Parameter Analysis and Future Development of the Periodic Shadowing Concept

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List of Abbreviations and Variables

PS - Periodic Shadowing
FFT - Fast Fourier Transform (Matlab function)
CCD - Charge-Coupled Device
FRED - An optics ray-tracing simulator, see References
f_g - Frequency of Ronchi gratings
ω - Fourier peak frequency
k - Exponent of the filter function
σ - Width (variance) of the filter function
a - Distance between the signal peak and the stray light peak in the Fourier domain

Abstract

Periodic Shadowing is a software post-processing technique for suppressing stray light. A proof-of-concept was recently published so an analysis of the involved parameters is needed to allow for a deeper understanding of the technique. In this project the three most important parameters in the technique are analyzed and their impact on the results of optical spectroscopy measurements is evaluated and discussed. The findings are then used in a successful initial attempt in a software-to-hardware conversion of the technique, which would remove the need for post-processing in the Periodic Shadowing technique altogether.

1 Introduction

1.1 Motivation

An optical spectrometer is a tool used to spatially separate and detect light of different wavelengths. Conclusions about the light source and its characteristics, such as which wavelengths the light consists of, can be drawn by examining light with an optical spectrometer. One useful application for optical spectroscopy is element identification, as each element radiates at a unique set of spectral wavelengths. Element identification is important when trying to determine for example the contents of distant stars [1], intermediate species in combustion processes [2] or the identification of electronic and molecular structure [3].

Despite being a well-used measurement technique, improvements in optical spectroscope design have been close to non-existent since its invention. Limiting factors still affect measurements, thus decreasing quality of results. There are ways to limit their effect but these have drawbacks such as being expensive, increasing measurement time drastically or limiting measurements in other aspects. If a method could be developed that mitigates the inherent limiting facts of optical spectroscopy without major drawbacks, the quality of the results from measurements using optical spectroscopy could improve significantly.

1.2 Background - Standard Setup

1.2.1 Spectroscopy

The basic setup of an optical spectrometer, the so-called Czerny-Turner spectrometer, is displayed in Figure 1. If an element is excited in e.g. a discharge lamp, it will de-excite and in the process emit the energy as a photon with spectral wavelength corresponding to the excitation energy. If this light enters an optical spectrometer it reflects off of a reflection grating, designed to reflect light at angles that depend on the wavelength of the light. Light with different wavelengths will travel slightly different paths through the spectrometer and hit the detector screen at unique locations for each wavelength, so that wavelength-discrimination is possible.

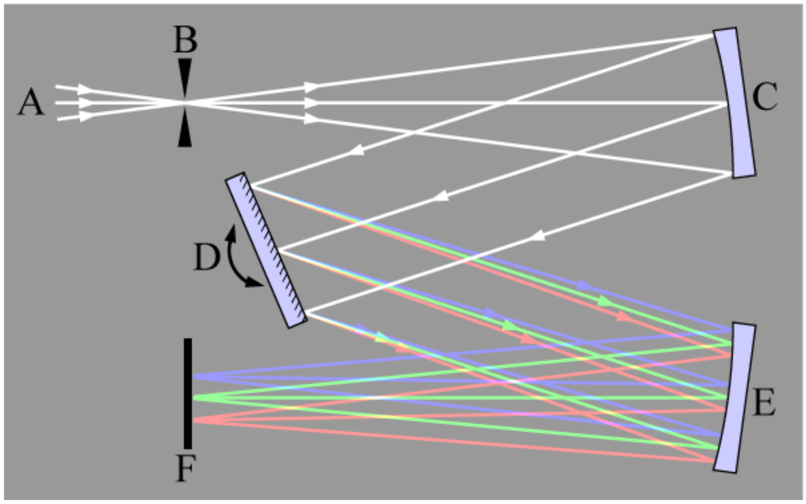

Figure 1: *The basic layout of a Czerny-Turner spectrometer. In the figure, A marks the incoming light. B is the entrance slit. C is the first collimating mirror. D is the reflection grating. E is the second collimating mirror. F is the location of the CCD-chip detector. Source: [4] (Modified)*

1.2.2 The Stray Light Problem

Since its creation, the design of the Czerny-Turner spectrometer has changed very little so very few of its initial problems have been dealt with. Imperfections in the mirrors and the reflective grating give rise to diffuse reflection and scattering. Also, leaks in the enclosure can introduce unexpected interfering background sources. Furthermore, higher order interference peaks from the reflective grating can scatter on the walls of the spectrometer and eventually reach the detector screen. These and other similar phenomena are summarized in the term *stray light* [5].

Stray light is a problem that potentially ruins measurements since high-amplitude peaks can be broadened so that they cover closely situated peaks of lower intensity, making them indistinguishable. Furthermore, in measurements that depend on small signal amplitude or a high signal-to-noise ratio, such as Laser-Induced Raman Spectroscopy [2], the signal can be so small or close to the measurement noise that it is very hard to distinguish signal from noise and stray light.

There are ways to reduce the problem of stray light, mainly using spectrometers equipped with a double monochromator [6] but they have drawbacks such as being large, cumbersome and relatively expensive. Furthermore, they do not produce a full spectrum as the double monochromator scans a narrow band of spectral wavelengths. If a full spectrum is desired the spectrum has to be scanned repeatedly, increasing the measurement time significantly. In an attempt to achieve similar levels of stray light suppression but with as few of the drawbacks of the double monochromator as possible, a method was recently presented by Kristensson *et al.* called Periodic Shadowing. This technique is new and there are several venues available when it comes to improving it. A better understanding of the technique, together with an analysis of relevant parameters, is therefore of importance before developing it further.

1.3 Background - Periodic Shadowing

Periodic Shadowing, henceforth shortened to PS, is a post-processing method for suppressing stray light in spectroscopic measurements. A brief explanation of the method and its inherent central concepts is presented here.

1.3.1 Fourier Transform

The first major concept of PS is the Fourier transform. The Fourier transform builds on the fact that any function can be described by a sum of sinusoidal functions with different spatial frequencies ω_n, similar to how a musical chord is made up from its constituent notes. Instead of looking at the spatial distribution of a measurement signal, a Fourier transform can be performed to give the base sinusoidal frequencies needed to recreate the signal. In the case of a one-dimensional signal, sinusoidal frequency is given on the x-axis and the amplitude of a given frequency is given on the y-axis. It is important to note that Fourier domain frequency does not have anything to do with the frequency (and thus wavelength) of light but is a purely mathematical concept in signal analysis and the two must not be confused.

A constant background noise or a constant off-set is a common feature in spectroscopic measurements. In the Fourier domain such a feature creates a peak at $\omega = 0$. If other kinds of interference are part of a signal they will also contribute with their own corresponding Fourier peaks, creating a Fourier spectra through superposition. The general shape of these spectra are determined by the types of interference present; if the interference is localized high amplitude signal, the contribution is high frequency peaks and if the interference is due to a constant off-set it contributes with low frequency peaks. If the source is random noise the Fourier spectrum is a varying offset since random noise gives contributions at almost all frequencies.

If instead a measurement signal is considered, the signal is a sum of the actual measurement signal as well as various unwanted contributions: background noise, stray light and similar effects. The Fourier transform will therefore be the sum of the individual Fourier transforms of all contributors. If the measure signal can be distinguished from the unwanted stray light and noise and isolated in the Fourier domain the same isolation would occur in the spatial domain. This is utilized in PS.

1.3.2 Ronchi Gratings

One way of isolating wanted from unwanted signal in the Fourier domain is by altering the spatial signal of interest through modulation with a known periodic pattern of spatial frequency f_g. If this is done before the light enters the spectrometer the result is that light following the intended path through the spectrometer will have this modulation while any stray light introduced in the spectrometer will not. This would separate the detected signal in the Fourier domain into two groups, signal that has been modified with this known frequency, the measurement signal, and signal that has not been modified, the stray light. Most of the signal that has been modified will be be located in a single pair of Fourier peaks at $\omega \propto \pm f_g$ while the location of the unmodified signal will be unchanged. This means that a pair of peaks will appear in the Fourier domain at a distance from $\omega = 0$ determined by the known frequency f_g. A higher f_g means the distance in the Fourier plane is larger while a lower f_g decreases the distance to $\omega = 0$.

If a constant-interval square wave transmission grating, known as a Ronchi grating, is placed in the signal path it effectively multiplies the spatial signal with a square wave pattern. In the case of the optical spectrometer a Ronchi grating can be placed in front of the entrance slit of the spectrometer in order to modulate the measurement signal.

In Figure 2 the difference between an ordinary spectrum and a spectrum modulated with a Ronchi grating can be seen, together with a Fourier transform of the 361 nm spectral lines from the corresponding image. The only difference between the two images is the periodic pattern of shadows introduced along the vertical axis (the rows) created by the Ronchi grating.

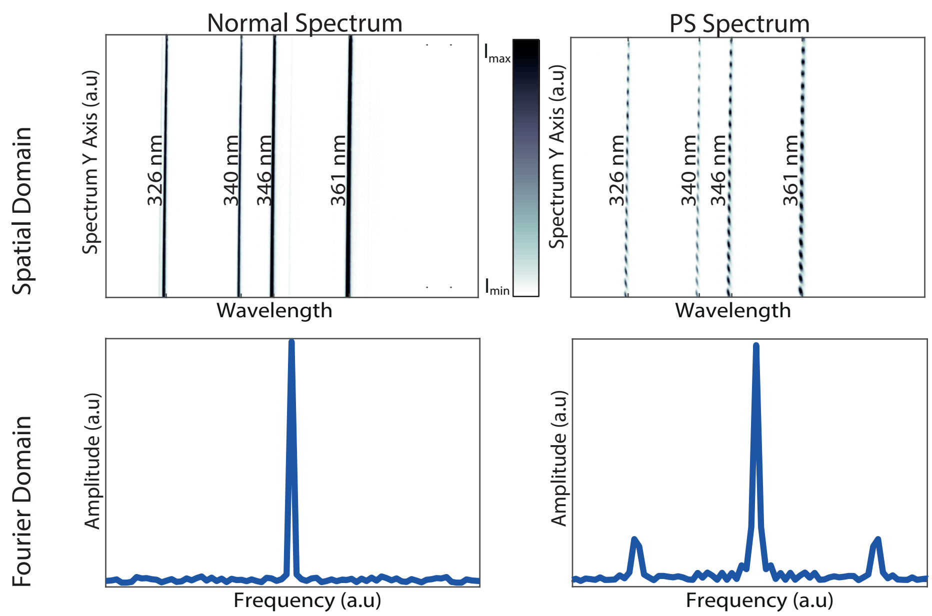

Figure 2: *Cadmium emission spectra,* 314.58 nm − 385.49 nm*. A regular spectrum (left) and a spectrum affected by a Ronchi grating (right) with their corresponding 1D Fourier spectra. On the right the mirroring Fourier peaks resulting from the introduction of a Ronchi grating are easily distinguishable.*

The peaks that arise from the introduction of a Ronchi grating and contains the measurement signal will henceforth be referred to as "signal peaks" while the peak centered at $\omega = 0$, that contains the stray light, will henceforth be referred to as "stray light peak". The ability to make this distinction is an important feature in PS.

1.3.3 Frequency Filtering and the Removal of Unwanted Signal in the Fourier Domain

A way to distinguish between measurement signal and stray light has been identified and the next step is to isolate the signal of interest. This is done by multiplication with a filter function centered on one of the signal peaks. A Super Gaussian function can be used to achieve this. A Super Gaussian has the same form as a Gaussian function with an extra exponent k, thus on the form

$$G(x) = e^{-\left(\frac{(x-\mu)^2}{2\sigma^2}\right)^k} \tag{1}$$

The main structural difference from a regular Gaussian is that, as k grows, the shape of the Super Gaussian approaches the shape of a top hat.

Since the goal is to isolate the measurement signal, σ and k are chosen so that the filter function only covers the signal peak. If an overlap between the filter function and the stray light peak were to occur stray light suppression would decrease and the procedure would not yield as good results. A visual representation of the effect of different values of k on the filter function, as well as an image showing the basic idea behind the frequency filtering, is displayed in Figure 3.

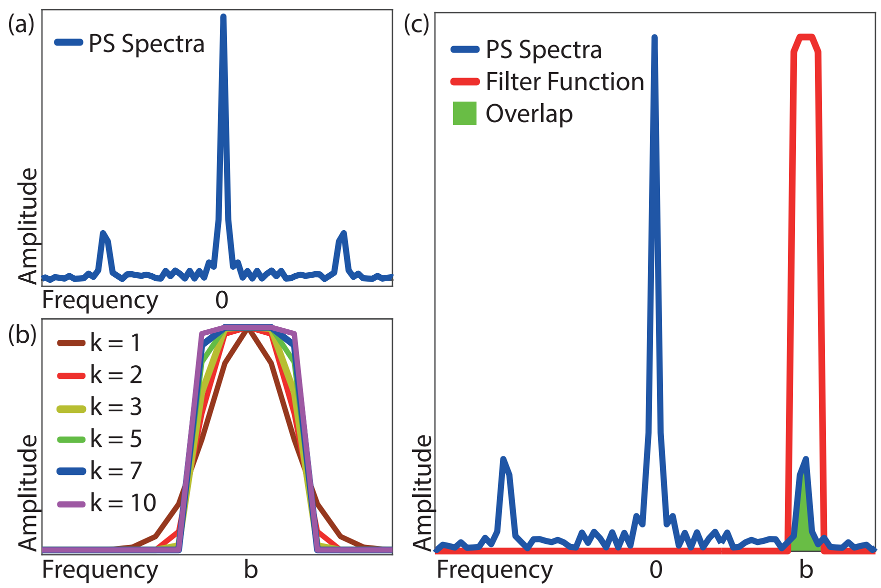

Figure 3: *(a) The sample PS Fourier spectra seen in Figure 2. The stray light peak is located at $\omega = 0$ and the signal peak pair at $\omega \propto \pm f_g$. (b) The effect on the filter function shape for different values of k. (c) The visualization of the multiplication between the PS Fourier spectra and the filter function. The overlap, the result of the multiplication, is highlighted in green. If the green area were to encompass any part of the stray light peak the suppression of stray light would decrease.*

In the way depicted in Figure 3 (c) much stray light is suppressed while the measurement signal is preserved. The resulting Fourier spectrum is then transformed back to the spatial domain and since no signal was removed the result is a spatial spectrum with suppressed stray light and more distinct spectral lines.

As already stated, if something affects a signal in the Fourier domain it also affects the spatial domain signal: Multiplication between two functions in the Fourier domain affects the spatial domain as if the Fourier transforms of the two functions were convoluted. Therefore, it is important to use an filter function that affects the spatial spectra as little as possible while still isolating the signal peak.

In terms of isolating the signal peak a top-hat function would be optimal but its Fourier transform is a sinc function, which would alter the spatial signal notably. Thus, a function with a Fourier transform that is well-known and easily predictable would be preferred. For this, a Gaussian would work well, since the Fourier transform of a Gaussian is another Gaussian. Convoluting a 2D spectrum (Top row, Figure 2) with a Gaussian along the Spectrum Y-axis would lower the signal intensity at the "top" and "bottom" of the 2D spectrum but the spectral lines would still be clearly displayed. The Super Gaussian works well when isolating the signal peak. Furthermore, its Fourier transform is a combination of a sinc function and a Gaussian, meaning that while it has elements of the sinc function the Gaussian contribution makes the effects on the PS spectrum more predictable.

1.3.4 Summary of PS

The PS technique is based on introducing a known periodic pattern into a measurement signal, in this case through the use of a Ronchi transmission grating placed in front of the entrance slit of the spectrometer. The detected signal is then Fourier transformed and the signal peak is isolated through multiplication with a filter function, effectively filtering out most of the stray light. Finally the result is inversely Fourier transformed, resulting in a measurement signal with suppressed stray light, hereafter referred to as a *PS spectrum*. A spectrum that has not been post-processed by PS is referred to as *raw spectrum*.

The most important parameters when it comes to affecting the stray light suppression are the ones that affect the likelihood of an overlap between the filter function and the stray light peak: the Ronchi grating frequency f_g as well as the width σ and the exponent k of the filter function. Consequently, these three are the parameters studied in this project.

1.4 Software-to-Hardware Conversion

One drawback of the PS method is the fact that the Ronchi grating inherently blocks about half of the measurement signal, significantly reducing signal-to-noise ratio. If a small and compact stray light suppressor could be constructed so that it could fit inside the spectrometer beam-line, removing the need for post-processing, the quality of spectroscopic measurements could be improved significantly through other post-processing techniques that reduces signal-to-noise ratio or that enhances the measurement signal. The goal of the PS software-to-hardware conversion is to investigate whether the PS software concept can be converted into hardware that can be integrated into a spectrometer so that no post-processing is needed in order to suppress stray light.

1.4.1 The Ronchi Grating and the Fourier Transform

Every software operation described this far can be preformed in hardware as well. The Ronchi grating is already a hardware component but it has another useful feature: Any optical component that creates diffraction, such as a Ronchi transmission grating, creates a Fraunhofer diffraction pattern with the same shape as the Fourier transform of the optical element in the far field (Fraunhofer region) [7]. If the Ronchi grating is introduced inside the spectrometer, where the light is collimated, such a pattern would appear. The Fourier transform is located in the far field of the Ronchi grating but since the light is focused onto a detector screen at the end of the spectrometer the detector screen becomes the far field. Thus, the Fourier transform of the measurement spectrum should be displayed onto the detector screen.

1.4.2 Hardware Frequency Filtering

With the Fourier transform of the measurement spectrum projected onto the detector screen, stray light have once again been discriminated from the measurement signal. To also remove the stray light from the detector screen a way to physically isolate the signal peak has to be found. One option would be to cover or deactivate the detector screen everywhere but where the signal peak is projected. This would, however, introduce the same complication as a software frequency filtering preformed with a top-hat function. Ideally, a transparency filter with a Super Gaussian profile would be used.

Assuming the signal peak can be physically isolated and detected without affecting the quality of the spectrum a hardware conversion of the PS method should be possible.

1.5 My Work

This bachelor thesis aims to improve the PS post-processing analysis and to further the understanding of the process as well as lay a foundation for a future software-to-hardware conversion proof of concept.

A Matlab script capable of testing how altering the three chosen variables affects the outcome of the method is to be created. The chosen variables are the frequency f_g of the Ronchi grating as well as the width σ and the exponent k of the Super Gaussian filter function. Consequently a set of PS spectra with different Ronchi gratings has to be recorded.

Lastly, a simulation environment has to be created so a ray-tracing simulation can be performed to test the theory behind a software-to-hardware conversion. A basic experiment is also to be performed to investigate whether a conversion of the PS method from software to hardware is possible in practice. The experiment is limited to the introduction of the Ronchi grating inside the spectrometer, since that is the only testable part based on the parameter analysis preformed on software PS so far. The goal is to see if stray light can be separated from measurement signal in this way.

2 Method

2.1 Laboratory Setup

The laboratory setup consisted of an optical spectrometer (Shamrock 750, Andor Technologies) in conjunction with a Cadmium discharge lamp. A CCD-camera (Luca, Andor Technologies) with 1002×1004 pixels resolution was mounted onto the spectrometer, acting as a detector screen.

The software Adobe Illustrator was used to create patterns for the Ronchi gratings. The patterns were then printed onto transparent overhead-paper. This method allowed inexpensive creation and testing of many different Ronchi grating frequencies without notably reducing the quality of the measured spectra. The gratings were fixed onto the outside of the spectrometer entrance slit with tape. This allowed the gratings to be as close to the entrance slit as possible while still being parallel to the slit opening.

Four series were acquired using a Cadmium discharge lamp and Ronchi gratings of varying line-widths in conjunction with the optical spectrometer. The line-widths of the gratings used were 0.7 mm 0.8 mm, 0.9 mm, 1 mm , 2 mm, 3 mm, 4 mm, 5 mm, 6 mm and 7 mm. The gratings were made so that the distance from one line to the next was equal to the width of the lines, creating a square-pulse profile. Their respective grating frequencies were:

Width (mm)	0.7	0.8	0.9	1	2	3	4	5	6	7
f_g (lines/mm)	1.43	1.25	1.11	1.00	0.50	0.33	0.25	0.20	0.17	0.14

The slit width of the spectrometer and the exposure time of the camera were set to 12 μm and 50 ms respectively, for all measurements. The spectrometer grating with a grating constant of 150 lines/mm was centered on 350 nm and the resulting observed spectral bandwidth was 314.58 nm to 385.49 nm.

Since the effect of PS on the measured images was of interest, the raw spectra was compared to their corresponding PS spectra. The spectra with the same Ronchi grating were summed and normalized to mitigate random background noise. The PS algorithm was then applied to the resulting 1D spectra. The resulting PS spectra was compared with its corresponding normalized image.

2.2 Matlab Script

A MATLAB script was developed in order to better understand the process of the PS method. The purpose of the script was to perform the PS algorithm when an image was loaded. The vital parts of the code are attached in Appendix 1, leaving out plotting and loading of images.

One feature that was emphasized in the Matlab script was that, since several different Ronchi gratings were to be used, the script would have to be able to identify the frequency of the grating in use without any input from the user. The script assumed that the Fourier peak with the highest amplitude in the Fourier spectra was the stray light peak and that the second highest peak was the signal peak. Since the distance between the two peaks is correlated to f_g of the Ronchi grating, the frequency was found by finding the distance between the two peaks.

2.3 FRED Simulation

A simulation environment was created in order to analyze one part of the Software-to-Hardware conversion. The ray-tracing program FRED [8] was used to create a replica of an optical spectrometer with a Ronchi grating introduced after the first collimating mirror. The Ronchi grating was used both to introduced the periodic pattern but also to create the hardware Fourier transform. Because of this, the Ronchi grating was placed after the first collimating mirror inside the spectrometer, where the light was collimated.

As stated, the spectrometer was designed so that the second collimating mirror focused the resulting spectrum onto the detector screen, which would allow the Fourier transform of the signal passing through the Ronchi grating to be projected onto it. An overview of the replica with labeled optical elements, as well as an overview after ray-tracing and a close-up image of the detector plate, can be seen in Figure 4.

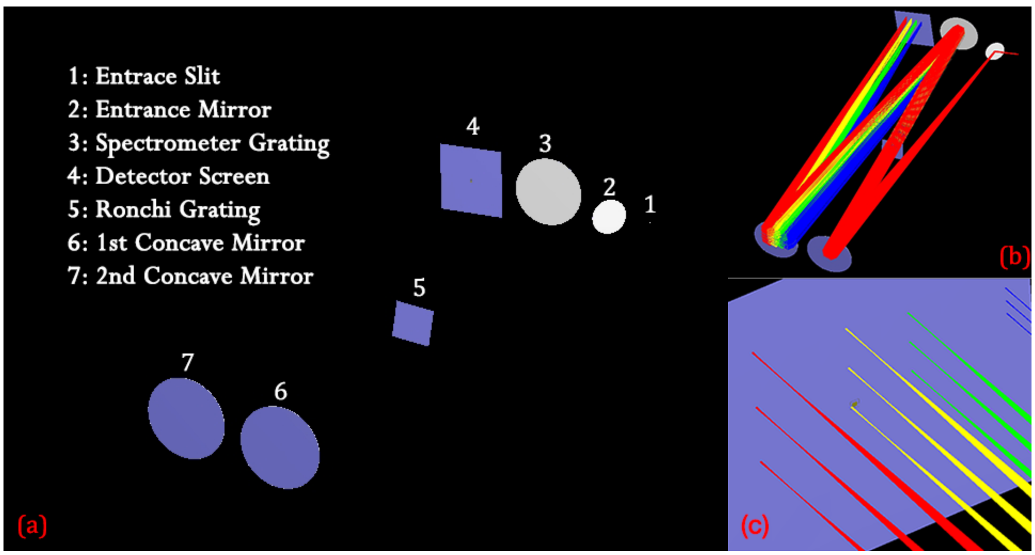

Figure 4: *(a) The replica of a spectrometer created in FRED, with optical components labeled. (b) The system after ray-tracing has been done, with rays displayed. (c) A close-up image of the detector screen. Four different wavelengths can be seen (Blue, Green, Yellow and Red) as well as the diffraction pattern created by the Ronchi grating in each wavelength.*

3 Results and Discussions

3.1 Study of Parameters in Periodic Shadowing

Three parameters in the PS method and their impact on the process are studied in order to improve the understanding of PS. Also, some interesting features concerning software-to-hardware conversion are touched briefly, in order to introduce an actual software-to-hardware conversion.

3.1.1 Result Evaluation and Area Ratio

There are several possible ways to evaluate the results of the PS method. The main feature of the PS method is to reduce the stray light broadening of spectral peaks meaning that a comparison of height-to-width ratio would be meaningful. Such an evaluation is however affected by the background radiation level and the background radiation level is suppressed by the PS method. This means that determining where the width of the spectral peaks are to be measured is a problem. Instead, the areas of the spectral peaks were compared by summing the intensities from the closest 25 detector pixels on each side of a peak maximum. The areas of the peaks from a raw spectrum were compared to those of the PS spectrum and an average peak area ratio was calculated. This quantity is hereafter referred to as *Area Ratio*.

3.1.2 Frequency Analysis

The first property to be analyzed was the influence of the spatial frequency of the Ronchi transmission grating. It was expected that a higher spatial frequency would provide better stray light suppression due to the increased distance between the signal peak and the stray light peak, in turn reducing the risk of an overlap in the frequency filtering process. Furthermore, a higher frequency allowed the Matlab script to make a more precise estimation of the actual frequency of the grating, reducing potential numerical errors. Results of this parameter analysis are displayed in Figure 5 and 6.

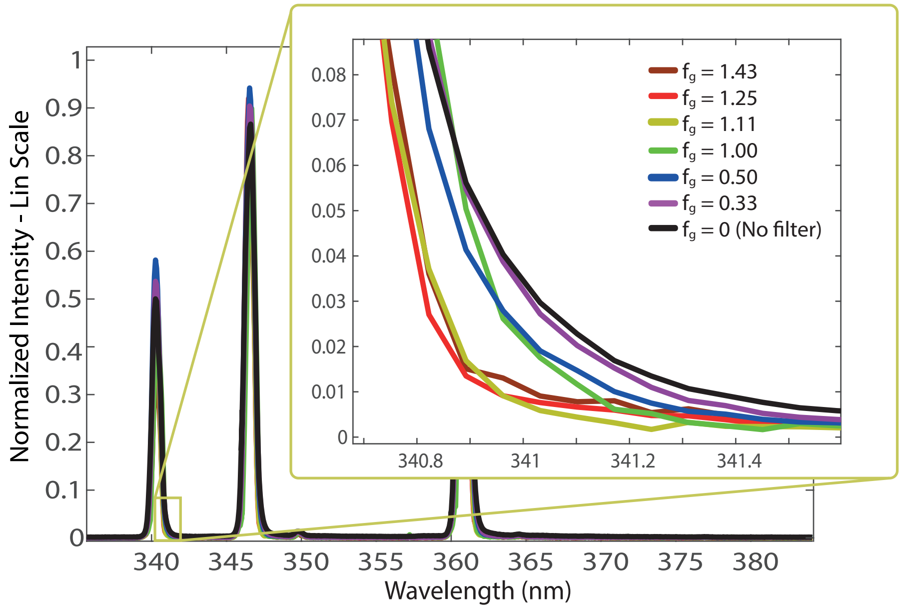

Figure 5: *Seven Cd spectra on a lin-lin scale; one raw spectrum and six PS-spectra. All PS-spectra, each with its own Ronchi grating frequency, (specified in the top right of the plot) have lower levels of stray light compared to the raw spectrum. The results further show that a higher Ronchi grating frequency leads to improved stray light suppression.*

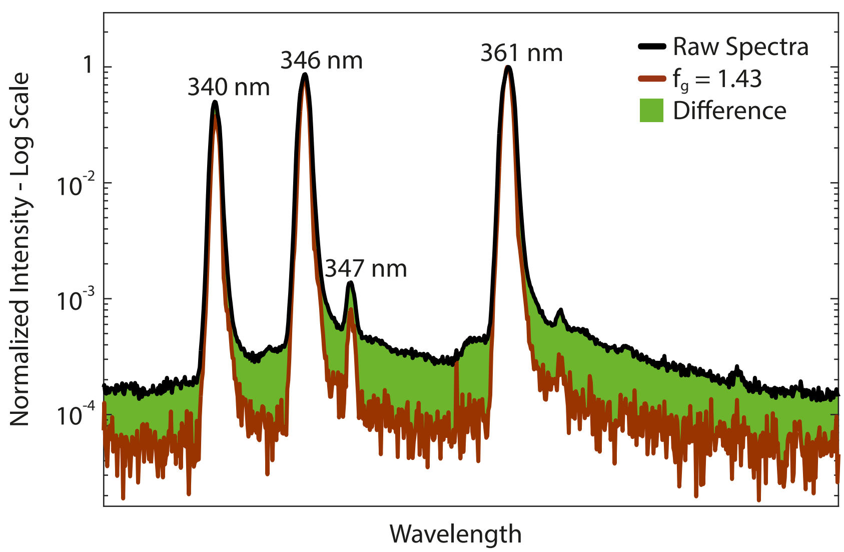

Figure 6: *The difference (green) between a raw emission spectrum (black) and the PS spectrum with the highest Ronchi grating frequency tested (brown) displayed in a lin-log plot.*

Figure 5 is a lin-lin plot showing the emission spectrum from a Cadmium spectral lamp in the previously specified wavelength band. The colors correspond to measurements with varying Ronchi-grating frequency. By comparing the different PS spectra to the raw spectrum (black) it is evident that using a higher f_g leads to narrower wings which is interpreted as improved stray light suppression.

Figure 6 shows a lin-log plot of the emission spectra from the same Cadmium spectral lamp. Only the raw spectrum as well as the highest f_g Ronchi grating are presented. The difference between the two is highlighted in green. It is seen that a higher f_g also provides background reduction, as well as stray light suppression.

We thus concluded that stray light suppression benefits from a higher Ronchi grating frequency. In the case of these experiments no upper limit was found for f_g so it cannot be stated whether one exists before the resolution of the detector screen limits the spectrum. Until such a limit is found the rule of thumb is that a higher Ronchi grating frequency provides better stray light and background suppression.

3.1.3 Analysis of the Filter Function

When analyzing how the characteristics of the filter function affects the outcome of the PS technique, there are two variables known to affect the result: the width of the filter function σ and the order of the exponent k. Both are important when it comes to isolating the signal peak as both quantities affect the risk of overlap with the stray light peak.

Prior to the parameter analysis, it was expected that a higher k would yield a lower area ratio since a higher k would reduce the wings of the filter function. Furthermore, a smaller σ was expected to yield better results since that would reduce the width of the filter function and thus decrease the chance of overlap with the stray light peak. The effect of these two variables depends on the frequency of the Ronchi grating, as the distance between the stray light peak and the signal peak in the Fourier domain determines what values σ and k can take so that there is no overlap. A high-frequency grating, $f_g = 1\,\text{line/mm}$, was chosen for the analysis in order to allow for a wider range of values for k and σ.

A parameter analysis was performed where k took values between 0 and 20, while σ took values between 0 and the value corresponding to the distance between the stray light peak and the signal peak in the Fourier domain. The aim was to identify points with sharp gradients in the area ratio indicating where there was an evident change in shape of the PS spectrum. If such points were found this change in shape could be identified as the values of σ and k causing an overlap. The method of comparison was the same as previously, an area ratio between raw image and PS image. Four spectral lines were analyzed. The result is presented in Figure 7.

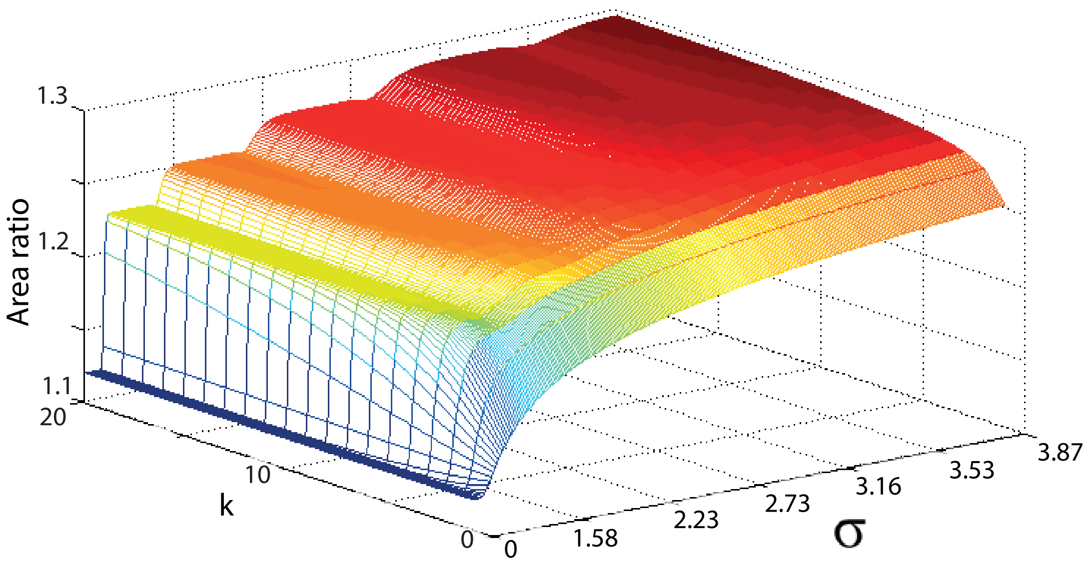

Figure 7: *The area ratio between raw spectrum and PS spectrum of one spectral peak as a function of the filter function width σ and exponent k. Plateaus of stability are observed around specific σ as long as k is sufficiently large. Generally, the results show that decreasing σ improves stray light suppression.*

In the analysis of σ a few things are important to note: If the exponent is high enough ($k > 5$) areas of stability form. The explanation for this behavior is that around $k = 5$ the filter function is close to a top hat function. The transition between areas of stability occurs when a new Fourier frequency of noticeable amplitude is included under the filter function due to an increased σ. As σ is decreased, a smaller area ratio with better stray light suppression was expected and this is supported by the results. However, an area ratio consistently larger than 1 was unexpected. After looking through the code (See Appendix) it turned out this was due to an unfortunate normalization of the PS spectra. While this does not affect the project outcome it is a bit counter-intuitive and therefore worth mentioning.

Stability in area ratio, and thus stray light suppression around σ, is desired when selecting σ in order to prevent computational problems such as rounding errors to affect the stray light suppression. Thus, the first conclusion to draw regarding k is that a higher exponent is preferred, as it makes the graphs more stable. However, it only has to be large enough so that the observed plateaus start to form to yield good results. However, larger k gives marginally larger areas of stability. No theoretical upper limit to k was found. However, when choosing an exponent, memory size has to be considered, since increasing the exponent rapidly increases the memory usage of the analysis. In the case of this project $k = 20$ was deemed a large enough value to be used. Furthermore, a small σ coupled with a large k yielded the best results for suppressing stray light, though improving only marginally as k grew from 10 to 20.

One risk with having a too large k is that the filter function becomes so much like a top-hat that it causes ripple effects in the final PS spectrum. A comparison was performed, investigating the intensity along the spectral lines in the resulting PS spectrum using different values for k in the process. If rippling is present regions of local decrease in intensity is expected to appear, most notably at the "ends" of the spectral lines. The result of the comparison is displayed in Figure 8.

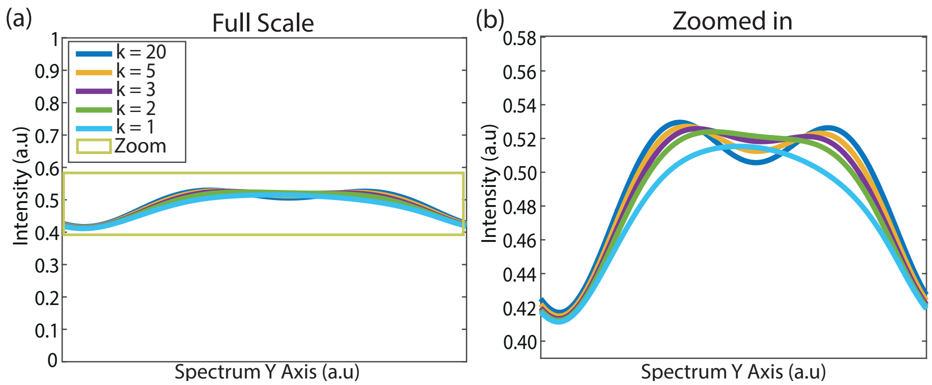

Figure 8: *The effect of different values of the filter function k on the resulting PS spectral lines. Rippling effects are visible as a local decrease in intensity at the edges of the Spectrum Y axis. While the rippling effect is present the value of k does not seem to affect the shape of the spectrum significantly. However, as k grows a local decrease seem to appear in the middle of the spectrum as well, seen in b). This means that a possible loss of intensity is a risk if k is allowed to grow very large ($k >> 20$). While negligible in the software version, rippling effects could very well be problematic in a hardware solution, where the shape of the filter function can be hard to control.*

While the rippling behavior is visible, the effect it has on the PS spectrum is negligible. Furthermore, it seems that the value of k does not affect the rippling shape very much as long as $20 \geq k > 1$. It is possible that a significantly higher value of k would cause a local decrease in intensity in the central region of the spectral line - such a trend is indicated in 8 (b) - but due to computational limitations such an analysis was not possible. Thus, it is concluded that, in the scope of this project, the value of k does not influence the final spectrum enough to become an issue, assuming a Ronchi grating of frequency $f_g = 1\,\text{line/mm}$ or higher is used.

3.1.4 Ronchi Grating Frequency f_g and Filter Function σ Analysis

Reasoning around the mathematical expression of the filter function led to the expectation that there should be some sort of relation between its width, σ, and the distance between the signal peak and the stray light peak, a. Since a depends on the frequency of the Ronchi grating f_g, there is a point in studying the relation between the two in this project. It was assumed that the exponent of the filter function was high enough so that the Super Gaussian could be approximated to a top hat function. In order for an overlap to occur the distance between the two Fourier peaks has to be smaller than half the width of the Super Gaussian.

The FWHM for a Gaussian is given by $2\sqrt{2\ln(2)}\sigma$ so the following relation has to be fulfilled in order to avoid an overlap if the filter function is a Gaussian:

$$a > \sqrt{2\ln(2)}\sigma \tag{2}$$

The expression of the FWHM of a Super Gaussian is changed slightly due to the introduction of the exponent k. Deriving the FWHM of the Super Gaussian was done in the following steps:

$$e^{-\left(\frac{(x-\mu)^2}{2\sigma^2}\right)^k} = \frac{1}{2} \tag{3}$$

$$\frac{(x-\mu)^2}{2\sigma^2} = \sqrt[k]{\ln(2)} \tag{4}$$

$$x - \mu = \pm\sqrt{2}\,\sqrt[2k]{\ln(2)}\sigma \tag{5}$$

Since a Super Gaussian with a large k closely resembles a top hat function it is assumed that the FWHM can be used as an indicator for overlap. If it is assumed that the signal peak is located at μ in the Fourier domain, the distance a to the stray light peak has to fulfill the relation $a > x - \mu$ in order to avoid overlap. Thus the following has to be true:

$$a > \sqrt{2}\,\sqrt[2k]{\ln(2)}\sigma \tag{6}$$

As long as equation 6 is valid, the PS method is expected to provide stray light suppression. If σ is chosen so that equation 6 is invalid, resulting in the stray light peak being completely included by the filter function, the PS method is expected to not provide any stray light suppression. When testing this, the expected outcome is as follows: When equation 6 holds, the PS method successfully suppresses stray light and, using the same method of evaluation as earlier, a smaller area ratio indicates better stray light suppression. The area ratios are still expected to be larger than 1. When equation 6 is invalid, the area ratio is expected to be close to 1, since very little stray light suppression occurs - the raw spectrum and the PS spectrum are practically the same.

The relation between the Ronchi grating frequency f_g and a was initially unknown so a correlation was made. The distance between the center of the left signal peak and the left wing of the stray light peak was found from Matlab plots displaying the FFT of the experimental data. Using this information, the largest allowed a, and thus also σ, for each Ronchi grating frequency was calculated. The resulting set of points was fitted to an exponential function, giving the largest allowed σ as a function of Ronchi grating frequency. This function was expected to mark the line where equation 6 becomes an equality.

Another parameter analysis was performed to analyze the aforementioned expected change in behavior with varying Ronchi grating frequency and Super Gaussian σ. The exponent of the Super Gaussian was set to $k = 20$ for this computation.

As can be seen in Figure 3, the signal- and the stray light peak are not delta functions. This means that a partial overlap is possible close to where equation 6 becomes equality. If a partial overlap occurs only some of the frequencies in the stray light peak are suppressed. This will most likely result in a region where the area ratio between the two spectra has a very large gradient. The goal of this analysis was to identify whether this region exists and, if so, if it coincides with the predicted correlation. The resulting height-map is displayed in Figure 9. The height map is graded from 1 to an area ratio much larger than 1, since the goal of the computation was mainly qualitative. Only Ronchi grating frequencies $f_g \leq 1$ line/mm are displayed, since nothing noteworthy is shown for larger f_g in the limited σ range.

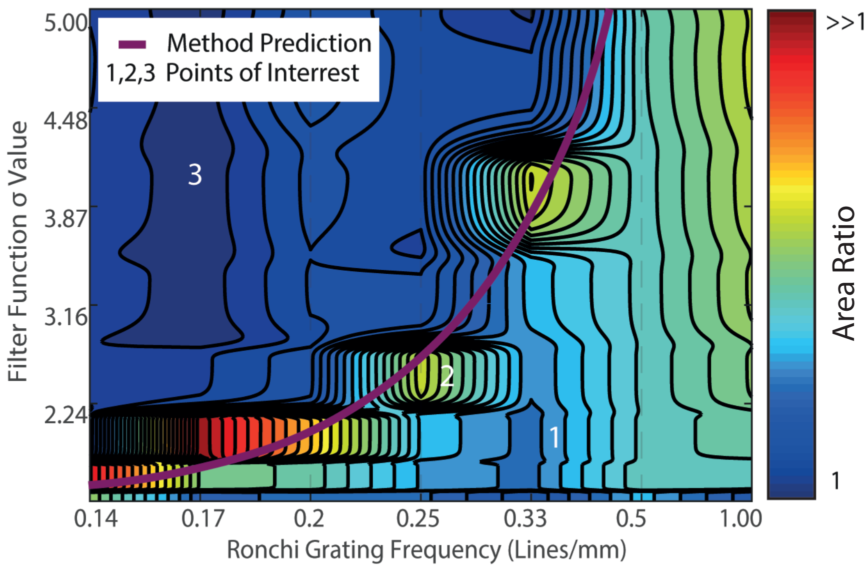

Figure 9: *The height map for different configurations of f_g and σ. (1) marks an area where σ has become low enough to result in no overlap between the Super Gaussian and the stray light peak for lower frequency gratings ($f_g \approx 0.33$). The purple line marked with (2) shows where equation 6 becomes an equality. To the left of the line, equation 6 no longer holds. The line passes near all points with a high gradient in the height map, suggesting that the analysis results coincides with the line of equality obtained through correlation. The area marked with (3) is where the overlap is so large that almost all of the stray light peak is underneath the Super Gaussian, causing very little stray light to be suppressed. When it comes to selecting Ronchi grating frequency f_g and filter function σ the aim is to be well to the right of the purple line in order to achieve stray light suppression.*

The main feature in Figure 9 is the emergence of an overall rather complex map. However, a few regions in it deserves to be explicitly mentioned, namely those marked $1-3$.

The area marked with (1) denotes the area where σ and f_g are such that no overlap occurs and stray light suppression is achieved. The purple line marked with (2) in the figure is the previously discussed correlation marking the predicted location where Equation 6 becomes an equality. It seems to accurately show where the threshold for overlap between the Super Gaussian and the stray light peak is, in accordance with previously discussed observations. As long as the grating frequency, in combination with the selected σ, is well to the right of this line, PS yields good results. This means that the area marked with (1) can be extended all the way to the top-right corner of the figure. The area marked with (3) is a large region where there is little difference between the raw spectrum and the PS spectrum. The overlap is so large that almost all the stray light peak is included underneath the filter function, causing very little stray light to be suppressed.

While equation 6 appears to hold for all cases, the correlation between f_g and a is unique for each measurement set-up and thus a new correlation has to be done if this is to be attempted again.

3.2 Software-to-Hardware Conversion

3.2.1 Basic Conversion

As previously stated, the Ronchi grating can be introduced inside the spectrometer and still modulate the spectrum the periodic pattern utilized in PS. Furthermore, this should create the Fourier transform of the signal passing through the Ronchi grating on the detector screen due to Fraunhofer diffraction. Hopefully, this would allow for the application of a spatial filter onto the detector screen, blocking anything but the signal peak and thus possibly obtaining a stray light suppressed spectrum without the need for software post-processing. The first step is to see whether the predictions about the Ronchi grating and its effects on the spectrum are correct.

The concept was briefly tested in the laboratory set-up by taking the lid off the spectrometer and holding the grating in the beam path. Results can be seen in Figure 10.

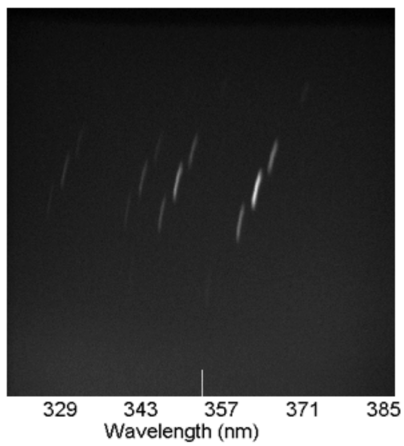

Figure 10: *The detector screen on the spectrometer when a Ronchi grating is introduced into the collimated beam inside the spectrometer. The image displays the hardware Fourier transform of the Cd atomic spectrum with an intense middle stray light peak and one signal peak on each side.*

When detecting at the same frequency bandwidth as earlier, and placing the Ronchi grating in the beam line, the expected shape, the Fourier transform of the modulated spectrum with a intense middle (stray light) peak and one signal peak on each side of it, is detected by the spectrometer. It is concluded that even this preliminary experiment agrees well with theory, the Ronchi grating can be used as a hardware stray light separator. This also agrees with the results of the FRED simulation, displayed in Figure 11.

Most spectrometers today are built to minimize the occupied space thus having beam paths cross each other to a maximum extent. Therefore, it was of interest to analyze whether the result would be affected by the angle of the Ronchi grating, with respect to the incoming light, or if the grating could be angled inside the spectrometer, to not block or affect other beam paths. Two ray-tracing simulations were carried out in a system where x was the horizontal axis in the plane of the grating, y was the vertical axis in the plane of the grating and z was the axis through the grating. The first simulation was made with the grating parallel to the collimated beam and the other with the grating rotated 12^o around the z-axis.

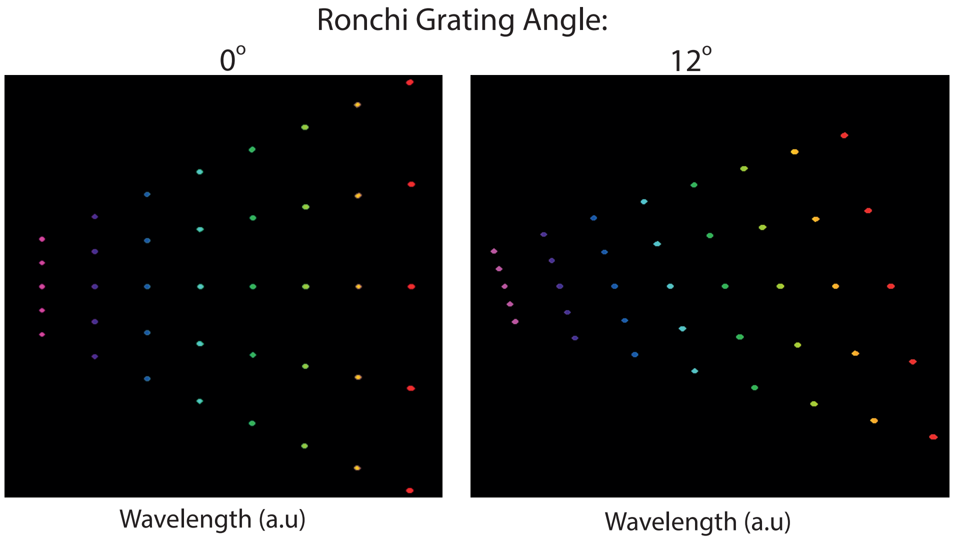

Figure 11: *FRED simulation results of a spectrum from a light source with eight evenly spaced spectral components in a system where x is the horizontal axis in the plane of the grating, y is the vertical axis in the plane of the grating and z is the axis through the grating: (a) - The grating oriented perpendicular to a collimated beam line, (b) - The grating rotated* 12^o *around the z-axis.*

The strong divergence of the positions of the signal peak in the vertical direction in both Figure 11 (a) and (b) is not due to the rotation of the grating, but because of wavelength-dependent diffraction introduced by the Ronchi grating. This is a possible concern when it comes to detection at long wavelengths. Since longer wavelengths have a larger spacing between their diffraction peaks, the risk that the signal peaks are projected outside the detector screen increases. This also means that the Ronchi grating frequency has to be low enough so that the signal peaks are projected onto the detector screen. This is more of a case-specific problem for different spectrometer designs and cannot be estimated generally. It is still important to take this into account however, since the spectrometer would be useless above or below a certain frequency, depending on the orientation of the grating.

Rotation around the z-axis leads to a loss of position, as can be seen in Figure 11 (b). This is most likely not an issue however, since it should be possible to calibrate or alter the experimental setup to take this into account. Another issue would be rotating the grating too much around the z-axis. Since there is a risk of signal peaks being projected outside the detector screen, this would limit the wavelength range of the detector screen further.

4 Conclusions

Three variables, f_g, σ and k, in the software version of PS have been analyzed and the following conclusions have been drawn:

The Ronchi grating frequency f_g should be as large as possible in order to maximize stray light suppression, and no upper limit was found in the course of this project.

The filter function width σ should be small enough to ensure no overlap between the filter function and the stray light peak. To further improve stray light suppression, σ should be as small as possible, in order for the filter function to filter out as many unwanted interfering signal components as possible.

The Super Gaussian exponent k should be sufficiently large, in order for areas of stability to form. In the case of this thesis $k = 20$ was deemed to be sufficiently large with a good margin. There were concerns with picking a too high value of k as this could affect the PS spectra in the form of ripple effects. These ripple effects were however negligible for $k \leq 20$.

f_g and σ can be selected to guarantee no overlap between the filter function and the stray light peak in the Fourier domain. The selection has to consider the correlation between f_g and a. While the correlation is specific in each experimental set-up, it proved to agree well with results from the corresponding parameter analysis.

In the software-to-hardware conversion, no problems was found when introducing the Ronchi grating into the spectrometer and allowing Fraunhofer diffraction to act as a hardware Fourier transform. Furthermore, no problems were found with introducing the Ronchi grating at an angle not perpendicular to the collimated beam line. This is true as long as the Ronchi grating frequency is low enough, and the grating is not angled in such a way, that the Fourier peaks are displayed outside the detector screen.

5 Outlook

Despite the thorough analysis of several important parts of the PS process, no direct flaws have been found that reduce the feasibility of a PS conversion from software to hardware. There still are unanswered questions, however. The wave profile of the Ronchi grating could be altered - could the signal-lowering properties inherent in PS be reduced by using gratings where the blocking areas in the periodic pattern are thinner than the transparent ones without affecting the PS results?

The shape of the filter function should be investigated further, both in order to optimize it for the software technique, but also to prepare for the next step in a software-to-hardware conversion - introducing the hardware filter function. Another interesting point is to investigate ripple effects in the PS spectrum for very large values of k. This ties together with preparing for the introduction of the hardware filter function, since a square pulse filter is one promising option.

Another possible project is writing a script that can be applied to any experimental setup consisting of an optical spectrometer, removing the need for case-specific information, to i) improve the experimental availability of the technique, and ii) to bring PS from a novel concept to an established component in applicable measurements.

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8 Appendix

```
Expo = 20;
DenomMax = 15;
DenomInt = 150;
Denom = linspace(0.001,DenomMax,DenomInt);

for j = 1:DenomInt
        for k = 1:size(ImgArray,3)

                Image = imresize(ImgArray(:,:,k),1);

                [~,Pos] = findpeaks(abs(fft(sum(Image,2))),...
                ...'SORTSTR','descend');

                f = Pos(1);

                [x,y] = size(Image);
                NewImageFFT1 = zeros(x,y);
                NewImageFFT2 = zeros(x,y);
                ImageFFT1 = zeros(x,y);
                ImageFFT2 = zeros(x,y);
                Data1 = zeros(x,y);
                Data2 = zeros(x,y);
                NewImage1 = zeros(x,y);
                NewImage2 = zeros(x,y);

                ImageFFT = abs(fft(Image));

                xCord = linspace(1, x, x);

                %%%***** Creating Filter **********************************

                for i = 1:length(ImageFFT)

                    [peaks,c] = findpeaks(ImageFFT(:,i),...
                    ...'SORTSTR','descend');

                    if c(2)<c(3)
                        d = c(1);
                    else if c(3)<c(2)
                            d = c(1);
                        end
                    end
```

```
                Freq_A = (f-1)/length(xCord);

                Ref1 = sin(2*pi*Freq_A*xCord);
                Ref2 = sin(2*pi*Freq_A*xCord + pi./2);

                Data1(:,i) = Image(:,i).*transpose(Ref1);
                Data2(:,i) = Image(:,i).*transpose(Ref2);

                ImageFFT1(:,i) = (fft(Data1(:,i)));
                ImageFFT2(:,i) = (fft(Data2(:,i)));

                SuperGauss = transpose(exp(-(...
                ...(xCord-1).^2./Denom(j)).^Expo));
                NewImageFFT1(:,i) = ImageFFT1(:,i).*SuperGauss;
                NewImageFFT2(:,i) = ImageFFT2(:,i).*SuperGauss;

                NewImage1(:,i) = abs(ifft(NewImageFFT1(:,i)));
                NewImage2(:,i) = abs(ifft(NewImageFFT2(:,i)));

            end

            PSImage = 2 * sqrt(NewImage1.^2+NewImage2.^2);
            Comp1 = mat2gray(sum(PSImage,1)./max(sum(PSImage,1)));
            Comp2 = mat2gray(sum(Image,1)./max(sum(Image,1)));

            A = sum(Comp1(150:200));
            B = sum(Comp1(350:400));
        C = sum(Comp1(430:480));
        D = sum(Comp1(640:690));

        RefA = sum(Comp2(150:200));
        RefB = sum(Comp2(350:400));
        RefC = sum(Comp2(430:480));
        RefD = sum(Comp2(640:690));

            A_val(k,j) = A./RefA;
            B_val(k,j) = B./RefB;
            C_val(k,j) = C./RefC;
            D_val(k,j) = D./RefD;

            disp(k)
    end
    disp(j)
end
```