ons allowed in MPFIT routine:	100,				
Number of MPFIT	Iterations in Final fit:	15,				
Standard Deviati	on of Residual [input - (baseline -	+ line fit)]:	7.6125505e-	D19,		
Continuum coeffi	cients are (*x^0,*x^1,*x^2): ,					
4.132438e+000, -	5.018580e-001, 1.650785e-002,					
Center (cm-1), C	Center Error (cm-1), Amplitude,	Amplitude Error,	FWHM (cm-1),	FWHM Error (cm-1),	Integrated Area,	Int. Area Error
15.374487,	1.345521e-003, 1.396960e-017,	8.585135e-019,	0.048107,	0.000000e+000,	5.567816e-019,	3.421749e-020
16.409259,	1.110517e-002, 1.683515e-018,	8.537485e-019,	0.048107,	0.000000e+000,	6.709932e-020,	3.402757e-020
17.750287,	1.716372e-002, 1.135580e-018,	8.556794e-019,	0.048107,	0.000000e+000,	4.526043e-020,	3.410453e-020
17.887244,	1.122227e-002, 1.735215e-018,	8.563802e-019,	0.048107,	0.000000e+000,	6.915991e-020,	3.413246e-020
18.372698,	2.031702e-003, 9.279633e-018,	8.569822e-019,	0.048107,	0.000000e+000,	3.698553e-019,	3.415646e-020
18.568120,	8.233513e-003, 2.288161e-018,	8.562407e-019,	0.048107,	0.000000e+000,	9.119846e-020,	3.412690e-020
19.219102,	5.945090e-004, 3.145791e-017,	8.506614e-019,	0.048107,	0.000000e+000,	1.253808e-018,	3.390453e-020
22.045262,	1.303566e-003, 1.434161e-017,	8.507187e-019,	0.048107,	0.000000e+000,	5.716089e-019,	3.390681e-020
23.064686,	5.552971e-002, 1.829396e-017,	2.405765e-016,	0.048107,	0.000000e+000,	7.291363e-019,	9.588576e-018
23.056432,	2.494446e-002, 4.072376e-017,	2.405766e-016,	0.048107,	0.000000e+000,	1.623113e-018,	9.588584e-018
24.542772,	1.080155e-002, 1.732346e-018,	8.515067e-019,	0.048107,	0.000000e+000,	6.904554e-020,	3.393822e-020
25.069844,	7.925211e-003, 2.367892e-018,	8.517787e-019,	0.048107,	0.000000e+000,	9.437631e-020,	3.394906e-020
25.614848,	6.333960e-003, 3.168819e-018,	8.581021e-019,	0.048107,	0.000000e+000,	1.262986e-019,	3.420109e-020
25.715695,	8.102384e-004, 2.475716e-017,	8.580720e-019,	0.048107,	0.000000e+000,	9.867380e-019,	3.419989e-020
26.899780,	2.066704e-004, 9.857867e-017,	8.672327e-019,	0.048107,	0.000000e+000,	3.929017e-018,	3.456501e-020
26.988551,	1.682255e-003, 1.211511e-017,	8.670906e-019,	0.048107,	0.000000e+000,	4.828680e-019,	3.455934e-020
27.850544,	2.919887e-003, 6.402876e-018,	8.507811e-019,	0.048107,	0.000000e+000,	2.551973e-019,	3.390930e-020
29.276685,	7.418303e-003, 2.578899e-018,	8.670229e-019,	0.048107,	0.000000e+000,	1.027863e-019,	3.455664e-020
29.388958,	5.557725e-004, 3.444191e-017,	8.673174e-019,	0.048107,	0.000000e+000,	1.372740e-018,	3.456838e-020
29.954610,	2.006005e-002, 9.335468e-019,	8.543155e-019,	0.048107,	0.000000e+000,	3.720807e-020,	3.405017e-020
30.739232,	1.213581e-004, 1.544247e-016,	8.561282e-019,	0.048107,	0.000000e+000,	6.154854e-018,	3.412242e-020

Figure 6.10: Text file output from the final stage of the line fitting routine, given an initial, user-supplied line list.

6.3.3 Detection of the Methylidyne cation

One of the exciting first detections of the FTS was the measurement of the methylidyne cation, observable in Figure 6.9, at $\sim 27.85 \pm 2.92 \times 10^{-3} \text{ cm}^{-1}$, represents the first detection of the fundamental rotational transition of CH⁺ [68]. The simultaneous detection of the CH doublet transition, as shown in Figure 6.11, solidifies this claim. One of the proposed routes to CH⁺ formation occurs with added energy liberated from the ISM via the endothermic reaction

$$C^+ + H_2 \to CH^+ + H \tag{6.2}$$

Possible energy sources supplying the ~ 0.4 eV needed to activate this reaction include interstellar molecular shocks [69]. However, both CH⁺ and CH (Figure 6.11) are found at the same velocities, which argues against the production of the methylidynium ion through shock chemistry. Additionally, the strong UV fields within photo-dissociation regions (PDRs) may satisfy the energy requirements, especially if H_2 is already in a vibrationally excited state

$$C^+ + H_2(v=1) \to CH^+ + H$$
 (6.3)

a reaction studied by Agundez et al. [70].

While the above routes to formation assume that H_2 is a necessary reactant, H_2 can also destroy the cation in collisions [71]. Indeed, Black et al. [72] concluded that the destruction rate exceeds the probability of formation, making the possibility of detection even more exciting.

Provided a source is optically thin,

$$\int I_{\nu} d\nu = \frac{N f A h \nu}{4\pi} \quad [W m^{-2}], \qquad (6.4)$$

where $\int I_{\nu} d\nu$ is the integrated line intensity, N is the total number of molecules along a line of sight of cross-sectional unit area, f is the fraction of molecules in the upper state of their rotational transition, A is an Einstein-A coefficient, h is Planck's constant, and ν is the frequency of the transition. Using the results from Naylor et al. [68], where

$$A = 5.96 \times 10^{-3} \text{ s}^{-1}$$
$$\nu = 835.079043 \text{ GHz}$$
$$\int I_{\nu} d\nu = 2.5 \times 10^{-16} \text{ W m}^{-2}$$



Figure 6.11: CH doublet as seen in the spectra for each of three SPIRE detectors along the Orion Bar, offset for clarity. In each, the continuum fit has been subtracted.

and the wavelength-dependent solid angle of the beam:

beam =
$$\frac{\pi}{4} \left(\frac{36''}{60'' \cdot 60''} \cdot \frac{\pi}{180} \right)^2$$
 [str] (6.5)

the CH⁺ column abundance is found to be $\sim 3.982 \times 10^{12}$ cm⁻². The above analysis required knowledge of the temperature of the source, assumed to be 85 K. However, if one is able to measure a series of rotational transitions of the same species, rotation diagrams can yield both a temperature and column abundance of the emitting region together.



Figure 6.12: Model of a two level atom, with absorption and emission between energy states l and u, lower and upper, respectively. E_l and E_u are the energies of the levels, while g_l and g_u are the degeneracies.

6.4 Rotation Diagrams

Rotation diagrams, or Boltzmann diagrams, [57] [58] are a powerful tool for determining two significant properties of a molecular cloud: the rotation temperature and the line-of-sight-column abundance. The next section outlines the theory behind rotational diagrams.

6.4.1 Emission Lines

Consider an optically thin molecular cloud (i.e. all radiation escapes local absorption), defined by a single excitation temperature, where the rotation temperature exceeds that of the background and all transitions are within the Rayleigh-Jeans limit [58]. For a two-level atom as in Figure 6.12, with upper energy state, u, and lower state, l, absorption and emission of radiation can occur by three different processes: induced absorption, spontaneous emission and induced, or stimulated emission. Each of these are represented in Figure 6.12 with their associated transition rate equations, or Einstein coefficients: B_{lu} , A_{ul} and B_{ul} , respectively. Rotational transitions occur due to changes in the angular momenta, quantum number J, such that a transition from J_u to J_l gives lines of amplitude

$$I_{ul} = N_u A_{ul} \frac{hc\sigma_{ul}}{4\pi}, \quad [W \text{ cm}^{-2} \text{str}^{-1}]$$
 (6.6)

where A_{ul} is the Einstein A coefficient (s⁻¹), N_u the upper energy state density (cm⁻²), σ_{ul} the emitted photon's wavenumber (cm⁻¹), and h and c are Planck's constant and the speed of light, respectively.

In local thermodynamic equilibrium (LTE) the upper state population is given by the Maxwell-Boltzmann distribution as

$$N_{u} = \frac{Ng_{u}}{Q_{rot}} e^{-E_{u}/kT_{rot}}, \quad [\rm{cm}^{-2}]$$
(6.7)

where g_u is the upper state degeneracy, Q_{rot} is the rotational partition function, T_{rot} is the excitation temperature (K), N is the total column density (cm⁻²) and k is the Boltzmann constant. In the case of a linear molecule rotating, the upper state energy is determined from

$$E_u = J_u (J_u + 1) Bhc, \quad [\mathbf{J}] \tag{6.8}$$

where B is a rotational constant for the molecule. With this definition, the transitions are found at frequencies given by

$$\sigma_{ul} = \frac{E_u - E_l}{hc} = 2BJ_u \quad [\text{cm}^{-1}].$$
(6.9)

In the case of a linear molecule the rotational partition function can be expressed as [57]

$$Q_{rot}(T) = \frac{kT_{rot}}{hcB}.$$
(6.10)

In the following section this theory will be applied to a SPIRE spectrum of DR21. With the line fitting tools developed to this point, it is possible to use the rotation diagram to determine or place constraints on physical conditions within the emitting region.

6.4.2 Rotation Diagram Method

The rotation diagram method requires three initial conditions: that the molecular transitions are optically thin, that they are all defined by a single rotation temperature, and that this temperature is significantly greater than the temperature of the background [57]. From Equation 6.7,

$$\frac{N_u}{g_u} = \frac{N}{Q_{rot}} e^{-E_u/kT_{rot}}, \quad \text{[molecules cm}^{-2]}$$
(6.11)

which, taking the logarithm of both sides of Equation 6.11, leads to

$$\ln L = \ln \left(\frac{N}{Q_{rot}}\right) - \left(\frac{\ln e}{T_{rot}}\frac{E_u}{k}\right) \quad [\mathrm{cm}^{-2}]$$
(6.12)

where $L = N_u/g_u$, and all other quantities are defined as before. Equivalently, from Equation 6.6, L can also be defined as

$$L = \frac{4\pi}{hc\sigma A_{ul}g_u} \int I_u \, d\sigma \quad [\text{ cm}^{-2}] \tag{6.13}$$

The linear relationship in Equation 6.12 has a slope, m, and intercept, b, which give a temperature of

$$T_{rot} = \frac{\ln e}{m} \quad [K] \tag{6.14}$$

and a column abundance of

$$N = Q_{rot} e^b \quad [\rm{cm}^{-2}]. \tag{6.15}$$

The following section uses SPIRE data of DR21 as an application of rotation diagram concepts.

6.4.3 DR21

Molecular cloud DR21 is an HII region within the Cygnus X complex of molecular clouds, located 1.7 kpc distant [73]. The DR21 complex itself is comprised of a molecular ridge with a number of separate CO clouds [74]. Altogether, the entire complex stretches over ~ 5 pc, and contains one of the most massive and most powerful molecular outflows in the galaxy [75]. Due to strong emission in the submillimetre, DR21 was chosen as one of the first observing targets for SPIRE.

SPIRE has provided uninterrupted broadband spectral coverage in the submillimetre, allowing the distinction between dust continuum and line emission. The high resolution mode of 0.04 cm⁻¹ will allow SPIRE to probe the physical characteristics of DR21. The positions of the ten CO lines present in the SPIRE band are marked in the SPIRE spectrum in Figure 6.13. Each of the ten lines with centers σ_{1-10} , and integrated line areas $\int I_u d\sigma_{1-10}$ were input to the line intensity ratio from Equation 6.13. The Einstein A coefficient A_{ul}



Figure 6.13: SPIRE spectrum of molecular cloud DR21, with the two wavelength bands superposed. The long wavelength band (SLW) extends from $14.9 - 33 \text{ cm}^{-1}$, while the short wavelength band covers $32 - 51.5 \text{ cm}^{-1}$.

can be expressed as

$$A_{ul} = \left(\frac{64\pi^4 \sigma_{ul}^3}{3h}\right) \frac{S\mu_{ul}^2}{g_u} \quad [s^{-1}]$$
(6.16)

where S is the line strength and μ_{ul} is the dipole moment. The product $S\mu_{ul}^2$ can be derived from a JPL document [76],

$$I_{ul}(T_0) = \left(\frac{8\pi^3}{3h}\right)\sigma_{ul}\frac{S\mu_{ul}^2}{Q_{rot}}\left[e^{-E_l/kT_{rot}} - e^{-E_u/kT_{rot}}\right] \quad [\text{nm}^2\text{MHz}]$$
(6.17)

where all quantities have been previously defined. Finally, one can obtain a linear relationship as depicted in Figure 6.14, where the two wavelength arrays have been treated



Figure 6.14: Rotation diagram for molecular cloud DR21, as calculated from five CO lines from each of the SLW and SSW arrays.

independently due to their different beam sizes. The black lines show the linear fit achieved by minimizing the chi-squared error. The resulting temperature and column abundance are 180.2 ± 3.60 K and $1.63 \times 10^{17} \pm 9.01 \times 10^{15}$ molecules cm⁻² respectively.

6.5 Conclusions

This chapter revisited some of the earlier topics in the thesis in the context of recently released *Herschel*/SPIRE data. High-resolution spectral data provided by SPIRE will make use of the line fitting tools that have been developed towards deriving physical information from both the underlying continuum and the lines themselves. Methods towards

this goal have been reviewed, including two parallel means which depend on the amount of information the user has about a spectrum pre-fit. Results from this process are essential to creating rotation diagrams: a key technique when interested in the rotation temperature and column abundance of a given source. Finally, all of the above is rigidly influenced by proper characterization of the instrumental line shape of the SPIRE FTS, work that was only introduced in the chapter.

Chapter 7

Conclusion

Two recent, ground-breaking observational projects are poised to provide astronomers with a new view of the submillimetre universe. The Herschel Space Observatory, currently in synchronous orbit with the Earth at the second Lagrangian point, is probing the submillimetre universe with three instruments, allowing unfettered access to this portion of the electromagnetic spectrum. Meanwhile, SCUBA-2, and its auxiliary instrumentation POL-2 and FTS-2, are awaiting arrival of its science-grade detector arrays with full commissioning expected toward the end of 2010. This thesis has addressed aspects both unique and common to each of Herschel and SCUBA-2, as they pertain to imaging spectroscopic observations of the submillimetre universe.

As with any large, internationally distributed high-tech collaboration, delays were to be expected. When I first began my Masters program, it was my intention to work exclusively on the spectrometer under development on SCUBA-2. However, the unanticipated delays in the delivery of the SCUBA-2 camera, which is still to receive its science-grade arrays, meant that halfway through my program it was realized that I would no longer be able to get data from FTS-2. As a result, my thesis has evolved into a survey of Fourier transform spectrometers on both Herschel and the JCMT.

Chapter 2 introduced topics relevant to Fourier transform spectroscopy in general, from measurement of a raw voltage signal to the calculation of a spectrum, along with many of the intervening advantages and disadvantages. Focus was limited to those aspects of the discipline that were to be addressed in later chapters. Chapter 3 examined the important aspects of detector nonlinearity, an issue that is important for both the SPIRE composite bolometer detectors and the ultra-sensitive FTS-2 TES detector technology. In particular, SPIRE has already devoted a large amount of effort to the correction of nonlinearity in both pre-flight and early flight data. Chapter 4 began the discussion of spectral line fitting, in the context of simulated FTS-2 data derived from the HARP heterodyne receiver. Here the importance of the instrumental line shape of a spectrometer, was introduced for the first time. Chapter 5 furthered the ideas of FTS-2 observation planning via the concepts of atmospheric/port cancellation and presented the assumed pixel positions on the sky for a group of well-studied sources. Finally, Chapter 6 showed some early SPIRE flight spectra towards the understanding of a number of topics previously developed. The line fitting algorithm was adapted and applied to SPIRE data.

The work that I have devoted to the topics in this thesis has resulted in authorship on a number of papers, owing partly to the privileged position of the AIG within these two world-class projects. Nevertheless, the impact of this effort cannot be understated. My time spent studying the phenomenon of nonlinearity has greatly increased its profile within the SPIRE working groups. Development is underway on a new temperature-based approach to correction that combines nonlinear correction with bath temperature drift correction. The two steps have been deemed inseparable, owing to the necessity of a proper T_0 value in many of the formulae of the bolometer model discussed in Chapter 3.

The line fitting program that I have helped to develop for SPIRE has already been partially distributed to the SPIRE working groups, with a full distribution in the near future. Much of the analysis towards recent SPIRE publications has utilized this tool. Results derived from the routine have been vetted against independent line fitting measures, such as those found in White et al. [73].

Additionally, with FTS-2 currently in boxes en route to Hawaii, my work modeling the spectra to be observed by FTS-2 is about to be put to the test. The work done in Chapter 4 represents the most realistic simulation of anticipated FTS-2 data currently available. Combined with my port rotation simulations, I have made a significant contribution to the transition of FTS-2 to an observatory-class instrument. In a similar fashion, I have made a significant contribution to the data analysis for SPIRE. I feel privileged to have been involved in both projects and now look forward to the discoveries that each will make, perhaps some of which will be as revolutionary as those by William Herschel over two centuries ago.

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Appendix A

Publications and Conferences Proceedings

A.1 Conference Proceedings

- S.C. Jones, D.A. Naylor, B.G. Gom and L.D. Spencer. Astronomical Submillimetre Fourier Transform Spectroscopy from the Herschel Space Observatory and the JCMT. In Celebrating 10 years of growth and scientific discovery in Canadian astronomy, page 46. Canadian Astronomy Society (CASCA), May 2010. CASCA Annual Meeting
- S.C. Jones, D.A. Naylor, B.G. Gom and L.D. Spencer. Spectral line fitting of an astronomical source. In Proceedings of the 30th Canadian Symposium on Remote Sensing (30th CSRS), pages 625-633. Canadian Remote Sensing Society, 2009.
- Scott C. Jones, David A. Naylor, Brad G. Gom, Locke D. Spencer and Nanyao Lu.
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A.2 Publications

- E. Habart, E. Dartois, A. Abergel, J.-P. Baluteau, D. Naylor, E. Polehampton, C. Joblin, P. Ade, L.D. Anderson, P. André, H. Arab, J.-P Bernard, K. Blagrave, F. Boulanger, M. Cohen, M. Compiegne, P. Cox, G. Davis, R. Emery, T. Fulton, C. Gry, M. Huang, S. C. Jones, J. Kirk, G. Lagache, T. Lim, S.Madden, G.Makiwa, P. Martin, M.-A. Miville-Deschênes, S. Molinari, H. Moseley, F.Motte, K.Okumura, D. Pinheiro Gocalvez, J. Rodon, D. Russeil, P. Saraceno, M. Sauvage, S. Sidher, L. Spencer, B. Swinyard, D.Ward-Thompson, G. J. White, A. Zavagno, SPIRE spectroscopy of the prototypical Orion Bar Photodissociation Region. Astronomy & Astrophysics (2010)
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