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In-situ determination of astro-comb calibrator lines to better than 10 cm s$^{-1}$

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Abstract: High precision wavelength calibrators for high-resolution astrophysical spectrographs will be key components of new precision radial velocity (RV) observations including the search for Earth-like exoplanets and direct observation of cosmological deceleration. The astro-comb, a novel high-precision calibrator, is a combination of an octave-spanning femtosecond laser frequency comb and a Fabry-Pérot cavity used to achieve calibrator line spacings that can be resolved by an astrophysical spectrograph. Systematic spectral shifts associated with the cavity can be 0.1-1 MHz, corresponding to RV errors of 10-100 cm/s, due to the dispersive properties of the cavity mirrors over broad spectral widths. Although these systematic shifts are very stable, their correction is crucial to high accuracy astrophysical spectroscopy. Here, we demonstrate an in-situ technique to determine the systematic shifts of astro-comb lines due to finite Fabry-Pérot cavity dispersion. The technique employed practically at a telescope-based spectrograph to enable wavelength calibration accuracy better than 10 cm/s.

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References and links
1. Introduction

High precision wavelength calibrators for astrophysical spectrographs will be key components of new precision radial velocity (RV) observations, including the search for Earth-like extrasolar planets (exoplanets) [1] and direct observation of cosmological deceleration [2, 3]. Recent work has demonstrated the potential of octave-spanning femtosecond lasers frequency comb [4] to serve as wavelength calibrators for astrophysical spectrographs (“astro-combs”) providing RV sensitivity down to 1 cm/s [5, 6]. Exoplanet searches place stringent demands upon such calibrators. For example, the RV induced on a Sun-like star due to a planet like the Earth in an orbit within the habitable zone is about 10 cm/s. The current state of the art astrophysical spectrograph, HARPS, has demonstrated stellar RV sensitivity \(\approx 60\) cm/s [1], largely limited by its thorium argon lamp calibrator [7, 8]. An astro-comb provides emission lines with uniform intensity and spacing, which can be referenced to atomic frequency standards and the global positioning system (GPS), yielding excellent long-term stability and reproducibility.

To date, astro-combs consist of a combination of an octave-spanning femtosecond laser frequency comb (source comb) and a Fabry-Pérot cavity (FPC), see Fig. 1. Spectral lines generated by the source comb are spaced by the pulse repetition rate \(f_r\), currently \(\approx 1\) GHz, which is too dense to be resolved by broadband astrophysical spectrographs [5]. The FPC serves as a mode filter with a free spectral range (FSR) set to an integer multiple of the repetition rate, \(\text{FSR} = M f_r\), with \(M \approx 10 – 100\), depending on the spectrograph resolution. Ideally, the FPC passes only every \(M^{th}\) source comb spectral line, providing thousands of calibration lines well matched to practical spectrograph’s resolution, with fractional frequency uncertainty limited only by the stability of the RF reference used to stabilize the source comb and FPC. This frequency can be \(< 10^{-11}\) using commonly available atomic clock technology which corresponds to \(\sim 3\) kHz uncertainty in the optical frequency or 0.3 cm/s in RV precision. However, because the spectrograph fails to resolve neighboring source comb lines, finite suppression of these neighboring lines by the FPC affects the lineshape and potentially the centroid of measured astro-comb lines. For example, in the results presented here, source comb modes neighboring the astro-comb line, with intensities after passing through the FPC that differ by 0.1% of the main astro-comb peak, shift the measured line centroid by 1 MHz, which corresponds to an RV systematic error of 1 m/s. In practice, such systematic RV shifts are inevitable over spectral bandwidths of 1,000 Å due to the dispersive properties of the FPC. Although these systematic shifts can be very stable over timescales of years, the correction of such shifts is crucial to high accuracy astrophysical spectroscopy.

In this paper, we demonstrate an in-situ technique to determine the systematic shifts of astro-comb lines due to FPC dispersion, which can be applied practically at a telescope-based spectrograph to enable wavelength calibration accuracy better than 10 cm/s. By measuring the intensity of astro-comb lines as the FPC length is adjusted, we determine (i) the offset of each FPC resonance from the nearest source comb line; (ii) FPC finesse as a function of wavelength; and
(iii) the intensity of individual source comb lines. These parameters can be determined quickly and reliably over the full 1,000 Å bandwidth of the astro-comb with only \( \approx 20 \) measurements at slightly different FPC lengths and can be performed quickly and reliably. The measurement has also been performed with a lower resolution commercial optical spectrum analyzer with consistent results. The astro-comb line characterization technique presented here builds on past work in which femtosecond lasers coupled to swept cavities were used to study both the medium in which the cavity was immersed and the cavity mirrors [9, 10].

2. Model

Imperfect suppression of unwanted source comb lines, e.g., due to finite FPC finesse, affects the astro-comb lineshape observed on a spectrograph. The lineshape can be modeled with knowledge of the FPC properties including mirror reflectivity and round trip phase delay. The intensity of a source comb line after the FPC is

\[
I'_m = I_m \frac{T_m}{1 + (2F_m/\pi)^2 \sin^2(\phi_m/2)}, \tag{1}
\]

where \( I_m \) is the intensity of the source comb line of optical frequency \( f_m \); \( T_m \) is the resonant transmission of the FPC at optical frequency \( f_m \); \( F_m \) is the finesse of the FPC near frequency \( f_m \); and \( \phi_m \) is the round trip phase delay. The phase delay may be expressed as [11]

\[
\phi_m = 2\pi \left( \frac{2L}{c} f_m n_m + \int_{0}^{f_m} \tau(f) \, df \right), \tag{2}
\]

where \( L \) is the length of the cavity, \( c \) is the speed of light in vacuum, \( n_m \) is the refractive index of the medium inside the cavity (air, vacuum, etc.) at optical frequency \( f_m \), and \( \tau(f) \) is the frequency-dependent group delay of the mirrors. The first term in parentheses in Eq. (2) is the distance between the mirrors expressed in wavelengths; while the second term, the integral of \( \tau(f) \), is the phase delay of the mirrors and represents the frequency-dependent penetration distance of light into the mirror. Maximum transmission occurs when a source comb line is resonant with the FPC, or equivalently \( \phi = 2\pi q \), with \( q \) an integer. The FSR, \( \Delta \), is the frequency difference between two consecutive FPC resonant frequencies. Assuming that \( \tau \) varies slowly with frequency, the FSR can be approximated by

\[
\Delta_m \approx \left[ \frac{2L}{c} \left( n_m + f_m \frac{dn_m}{df} \right) + \tau_m \right]^{-1}. \tag{3}
\]
For our typical astro-comb settings, $\Delta_m \approx 31$ GHz, $F_m \approx 180$ and source comb lines nearest the astro-comb peak are suppressed by $\approx 22$ dB. This imperfect suppression leads to systematic inaccuracies in astro-comb line centers at the 50 cm/s level, as observed on a high resolution astrophysical spectrograph across a 1,000 Å bandwidth (see Fig. 2). The effects of these systematic shifts can be characterized by determining the FPC finesse ($F_m$) and the frequency difference between astro-comb lines and the FPC resonance over the full spectral width. Compensation can then be applied to determine wavelength solutions (conversions from spectrograph pixel number to wavelength) with accuracy better than 50 cm/s.

We determine $F_m$ and the frequency offset of the FPC resonance from the astro-comb lines by adjusting the length of the FPC and measuring the intensities of astro-comb lines over the full spectral bandwidth. When we change the frequency of one FPC resonance from $f_d$ to $f_d + \delta f$ the cavity length changes by

$$\delta L \approx - \frac{c}{2n_d f_d} \left[ \tau_d + \frac{2L}{c} \left( n_d + f_d \frac{dn}{df} \bigg|_{f_d} \right) \right] \delta f,$$

where $\Delta_d$ and $\tau_d$ are the FSR of the FPC and the phase delay of the mirrors, respectively, at the frequency of the controlled resonance. The change of the cavity length leads to a change of the

$$\delta L \approx - \frac{c}{2n_d f_d \Delta_d} \delta f,$$
Fig. 3. Source comb spectrum as measured with a commercial optical spectrum analyzer. The source comb consists of \( \sim 10^5 \) narrow lines (width < 1 MHz), equally spaced in frequency (\( \approx 1 \) GHz, not resolved here), and spanning more than an octave between 6,000 Å and 12,000 Å.

The round trip phase delay of an astro-comb line \( f_m \) by

\[
\delta \phi_m = \frac{4\pi n_m f_m}{c} \delta L \approx -2\pi \frac{n_m f_m}{n_d f_d \Delta d} \delta f.
\]

As a result, the intensity of the astro-comb line varies with the change of the frequency of one FPC mode according to Eq. (1), from which we can derive the finesse and the phase errors at all astro-comb line frequencies.

3. Experiment

The astro-comb is shown schematically in Fig. 1. The octave-spanning source comb spectrum (Fig. 3) is generated by a mode-locked titanium-sapphire femtosecond laser (Octavius, Menlosystems Inc. with repetition rate \( f_r \approx 1 \) GHz). The absolute frequencies of the comb lines can be expressed as \( f_m = f_0 + m f_r \), where \( m \) is an integer and \( f_0 \) is the carrier-envelope offset frequency. A pin diode detects \( f_r \), which is then stabilized by adjusting the laser cavity length. The \( f-2f \) self-referencing method is used to produce a signal at \( f_0 \) on an avalanche photodiode: comb lines around 11,400 Å are frequency doubled in a 1 mm thick LBO crystal and beat with comb lines around 5,700 Å. \( f_0 \) is then stabilized by intensity modulation of the 7.6 W, 5,320 Å pump laser. Both \( f_r \) and \( f_0 \) are referenced to low-noise radio-frequency synthesizers, which are stabilized to a commercial rubidium frequency reference. For our source comb, typical values of these frequencies are: \( f_r = 1.042048458 \) GHz and \( f_0 = 0.09 \) GHz, and the resulting comb linewidth is < 1 MHz.

The source comb beam passes through the FPC, filtering out unwanted comb lines and increasing the transmitted line spacing. Two flat mirrors with \( \approx 98.5\% \) reflectivity and minimal group delay dispersion (< 10 fs\(^2\) from 7,500 Å to 9,000 Å) comprise the FPC. Due to the low dispersion mirrors, the FSR of the FPC is almost constant: within the 1,000 Å bandwidth, typically one in thirty comb lines is resonant with the FPC (Fig. 2a). The measured finesse of the FPC is \( \approx 180 \), which is consistent with the theoretical limit estimated from the mirror reflectivity.

We stabilize the FPC by locking one transmission resonance to an injected diode laser. The diode laser is modulated at 30 MHz with an EOM and injected into the FPC with a polarization orthogonal to the comb light. After the FPC, the diode beam is separated from the comb, demodulated, and used to derive a feedback signal that stabilizes the FPC to the diode laser.
diode laser itself is offset-locked to one of the source comb lines at a wavelength $\approx 7,950 \text{ Å}$. This wavelength is close to the Rb D1 transition. Absorption spectroscopy of the diode laser light using a thermal rubidium vapor cell thus identifies the diode frequency to within one source comb line. The offset lock then determines the absolute frequency of the diode laser with the accuracy of the underlying atomic frequency reference.

In its current incarnation as a wavelength calibrator for an astrophysical spectrograph, the astro-comb spectrum is analyzed by the Tillinghast Reflector Echelle Spectrograph (TRES), a fiber-fed multi-order echelle spectrograph at the 1.5 m telescope of the Whipple Observatory. Spectral dispersion is provided by an echelle grating with cross-dispersion from a prism operated in double-pass mode. TRES covers a spectral bandwidth from 3,700 Å to 9,100 Å with a resolving power of $R = \lambda / \delta \lambda \approx 50,000$ [12] corresponding to a resolution of $\approx 7 \text{ GHz}$ at 8,000 Å. The astro-comb is injected into an integrating sphere and then sent to TRES on a 100-µm multimode fiber. The integrating sphere reduces lineshape fluctuations due to fiber alignment, which is essential for high accuracy astrophysical spectroscopy but is not crucial to the work described in this paper. Each astro-comb spectral measurement by TRES is typically integrated for 60 s and recorded on a cooled (100 K) two dimensional CCD (see Fig. 2b). The separation of the FPC mirrors is set such that astro-comb lines are separated by $\approx 4$ resolution elements of the spectrograph.

We also characterized the astro-comb spectrum with a commercial optical spectrum analyzer (ANDO AQ6315), which has much lower resolution ($\approx 300 \text{ GHz}$) when operated in broadband (1,000 Å) mode. There are then $\approx 10$ astro-comb lines in one resolution element. We find that all parameters measured with the commercial analyzer are consistent with those measured with TRES.

4. Results and Analysis

We find good agreement between TRES measurements of the astro-comb spectrum the model presented above. For example, Figure 4 shows the measured variation of the peak intensity of one astro-comb line vs diode laser frequency (and thus cavity length) and a fit of Eq. 1 to the data. From the fit, we derive the astro-comb resonant intensity $I_m$; the FPC finesse $F_m$; and the phase deviation $\delta \phi_m$. The phase deviation is the offset of the round trip phase from an integer multiple of $2\pi$ at an astro-comb line, and is determined from the detuning of the astro-comb peak at frequency $f_m$ from center of the FPC resonance at nominal diode laser setting $f_{\text{FPC}}$. The phase deviation is then given by

$$\delta \phi = 2\pi \frac{f_{\text{FPC}} - f_m}{\Delta \phi},$$

(7)

where $\Delta \phi$ is the free spectral range near frequency $f_m$. The finesse, $F$, of the FPC can be derived from the fit as

$$F = \frac{2\pi}{\Delta \phi_{\text{FWHM}}},$$

(8)

where $\Delta \phi_{\text{FWHM}}$ is the full width at half maximum in phase of an FPC resonance. The uncertainties in measured FPC resonance centers and widths are approximately 1 MHz, corresponding to phase uncertainties of 0.2 mrad. The variation of these parameters as a function of wavelength provides the information needed to characterize the astro-comb spectrum as a wavelength calibrator.

Finesse and phase deviation are found to vary slowly across the entire astro-comb spectrum. The FPC finesse is approximately 180 (Fig. 5a) and the phase deviation of the FPC relative to astro-comb lines is $< 2\pi \times 10^{-3}$ (Fig. 5b). Reflections from the back surfaces of the FPC mirrors used in these measurements produce the small, rapid phase variations observed in the fig-
Fig. 4. Measurements using the TRES spectrograph of the peak intensity of one astro-comb spectral line as the diode laser frequency, and thus the Fabry-Perot cavity length, is varied (solid circles) and a fit of Eq. 1 to the data (solid line). Uncertainties in the linewidth and in the offset of the peak from zero diode detuning are approximately 1 MHz.

Fig. 5. (a) TRES measurements of the finesse of the Fabry-Pérot cavity and (b) phase variation of the astro-comb lines in the range of 7,700 Å - 8,700 Å. The small, rapid phase variation in (b) is due to 0.1% reflections from the back surfaces of the cavity’s antireflection coated mirror substrates (see text).

ure. Despite antireflection-coatings the mirror substrates reflected 0.1% of the incident power. A simple model with realistic parameters reproduces the observed phase variations and allows systematic effects associated with these reflections to be eliminated. In future work, slight wedging of the substrates will eliminate these variations. After fitting the phase deviation with a sixth order polynomial, we compared our result with the phase deviation derived from a model of air dispersion [13] and the mirror phase delay measured with a white light interferometer (Fig. 6). The two different methods agree well, but the TRES measurement has much lower noise.

Using these in-situ measurements of the FPC finesse and the phase deviation, along with the source comb intensity variation and resonant FPC transmission, we can determine the suppression of unwanted source comb lines and the resultant frequency shifts of astro-comb line centers. The variation with optical frequency of source comb line intensity and resonant FPC transmission ($t_m \cdot I_m$ in Eq. 1) is measured by offseting the diode laser frequency from its nominal value by the source comb repetition rate, and thereby tuning the FPC to resonance with a neighboring (and normally suppressed) source comb mode. The maximal transmission of each
transmitted source comb line and thus $t_m \cdot I_m$ is measured; and then the procedure is repeated for all normally suppressed source comb modes. We find that the variation of $t_m \cdot I_m$ is within our measurement uncertainties ($< 1\%$). Evaluating Eq. 1 for a single astro-comb line and all of its neighboring (suppressed) source comb lines within one spectrograph resolution element, and determining the net transmitted spectrum weighted by the frequency offset from the central astro-comb frequency, allows us to evaluate the effective line center shift in the astro-comb spectrum. For moderate finesse and $f_r >> \Delta m/F$, the systematic shift $\delta f_m$ of an astro-comb line of frequency $f_m$, as measured on a spectrograph, can be approximated as

$$\delta f_m \approx f_r \left( \frac{\Delta m}{2F} \right)^2 \left[ \frac{t_{m+1}I_{m+1} - t_{m-1}I_{m-1}}{t_mI_m} - 2 \frac{\delta \phi_m \Delta m}{\pi f_r} \right]$$

where the term in parentheses parameterizes the mean suppression of nearest source comb side modes, the first term in square brackets results from the difference in source comb intensity between the upper and lower side modes, and the second term in square brackets results from FPC phase deviation leading to asymmetry of the comb lines relative to the FPC mode. The frequency shift in an astro-comb line centroid due to variations of neighboring source comb line intensities at the 1% level is thus $\approx 70$ kHz or 7 cm/s. Note that we do not expect neighboring source comb lines to differ as much as 1% level; also a Gaussian distribution of comb-line intensities will average away much of this astro-comb centroid frequency shift. Nonetheless, we expect that moderately higher FPC finesse ($F \approx 500$) or more precise measurements of line to line intensity variations will be required to assure 1 cm/s accuracy. In Fig. 7, we show the shift of the estimated systematic error in the wavelength calibration of TRES as a function of wavelength, when using the astro-comb as the calibration reference, if the effect of nearest suppressed source-comb lines are not included in the fit model. With proper inclusion of such effects, residual uncertainty in the wavelength calibration is at the 1 cm/s level. In general while astro-comb line frequency shifts caused by mirror dispersion and resultant wavelength dependence of FPC finesse and phase deviation can be absorbed into the wavelength calibration if reproducibility is all that is desired, at the few cm/s level these corrections must be applied to the spectrograph calibration to achieve accurate stellar radial velocity measurements.

Fig. 6. TRES measurement of the cavity phase deviation as described in the text (solid curve) compared to a model derived from air dispersion and mirror phase delay as measured with a white light interferometer (dashed curve). The constant and linear phase variation which depend upon the absolute cavity position and length are removed from both curves for clarity.
5. Conclusion

In summary, we have demonstrated an *in-situ* method to determine systematic shifts of astro-comb spectral lines due to imperfect suppression of source comb lines by the Fabry-Perot filter cavity (FPC). This method involves measurement of FPC finesse as well as the phase deviation of all astro-comb lines over a bandwidth of 1,000 Å. Such measurements can be performed *in-situ* at a telescope with either an astrophysical spectrograph or a commercial optical spectrum analyzer of lower resolution. From the measured phase deviation, the dispersion of the FPC is derived and found to be consistent with that calculated from the intra-cavity air dispersion and the group delay dispersion of the FPC mirrors. Applying resultant corrections for shifts in the centroid of astro-comb spectral lines allows us to model the astro-comb spectrum as measured on an astrophysical spectrograph with accuracy to better than 0.1 MHz, i.e., 10 cm/s for measurement of a stellar radial velocity. Such high accuracy is important to many applications of astro-comb wavelength calibrators, such as the search for habitable exoplanets, direct measurement of the expansion of the universe, and searches for a temporal variation of physical constants.