Measuring the Yellow Doublet Wavelengths in the Mercury Spectrum

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Abstract—The mercury yellow doublet has been found and measured using a modified Fourier transform interferometer. The wavelengths of the doublet are $5.769 \pm 0.002nm$ and $5.790 \pm 0.004nm$. The interferograms of the mercury green line and the yellow doublet are processed and corrected, which allowed the reconstruction of the yellow peaks through the fast Fourier transform algorithm. The wavelengths are determined through curve fitting using a Gaussian.

I. INTRODUCTION

Fourier transform spectroscopy is a technique for measuring light spectra based on coherence [1]. A mercury discharge lamp is used as the light source in a Fourier transform spectrometer. The beamsplitter splits the light emitted from the mercury lamp to two mirrors (M1 and M2): one stationary and one that is moved by a stepper motor with an unknown pattern of movement. The lights then reflect back from the mirrors and reach the detector. An interference pattern can be observed if the difference in distance, x, between the distance from M1 to the beamsplitter and M2 to the beamsplitter is within coherence length of the light source. The light detector detects the interference pattern which is the Fourier transformation of the wave function of the light source. Reapplying the Fourier transform on the interference pattern will reconstruct the wave function hence giving the spectrum of the light source. By adding an additional beamsplitter, detector and two filters(green and yellow), the systematic errors of the interferometer can be corrected by stretching and shrinking the x-position of each point for the green line, which can be used, together with the cubic spline for the yellow doublet interferogram, to reconstruct the yellow doublet.

II. THEORY

A. Fourier Transform

The Fourier transform converts signals from their current domain to a frequency domain, which can also be reversed. The transform of a time domain signal is given by:

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i2\pi\omega x}dt$$
(1)

It transforms a integrable function $f : \mathbb{R}$. The Fourier transform of a signal that consists of two frequencies will result in a frequency domain which reflects that spectrum of two frequencies. Fig.1 demonstrates the two signals both separately and superposed as an interference pattern. It also shows the Fourier transform of the signal which is what is

expected for the yellow doublet. The discrete Fourier transform computes the Fourier transform of a discrete sequence. The discrete Fourier transform can transform N complex number in sequence $x_n = x_0, x_1, ..., x_{N-1}$ to another sequence $X_k = X_0, X_1, ..., X_{N-1}$ expressed as [2]:

$$X_{k} = \sum_{n=0}^{N-1} x_{n} \cdot e^{-\frac{i2\pi}{N}kn}$$
(2)



Fig. 1. The Fouier transform of a two-frequency signal: the upper time domain plot shows two separate sinusoidal signals and the lower time domain plot shows their superposition; the frequency domain plot shows the Fourier transform of the signal.

In this investigation, the Fast Fourier Transform algorithm form the SciPy library is used as it significantly reduces computation time. The computational complexity of the DFT is $O(n^2)$ while that for the FFT is O(nlog(n)) [3]. The difference in complexity has a great impact for computation time as N is large in this investigation.

B. The Uncertainty Principle

The statistical interpretation for the Fourier transform of wavefunctions convey the uncertainty principle. Let f(t) be a normalized Gaussian wavefunction of the form:

$$f(t) = \frac{1}{\tau \sqrt{2\pi}} e^{-\frac{t^2}{2\tau^2}}, \qquad -\infty < t < \infty$$
(3)

Let \tilde{f} be the Fourier transform of the wavefunction of the form:

$$\tilde{f}(\omega) = \frac{1}{\sqrt{2\pi}} e^{-\frac{\tau^2 \omega^2}{2}} \tag{4}$$

The intensity distribution of f(t) in time domain is given by $|f|^2$, which is also a Gaussian. Similarly the frequency domain has an intensity distribution of $|\tilde{f}|^2$. In the above example the bandwidth for t and ω are inversely related, which gives [4]:

$$\Delta \omega \, \Delta t = 1 \tag{5}$$

The value of 1 is specific to the normalized Gaussian; any wavefunction f(t) will have a $\Delta \omega \Delta t$ product. Therefore, a signal that is narrow in the time domain must have a greater spread in the frequency domain and vice versa.

III. METHOD

A. Experimental Setup

Fig. 2 shows the experimental setup of a modified Fourier transform spectrometer. M1 is a mirror that is fixed in position whereas M2 is connected to a lever which is connected to a stepper motor [5]. By entering different commands in the terminal, M2 will be able to move for different distances at different velocities. The yellow filter is a Thorlabs FB580-10 Bandpass Filter with a central wavelength (CWL) of $580 \pm$ 2nm and a full width at half maximum (FWHM) of $10\pm 2nm$. The green filter is a Thorlabs FL543.5 laser line filter with a CWL of $543.5 \pm 2nm$ and a FWHM of $10 \pm 2nm$ [6]. A Fourier transform spectrometer is chosen due to the Fellgett advantages. Unlike conventional grating spectrometers, each scan performed by a Fourier transform spectrometer receives information of the entire source spectrum. Moreover, its ability perform microsampling and to obtain a high signal-to-noise ratio makes it a suitable instrument for this investigation [1].



Fig. 2. Modified Fourier transform spectrometer, the red arrows indicate light paths

B. Data-taking

Before executing a command in the terminal, it is necessary to ensure that a interference pattern can be observed by intercepting the light between the two beamsplitters with a piece of paper, and the position of M2 should be approximately at the null point. This must be done using the blue LED first and then switching to a white LED when an interference pattern is observed using the blue LED. The blue LED has a longer coherence length as the bandwidth of it is significantly smaller than that of the white LED. Hence the interference pattern, which is its Fourier transformation, will have a larger coherence length than that of a white LED. The range of the scan is then determined and M2 will be moved to the starting position to start the scan. The rate of data collection can be chosen from the terminal; a sampling rate of 500 Hz is chosen for this Investigation.

C. Correcting the Spectrum

Knowing that the wavelength for the green line in the mercury spectrum is 546nm, the distance between zero crossing points in the interferogram for the mercury spectrum with a green filter could be stretched and shrank. The distance between two zero crossings remains 273nm throughout the entire spectrum, this width corresponds to half of the green line wavelength. The new positions for the corrected x coordinates are expressed by:

$$x_{corr} = L_{corr} + \frac{\lambda_{true}}{\lambda_{measured}} (x_{uncorr} - L)$$
(6)

Where x_{corr} is the corrected x coordinate, L_{corr} is the corrected x coordinate of the previous point, λ_{true} and $\lambda_{measured}$ are the true and measured wavelengths for the mercury green line, x_{uncorr} is the current uncorrected x coordinate and L is the previous uncorrected x coordinate. Although the data was collected at 500 Hz, an average needs to be taken every 10 points as the mercury discharge lamp is running on A alternative current. Taking a binned average can reduce the noise measured by the detectors. Since the interferograms were taken at discrete intervals, the exact values of the zero crossings for the mercury green line are not given in the data. Instead, linear interpolation is used to approximate the position of the zero crossings by locating the two points near the zero crossing and taking their mid point. After correction, the distance between the largest and smallest x coordinates are split into n arbitrarily large (10^7) discrete segments. The resampled x coordinates and the y coordinates for the mercury yellow doublet are then input into the Cubic Spline data interpolator in SciPy. Given a set of n+1 data points (x_i, y_i) where x_i is monotonically increasing, the spline function S(x)is a polynomial of degree 3 on each sub interval $[x_{i-1}, x_i]$ and $S(x_i) = y_i$ for all i = 1, 2, ..., n [7]. The Cubic Spline is used to re-sample the corrected interferogram for the yellow doublet with more equidistant points for the Fast Fourier transformation, which gives the re-constructed spectrum of the mercury yellow doublet.

IV. RESULTS AND ANALYSIS

A. Position Correction

The M2 mirror moved for approximately $7 \times 10^{-4}m$ during the scan, with the null point centered at the midpoint. Fig. 3 shows the interferograms of the mercury yellow doublet and green line. Both interferograms show a long coherence length as expected according to Fourier theory. The intensity for the interferogram of green line is higher than that of the yellow doublet, which means the intensity of the green line is higher than the intensity of the yellow doublet in the mercury spectrum. After correcting the 'x' coordinates for the green line interferogram using Eqn. 6 with the reference wavelength of 546nm, the yellow doublet spectrum is also corrected as



Fig. 3. The interferograms of intensity in arbitrary unit against M2 displacement in meters for mercury yellow doublet (above) and mercury green line (below).

they share the same x coordinates. Fig. 4 shows the enlarged vellow doublet interferogram before and after correction, as well as the change in the x coordinate at each point. Before correction, the mean distance between two zero crossings, which is half a wavelength, is 274.01nm and the value after correction is 272.96nm. The uncertainty of the stepper motor movement can therefore be estimated from the the difference in the two values. However, the uncertainty is eliminated by using the known wavelength of the mercury green line which corrects the entire interferogram. It can be observed on the plots that the curves are not completely smooth. This could be caused by dusts floating in the air of the shaking of the workbench, as multiple groups share the same one. Fig. 5 shows the correction for x against M2 displacement. The reason for the observed correction pattern is unclear but it is very likely to be caused by asymmetrical rotation of the motor as the stepper motor's error in motion is sinusoidal of a wavelength of approximately 0.0002m. However, the magnitude of the correction tends to be larger in the negative direction which is evidence for another systematic error. Further investigation could be done on the effects induced by the uncertainty of the stepper motor motion on the wavelengths of the yellow doublet obtained. Beyond the stepper motor, the detectors will also have uncertainties, but since they are 3-d printed there is no specific specification for their uncertainties and the uncertainties were not measured in the interest of time as it has no effect on determining the yellow doublet wavelengths. The error of the interferometer will not be discussed beyond this point as the x coordinates have been corrected.

B. Finding the Yellow Doublet

Fig. 6 shows a zoomed-in part of the FFT of the mercury yellow doublet after Fourier transform at 575 - 581nmwavelength. Each diamond points on the plot represents a coordinate. although two peaks can be observed in the region corresponding to the yellow wavelengths that are approximately 2nm away from each other, the resolution of the plot is low therefore a curve fitting algorithm needs to be used to determine the peak as well as the uncertainty. The $curve_fit$



Fig. 4. Above: The intensity in arbitrary unit against M2 displacement in meters for mercury yellow doublet before correcting the x coordinates. Below: The intensity in arbitrary unit against M2 displacement in meters for mercury yellow doublet after correcting the x coordinates (solid line) and the position correction for x in nanometers against M2 displacement in meters(dotted line).



Fig. 5. The correction for x in nanometers against M2 displacement in meters throughout the entire scan.



Fig. 6. The scaled fast Fourier transform of the corrected spectrum for the yellow doublet and the Gaussian fit of the two peaks.

function from the SciPy library is imported and used to fit the coordinates. A Gaussian function is used to approximate the peaks and is defined as:

$$f(x) = ae^{-\frac{(x-\mu)^2}{2\sigma^2}}$$
(7)

Where a is the height of the peak, μ is the center of the peak, and σ is the standard deviation. Table 1 shows the four coordinates used to fit the Gaussian shown in Eqn. 7, table 2 shows the curve fitting constants for both peak 1 and peak 2, and table 3 shows the covariance matrices of the Gaussian curve fit constants. The wavelength for the first peak of the yellow doublet is $5.769 \pm 0.002nm$ and the wavelength for the second peak is $5.790 \pm 0.004nm$. The curve fitting function gives the uncertainties for for both μ and σ through covariance matrices. For the 577nm peak the uncertainties for μ and σ are 5.722×10^{-21} and 3.032×10^{-21} while for the 579nm peak the uncertainties are 1.687×10^{-23} and 2.037×10^{-23} respectively. These uncertainties are really small compared to the value of μ and σ for both peaks, hence they have no significant effect on their values.

TABLE I COORDINATES FOR GAUSSIAN FIT

	Coordinates		
Peak	x	y	
1	$5.761123208408274 \times 10^{-7}$	1185554474.416151	
1	$5.765494318581571 \times 10^{-7}$	2494953092.3225217	
1	$5.769872066735392 \times 10^{-7}$	8459981371.704788	
1	$5.774256468001908 \times 10^{-7}$	639985766.5091902	
2	$5.783045290632048 \times 10^{-7}$	1267325099.8399014	
2	$5.787449742490869 \times 10^{-7}$	6158429728.143193	
2	$5.791860908453134 \times 10^{-7}$	7227677970.128546	
2	$5.796278803882923 \times 10^{-7}$	1856480870.8734212	

TABLE II GAUSSIAN CURVE FIT CONSTANTS

Peak	a	μ	σ
1	8.95678×10^9	$5.76910 imes 10^{-7}$	2.26475×10^{-10}
2	8.09908×10^9	$5.79010 imes 10^{-7}$	3.62100×10^{-10}

V. CONCLUSION

The measurement of the mercury yellow doublet is obtained through the use of a modified Fourier transform spectrometer with a mercury discharge lamp as the light source. the xcoordinates in the green interferogram is then fitted against the standard mercury green line spectrum of 546nm which also corrects the yellow doublet interferogram. Next, the corrected yellow doublet interferogram is re-sampled using the cubic spline interpolator to increase the number of samples which are also equidistant in x. The fast Fourier transform is then performed on the interferogram, which gives the two peaks corresponding to the yellow doublet after scaling. By fitting a Gaussian curve on the two peaks, the wavelengths of the yellow doublet can be obtained which are $5.769 \pm 0.002nm$ and $5.790 \pm 0.004nm$. This concludes the existence of the mercury yellow doublet as well as their values. Further investigation to improve the results could be done by investigating the error induced through linear interpolation in estimating the crossing points and investigating the error induced through the motion of the stepper motor.

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