Impact of instrumental systematic errors on fine-structure constant measurements with quasar spectra

Jonathan B. Whitmore* and Michael T. Murphy
Centre for Astrophysics and Supercomputing, Swinburne University of Technology, Hawthorn, VIC 3122, Australia

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ABSTRACT
We present a new ‘supercalibration’ technique for measuring systematic distortions in the wavelength scales of high-resolution spectrographs. By comparing spectra of ‘solar twin’ stars or asteroids with a reference laboratory solar spectrum, distortions in the standard thorium–argon calibration can be tracked with $\sim 10 \text{ m s}^{-1}$ precision over the entire optical wavelength range on scales of both echelle orders ($\sim 50–100 \text{ Å}$) and entire spectrographs arms ($\sim 1000–3000 \text{ Å}$). Using archival spectra from the past 20 yr, we have probed the supercalibration history of the Very Large Telescope-Ultraviolet and Visible Echelle Spectrograph (VLT-UVES) and Keck-High Resolution Echelle Spectrograph (HIRES) spectrographs. We find that systematic errors in their wavelength scales are ubiquitous and substantial, with long-range distortions varying between typically $\pm 200 \text{ m s}^{-1}$ per 1000 Å. We apply a simple model of these distortions to simulated spectra that characterize the large UVES and HIRES quasar samples which previously indicated possible evidence for cosmological variations in the fine-structure constant, $\alpha$. The spurious deviations in $\alpha$ produced by the model closely match important aspects of the VLT-UVES quasar results at all redshifts and partially explain the HIRES results, though not self-consistently at all redshifts. That is, the apparent ubiquity, size and general characteristics of the distortions are capable of significantly weakening the evidence for variations in $\alpha$ from quasar absorption lines.

Key words: atomic data – line: profiles – methods: data analysis – techniques: spectroscopic – quasars: absorption lines.

1 INTRODUCTION
The Standard Model of particle physics requires a number of fundamental physical constants as inputs. These constants are defined by dimensionless ratios of physical quantities, e.g. the charge of the electron, or the speed of light, but, as dimensionless ratios, they have the same value for any choice of physical units. No physical theory predicts their values, so we must derive their values from measurements. The fine-structure constant, $\alpha \equiv e^2/\hbar c$, is the coupling constant that sets the scale of electromagnetic interactions, and its possible variation will be the focus of this paper:

$$\Delta \alpha/\alpha \equiv \frac{\alpha_z - \alpha_0}{\alpha_0},$$

with the value of $\alpha$ at some redshift $z$ denoted as $\alpha_z$ and the current laboratory value as $\alpha_0$.

Experimental and observational limits have been placed on $\Delta \alpha/\alpha$ over a range of precisions and time-scales, with Uzan (2011) reviewing the various methods and constraints. These generally range from a very tight constraint over several years in laboratories, e.g. a few parts per $10^{17}$ (e.g. Rosenband et al. 2008), to somewhat looser constraints at cosmological scales, e.g. a few per cent with the cosmic microwave background (e.g. Menegoni et al. 2012). However, measurements of $\Delta \alpha/\alpha$ in absorption systems found within quasar spectra probe values of $\alpha$ over cosmological time and distance with a typical precision of several parts per million (ppm). The interest in the possibility of the variation of two fundamental constants ($\alpha$ and $\mu$) has intensified over the past 15 yr since the emergence of some evidence for a cosmological variation of $\alpha$ from quasar studies. This evidence came with the increased sensitivity to $\alpha$ variation enabled by the ‘Many-Multiplet’ (MM) method (Dzuba, Flambaum & Webb 1999; Webb et al. 1999): the comparison of many different metal ion transitions whose frequencies have widely differing dependence on $\alpha$. Absorption systems that lie along the line of sight to a quasar imprint a number of narrow metal absorption lines on to its spectrum, and $\Delta \alpha/\alpha$ is measured by comparing the relative wavelength spacing of these features.

The MM method was first applied to a sample of 30 quasar absorption systems with the Keck-High Resolution Echelle Spectrograph (HIRES) in Webb et al. (1999). In the years since, the MM method has been applied to several other individual
absorption systems (e.g. Quast, Reimers & Levshakov 2004; Levshakov et al. 2007; Molaro et al. 2008a, 2013a). However, the most statistically significant results have come from two large samples: a substantially increased Keck-HIRES sample and a more recent sample measured with the Very Large Telescope–Ultraviolet and Visible Echelle Spectrograph (VLT-UVES) spectrograph. HIRES and UVES are high-resolution ($R \approx 50,000$–80 000) echelle spectrographs on 8-to-10-m class telescopes: Keck (Hawaii) and VLT (Chile), respectively. The final Keck sample combined $\Delta \alpha/\alpha$ measurements from 140 absorption systems, along 78 lines of sight, to yield a statistically significant non-zero weighted average of $\Delta \alpha/\alpha = -5.7 \pm 1.1$ ppm (Murphy, Webb & Flambaum 2003; Murphy et al. 2004). King et al. (2012) later analysed 154 systems with the VLT and found a statistically significant positive average value. However, by combining the VLT sample with the Keck sample, Webb et al. (2011) and King et al. (2012) found evidence for a spatial dipole in the value of $\alpha$ across the sky. These surprising results demand detailed investigations into possible systematic effects in high-resolution spectrographs that might mimic this possible evidence for a varying $\alpha$ (e.g. Murphy et al. 2001b; Murphy, Webb & Flambaum 2003; Molaro et al. 2008b, 2013a; Griest et al. 2009; Whitmore, Murphy & Griest 2010; King et al. 2012; Evans & Murphy 2013; Rahmani et al. 2013; Evans et al. 2014). We continue that effort here.

Any significant distortion of the wavelength scale, especially over long wavelength ranges ($\gtrsim 1000 \text{Å}$), could have a serious impact on the accuracy of $\Delta \alpha/\alpha$ measurements from quasar absorption spectra. The predicted relative wavelength shifts for $\Delta \alpha/\alpha \sim \sim 1$ ppm correspond to 1/10th of a pixel wavelength accuracy across the wavelength range of the spectrograph. Thus, having an accurate wavelength scale is extremely important. The standard method used to calibrate the wavelength scale of quasar exposures on high-resolution spectrographs is by comparison with a separate ThAr arc lamp exposure. The sharp ThAr emission lines have known wavelengths, and the positions at which they fall on the CCD are used to create a wavelength solution for the separate quasar exposure.

There have been a number of tests of the wavelength solution provided by ThAr spectra, especially with regards to fine-structure constant work, including Valenti, Butler & Marcy (1995), Murphy et al. (2001b), Molaro et al. (2008b), Griest et al. (2009), Whitmore et al. (2010), Wilken et al. (2010), Wendt & Molaro (2012), Rahmani et al. (2013) and Bagdonaite et al. (2014). These studies uncovered and quantified new systematic errors, such as a varying instrument profile (IP), intraorder wavelength-scale distortions, CCD pixel-size irregularities and, more recently, long-range wavelength-scale distortions: in their study of possible variations in $\mu$, Rahmani et al. (2013) cross-correlated asteroid spectra, observed with VLT-UVES, with laboratory solar spectra and found differential velocity shifts between them of up to 400 m s$^{-1}$ over $\sim 600$-Å scales. They found these distortions to be an important correction and potential source of systematic error for all previous $\mu$ measurements using VLT-UVES spectra. Bagdonaite et al. (2014) used a similar asteroid technique – one we describe in detail here – finding that a similar correction for long-range distortions was required for an accurate measurement of $\mu$ from their quasar spectra. These long-range distortions and the other systematic errors mentioned above have also been factored into more recent $\Delta \alpha/\alpha$ measurements (e.g. Evans & Murphy 2013; Molaro et al. 2013a; Evans et al. 2014). However, it remains to be assessed in detail whether these effects may help explain the systematically non-zero $\Delta \alpha/\alpha$ measured from the large Keck and VLT samples.

In this paper, we introduce a new ‘supercalibration’ method of identifying long-range wavelength-scale distortions by using high-resolution echelle spectra of ‘solar twin’ stars and significantly improve the use of asteroid spectra for this purpose. We apply this method to HIRES and UVES spectra taken during the epochs contributing to the previous evidence for a varying $\alpha$ and quantify the effect of these errors on previous $\Delta \alpha/\alpha$ measurements by modelling the effect on simulated data. The outline of the paper is as follows. In Section 2, we discuss the archival observations and data reductions that have been used in this paper to quantify long-range wavelength miscalibrations. In Section 3, we elaborate on the supercalibration method, giving an update to the methods used in Griest et al. (2009) and Whitmore et al. (2010). In Section 4, we present the results of its application to different spectrographs, and in Section 5 we use simulated spectra to uncover the implications that these wavelength miscalibrations are likely to have had on previous $\Delta \alpha/\alpha$ studies. We summarize and discuss our findings in Section 6.

2 ASTEROID AND STELLAR DATA REDUCTION

In this paper, we do not consider directly the quasar spectra that led to evidence for a varying $\alpha$ in Murphy et al. (2003, 2004) and King et al. (2012). Instead, we focus on observations using different techniques to quantify the likely types and magnitude of systematic calibration errors in those data. Most of the observational data used in this paper for calibration purposes is spectra of either asteroids or stars. Our main analysis uses archival, publicly available spectra for both UVES and HIRES across more than 15 yr. The spectra were taken across many different nights, sky/telescope positions, weather conditions, temperatures, pressures and spectrograph set-ups.

2.1 VLT-UVES

The UVES (Dekker et al. 2000) on the VLT consists of two arms: a blue arm and a red arm. The light path when observing an astronomical object is as follows. The light reflects off the primary, secondary and tertiary mirrors of the telescope, into a pre-slit unit (containing calibration lamps and optics) where it passes through an image derotator$^1$ and then into the Nasmyth-mounted UVES enclosure. When a dichroic mirror is in use, the light is split into red and blue light to pass through to the different arms. The blue (red) light propagates through the blue (red) slit, a series of optics, the echelle and cross-disperser gratings and is finally imaged on to the CCD. UVES has a total of three CCDs, one in the blue arm and two (denoted ‘upper’ and ‘lower’) in the red arm. The ThAr calibration lamp is housed in the UVES enclosure and when a calibration exposure is taken, a mirror is swung into the light path immediately after the telescope shutter, where it reflects the lamp light through the rest of the spectrograph. When an iodine cell is being used, it is heated and placed in the light path in front of the derotator within the UVES enclosure.

We use the standard European Southern Observatory (ESO) data reduction software, Common Pipeline Library (cpl) version 4.7.8. The reduction scripts are created using UVES_headsort.$^2$ We also used the carefully selected ThAr line list found in Murphy et al. (2007) for our reductions and we fit the wavelength solution with

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$^1$ ‘Derotator’ is the name used for the UVES image rotator and we use that convention here.

$^2$ Available at http://astronomy.swin.edu.au/~mmurphy/UVES_headsort
a sixth-degree polynomial. We discuss the differences and implications of using ‘attached’ and ‘unattached’ ThAr exposures in Section 4.1.1.

2.2 Keck-HIRES

The HIRES on the Keck telescope is a cross-dispersed echelle spectrograph with resolving power of $R \approx 25,000–85,000$ (Vogt et al. 1994). During an exposure, an astronomical object’s light reflects off the primary, secondary and the tertiary mirrors into the Nasmyth-mounted HIRES enclosure. There it passes through the image rotator, through the slit, off the collimator, echelle grating, cross disperser, more mirrors and optics, and is finally imaged on the CCD.

The principle aim of this paper is to understand the effect of any wavelength miscalibration on quasar spectra that could lead to errors in previous $\alpha$ measurements. As most of the Keck spectra used in Murphy et al. (2003, 2004) were reduced with the reduction software MAKEE, we use MAKEE to reduce the supercalibration spectra throughout this paper. The other main reduction software available is HIRESREDUX3 maintained by J. X. Prochaska. We tested the two software packages by comparing their relative wavelength solutions to the same supercalibration exposures and our tests did not find substantive differences.

3 SUPERCALIBRATION METHOD

3.1 General method overview

The standard method for wavelength calibrating a quasar exposure on a slit spectrograph is by comparison with a ThAr arc lamp exposure. The calibration source is a ThAr lamp that emits a spectrum with very sharp emission lines at known wavelengths. A 2D wavelength solution maps the detector’s CCD pixels to wavelengths. The ThAr wavelength solution is simply adopted as that of the quasar exposure. When accurate wavelength scales are needed, ThAr exposures should clearly be taken before slewing the telescope after the quasar exposure and without changing any of the spectrograph settings. However, even when such care is taken, the ThAr light may still follow a different light path through the spectrograph compared to the quasar exposure because the ThAr lamp light is reflected through the spectrograph by a mirror. And, at the very least, the ThAr light typically illuminates the slit (close to) uniformly, whereas most science objects, e.g. quasars and stars, are point-like, so different point spread functions are to be expected. If those differences are wavelength dependent, a potentially important calibration error will ensue.

In principle, the accuracy of the ThAr calibration method can be tested by comparing a ThAr-calibrated spectrum with a reference spectrum of the same science object on a different ‘absolutely calibrated’ spectrograph. The supercalibration method that we use in this paper follows this basic procedure. We take an exposure of a source with the telescope’s spectrograph, and compare its final calibrated spectrum with the reference spectrum of the same source from a Fourier Transform Spectrometer (FTS). We then solve for a relative velocity shift between these two spectra as a function of wavelength. In general, the most useful reference spectra have a large amount of spectral information, i.e. containing many sharp, narrow absorption features. We call this the ‘supercalibration’ method: it aims to check the normal calibration against a more reliable reference.

The basic implementation of the supercalibration method takes advantage of two different reference spectra: a molecular iodine ($I_2$) absorption spectrum and the solar spectrum. These spectra have a nearly continuous forest of narrow absorption features that allows us to consider small chunks of each spectrum, typically $500 \text{ km s}^{-1}$ wide ($\approx 8 \text{ Å}$ at $5000 \text{ Å}$). We determine the relative velocity shift between the reference chunk and the object spectrum using the following five transformations to each reference chunk: (1) a constant wavelength shift, (2) a flux scaling factor, (3) a constant flux offset, (4) a linear continuum slope correction and (5) the velocity width of a Gaussian IP. Because we are solving for transformations of the entire spectrum within each chunk, we are using all of the spectral information available. We solve for the best-fitting model parameters by minimizing $\chi^2$ between the transformed reference chunk and the object spectrum using MINUIT, the PYTHON implementation of SEAL MINUIT.4

In all that follows, the reference will be a high signal-to-noise ratio (SNR) FTS spectrum of the relevant reference source, either the solar spectrum or the iodine cell absorption spectrum. The FTS is an instrument that works under a fundamentally different process than the echelle spectrographs on telescopes, and we expect the relative FTS frequency scale (and thus wavelength scale) to be much more accurate. Therefore, the reference FTS spectrum’s wavelength scale is assumed to be correct; this assumption can be relaxed in certain ways that are detailed later (see Section 3.3.3). The best-fitting wavelength shift for each chunk is given by the following relation: $\lambda_{\text{shift}} = \lambda_{\text{FTS}} - \lambda_{\text{ThAr}}$. We plot our results in this paper with this wavelength shift turned into a velocity shift via

$$v_{\text{shift}} = c \times \frac{\lambda_{\text{shift}}}{\lambda}.$$  

(1)

The final, reported shift should be added to the standard ThAr calibration solution to obtain the ‘correct’ wavelength, i.e. that matching the FTS reference. For example, a $v_{\text{shift}}$ for a given chunk of $+50 \text{ m s}^{-1}$ means that the science spectrum needs $50 \text{ m s}^{-1}$ added to its wavelength scale for that chunk to align with the reference spectrum.

We note two practical details here about implementing the supercalibration method before describing our two implementations in the following two subsections. First, for all the analysis that follows, we mask atmospheric lines by removing the portion of the spectrum around and including the wavelength of known telluric emission and absorption lines.5 The presence of strong atmospheric lines can cause a spurious value for the $v_{\text{shift}}$ derived from the supercalibration method. Secondly, our method is applied to each echelle order separately and not on order-merged or redispersed exposures, so no artefacts or spurious velocity shifts can enter from redispersing or combining overlapping edges of adjacent orders.

3.2 Supercalibration method: iodine cell implementation

The UVES and HIRES instruments each contain a glass enclosure containing molecular iodine gas ($I_2$) called an iodine cell. This is heated to either 70°C (UVES) or 50°C (HIRES) and, at the observers’ request, placed directly in the light path of the spectrograph.

3 Available at http://www.ucolick.org/~xavier/HIRedux/
4 Available at https://github.com/minuit/minuit
5 Available at http://www.astro.caltech.edu/~tb/makee/OutputFiles/skylines.txt
As light passes through the iodine cell, a forest of narrow absorption features is imprinted from roughly 5000–6200 Å. The iodine cell has been used extensively for exoplanet detection (Valenti et al. 1995; Butler et al. 1996, 2003; Bedding et al. 2001; Marcy et al. 2005).

We make use of the iodine cell as an independent check of the ThAr wavelength solution. The first implementation of this method used the iodine cell spectra imprinted on to a quasar spectrum (see Griest et al. 2009; Whitmore et al. 2010, for details), and we use it again for the current work with a few minor improvements (allowing a constant flux offset, for example). The main difference is that here we use a fast-rotating bright star as the source because these are much brighter than quasars. The rotation effectively blurs any sharp spectral features from the star itself. After calibrating this exposure with a ThAr exposure in the standard way, we use the supercalibration method to compare it with a laboratory FTS spectrum of the iodine cell as the reference.

The FTS spectrum of the iodine cell has much higher resolving power ($R \approx 800,000$) than the telescope echelle spectrographs, UVES or HIRES ($R \approx 50,000–80,000$), used in the relevant quasar studies. Fig. 1 shows the iodine cell reference spectrum with the corresponding telescope spectrum. The much higher resolving power of the FTS is clearly visible. During the fitting process, each ($\approx 8$ Å) chunk of the FTS spectrum is transformed via the free parameters listed in Section 3.1 until $\chi^2$ is minimized. Fig. 1 shows an example best-fitting solution. The best-fitting transformed FTS spectrum produces the bottom panel in Fig. 1 and clearly shows the good match between the model and the data. We use the iodine supercalibration method in Section 4.2, where we characterize the effect of object placement within the spectrograph slit.

### 3.3 Supercalibration method: solar implementation

The main results of this paper derive from using the supercalibration method with the solar spectrum. We extend the same supercalibration method used by the iodine cell, but instead of iodine, we use the solar atmosphere as the reference source. The main advantage of using the solar spectrum is that sharp, narrow absorption lines are present at all optical wavelengths, not just at 5000–6200 Å as in the iodine method. Another advantage is that no change in the telescope’s optical path is required. In contrast, after placing the iodine cell in the light path, adjustments usually have to be made to the focus and slit alignment. The solar FTS reference spectrum we use comes from the Chance/Kurucz FTS vacuum solar spectrum Chance & Kurucz (2010), which they refer to as KPN02010. To access the solar spectrum at the telescope, we observe two types of astronomical objects: asteroids and ‘solar twins’. The first uses the Sun’s spectrum itself reflected off Solar system objects, in this case asteroids (moons are another possibility). The second uses stars that have almost identical spectra to our Sun and, for the intents and purposes here, can be treated as real solar spectra. We present the latter method here for the first time, demonstrating that it is effective and has several advantages over the other methods.

#### 3.3.1 Asteroid supercalibration

The asteroid-reflected solar spectrum has been used before for spectrograph calibrations. Molaro et al. (2008b) first fitted for a relative radial velocity difference between the centroids of a small number of selected, individual absorption lines and others in the same spectrum and also with the corresponding lines in a laboratory FTS solar spectrum. Rahmani et al. (2013) instead used a cross-correlation technique to compare spectral regions approximately one echelle order wide ($\approx 80$ Å), containing many absorption lines, between asteroid and laboratory FTS spectra. Our technique uses small spectral chunks, 500 km s$^{-1}$ ($\approx 8$ Å) wide, which allows us to map wavelength calibration distortions not only over long wavelength ranges, but also in detail across each echelle order.

#### 3.3.2 Solar twin supercalibration

We present a new technique for comparing spectra of ‘solar twin’ stars and solar FTS spectra. This technique is the same as for the asteroids in all respects (same reference FTS, same velocity chunk size, etc.), except that it uses a solar twin as the object spectrum, rather than solar light reflected from Solar system objects. In this work, we restricted observations to stars defined as ‘twins’ or ‘analogues’ of the Sun in Takeda et al. (2007), Meléndez et al. (2009), Onehag et al. (2011) and Datson, Flynn & Portinari (2014). However, we have recently observed other ‘solar-like’ stars — those with

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Figure 1. An example wavelength chunk of the iodine cell supercalibration method. The top panel shows the iodine cell spectrum imprinted on the spectrum of HR9087, a fast-rotating bright star, observed with the UVES spectrograph on 2009 December 9. The second panel shows the same region of the iodine cell spectrum as measured by an FTS. The third panel shows the normalized residuals of the best-fitting ‘supercalibration’ for the chunk shown in the fourth panel.

\[\text{UVES iodine cell FTS scan available from ESO at } \text{http://www.eso.org/sci/facilities/paranal/instruments/uves/tools.html}\]

\[\text{Available at } \text{http://kurucz.harvard.edu/sun/irradiance2005/irradthu.dat}\]
This means that they offer the ≈ −2010 8 chunk when the spectral SNR is ≲ 50 000), the latter is not generally true. Therefore, the statistical illustration that,

Some bright asteroids project angular sizes of ≳ 2003 R 447, relative velocity distortions of 120 per 1.3-km s⁻¹. Line-to-line random shifts are diminished in our technique because each chunk includes many lines, while the systematic component should not be important for determining wavelength calibration distortions (i.e. systematic velocity shift variations with wavelength). Due to similar activity variations in our own Sun, our asteroid technique will also suffer from some of these effects. However, a line-by-line analysis, like that first conducted by Molaro et al. (2008b), coupled with monitoring of solar activity, can in principle remove these effects.

Finally, if wavelength calibration distortions are driven by drifts in the spectrographs, it may be a problem that there is a substantial difference in the exposure times between solar twins and quasars. However, the benefit of a short exposure time is that the calibration check is relatively rapid and can be taken during the night. A possible advantage of this technique over using reflected solar light from Solar system objects (e.g. asteroids like in Section 3.3.1, or the moon) or sky emission spectra (e.g. Valenti et al. 1995), is that stars are unresolved point sources. This means that they offer the closest comparison to the quasar observations [aside from directly comparing two spectra of the same object, which can provide information about relative calibration distortions, e.g. Evans & Murphy (2013)]. Solar twins are also at fixed positions in the sky – they do not move at substantially non-sidereal rates like asteroids and other Solar system objects. This increases the practicality of solar twin supercalibration.

3.3.3 Test of solar FTS spectrum

Another possible concern about using the solar FTS reference is the assumption that its wavelength scale is correct and does not suffer from any systematic distortions itself. The FTS spectrum was constructed by stitching together several overlapping FTS scans of the solar spectrum (Chance & Kurucz 2010), and this stitching could introduce long-range wavelength distortions. A few of these concerns can be addressed by some relatively simple checks.

The High Accuracy Radial velocity Planet Searcher (HARPS) spectrograph is a stable, well-calibrated, temperature controlled and, most importantly for the present considerations, fibre-fed vacuum spectrograph on the ESO La Silla 3.6m telescope (Mayor et al. 2003). It differs in a number of ways from a slit spectrograph in air (UVES and HIRES): the optical fibre feeds the light directly to the instrument, the instrument is held to a constant

\[^8\] Some bright asteroids project angular sizes of \(\lesssim 0.2\) arcsec which, for the purposes of most optical observations, where the seeing is typically \(\gtrsim 0.5\) arcsec, is unresolved. However, the brightest asteroids (e.g. Ceres and Vesta) can be marginally resolved in such conditions.
tortions. However, our results are not identical to the frequency-comb technique returns reasonably reliable information about relative distortions. However, our results are not identical to the frequency-comb results: our intraorder distortions typically span approximately \pm 100 \text{ m s}^{-1} across each order, with either a flattening or slight reversal of the intraorder slope towards the order edges, whereas the results of Wilken et al. (2010) and Molaro et al. (2013b) generally show a \pm 70 \text{ m s}^{-1} span with the slope reversing completely towards the order edges. An important possibility is that the intraorder distortions are somewhat variable within HARPS, so further testing of different supercalibration techniques with HARPS is desirable. There may be some evidence in Fig. 3 for a small, \sim 45 \text{ m s}^{-1} per 1000 Å long-range distortion in the HARPS results and/or a \sim 50 \text{ m s}^{-1} shift at \sim 4750 Å. Given the lack of evidence for long-range slopes of this magnitude in the previous HARPS asteroid tests (Molaro & Centurión 2011; Molaro et al. 2013b), it may be that the slope and/or shift we observe is due to systematic effects in the Chance & Kurucz (2010) solar FTS spectrum. We do not attempt to correct this possible effect in the results of this paper because it is significantly smaller than the typical distortions we find in the UVES and HIRES instruments. Nevertheless, it highlights the importance of obtaining a more accurate solar reference spectrum for use in supercalibrating astronomical spectrographs.

Fig. 3 also shows an example solar twin supercalibration from both UVES and HIRES. The relative differences between the results from these slit spectrographs and the fibre-fed HARPS instrument is striking and compelling. There appear to be substantial long-range wavelength calibration distortions in both UVES and HIRES. Interestingly, it appears that each arm of UVES suffers from a long-range distortion with a similar slope, while the single arm of HIRES is characterized by a single distortion. The supercalibration for each of these three instruments uses the same FTS reference, so any intrinsic distortions from the supercalibration method itself must be much smaller than the effect we are detecting in UVES and HIRES. Finally, even if there is some conspiratorial way that the FTS and HARPS spectrographs have wavelength distortions that effectively cancel each other, the relative differences between HIRES and UVES still remain (though their absolute levels of distortion would be unknown).

In summary, the solar twin supercalibration is a new approach that reliably exposes and quantifies distortions in the ThAr wavelength solution. The next section details the different long-range wavelength-scale distortions in both the UVES and HIRES instruments.

4 VELOCITY DISTORTIONS IN VLT-UVES AND KECK-HIRES

One key advantage of the solar twin supercalibration method is that exposures of various solar twin stars have been taken with Keck-HIRES and VLT-UVES over many years. Applying the solar twin supercalibration method to both the Keck-HIRES and VLT-UVES archival exposures, taken across a wide range of dates and conditions, therefore allows us to quantify the historical record of long-range velocity distortions of the instruments. Below, we find significant long-range velocity distortions in both Keck-HIRES and VLT-UVES over most of their lifetimes, albeit somewhat sparsely sampled. We examine the distortions themselves in this section, while we analyse the impact that these distortions may have had on previous fundamental constant measurements in Section 5.

4.1 Long-range velocity distortions

4.1.1 VLT-UVES

As described in Section 2.1, the UVES spectrograph has the option of using a dichroic mirror to split incoming light into two arms (red and blue). The red arm consists of two CCDs, while the blue arm has a single CCD. There are a number of standard wavelength settings for UVES that are referred to by their central wavelength in nm for the two arms. For example, the 390/580 setting centres the blue arm at 3900 Å and the red arm at 5800 Å. The central wavelength of the blue arm falls in the centre of the blue CCD, while in the red arm the central wavelength falls between the two CCDs.
The supercalibration of solar twin HD76440 (upper) and asteroid Eunomia (lower) observed with UVES on 2013 May 15. The blue CCD is plotted in blue (left), the two red CCDs are plotted in green (middle) and red (right). In each exposure, the same arbitrary velocity shift has been applied to the results of all three CCDs so that the results roughly centre on zero velocity shift.

UVES was designed so that the gratings could be reliably set, changed and reset to the same position such that dispersed wavelengths were directed to the same CCD location to within $\pm 1/10\text{th}$ of a pixel. The goal of this design was to maximize time during the night spent taking science exposures, with the ThAr calibration exposures to be taken at the end of the night. Because of this design, the gratings are automatically reset after each observation block (OB) during the standard observation protocol. ThAr exposures taken in this way are referred to as ‘unattached’. However, OBs may include an ‘attached’ calibration exposure in which the science exposure is followed immediately by a ThAr exposure without any intervening grating reset. Such an ‘attached’ ThAr is clearly preferred when accurate wavelength calibrations are required. Note that the spectra used by King et al. (2012) in the larger VLT quasar sample of $\Delta\alpha/\alpha$ measurements were taken predominantly in the ‘unattached’ mode.

On 2013 May 15, the solar twin HD76440 and the asteroid Eunomia were observed several times, each with an ‘attached’ ThAr exposure, over a 30 min period. The telescope was slewed between these exposures. We plot the resulting supercalibration method results for both objects in Fig. 4. Intraorder (across a single echelle order) velocity distortions are prevalent in all orders and an approximately linear long-range velocity distortion appears across the wavelength range of each arm separately. The long-range velocity slope is found by fitting an unweighted line to the average $v_{\text{shift}}$ per order for each arm. There appears to be a similar slope in each arm such that the total velocity shift over the wavelength range of each arm is approximately the same. There also appears to be little or no velocity shift between the central wavelengths of the two arms. We find this to be a common distortion pattern for UVES and, from the archival data we have, find that it appears to be independent of the wavelength setting used in each arm. Because the centre of the arms are aligned in velocity space, at least in these particular exposures, the common slope effectively translates into an overall ‘lightning-bolt’ shaped distortion across the wavelength coverage of the exposure.

We have sparse archival data that irregularly samples the wavelength miscalibrations over the time range of the quasar observations we consider. None the less, we find a few overall characteristics that are shared generally by most of the supercalibration exposures we analysed. The slope of the distortions appear to be of similar slope and sign between the two arms, i.e. if the blue arm has a high positive slope, the red arm will also have a high positive slope. We also find that positive slopes are more common in the archival supercalibration spectra we were able to identify. To plot this slope, we adopt the following simple procedure. A weighted average $v_{\text{shift}}$ for each order was first calculated, then an unweighted straight line was fit to each average order value within each arm of the spectrograph.

As a visual summary of this best-fitting linear slope to the long-range velocity distortions, we plot the slopes found as a function of observation date in Fig. 5. This figure shows the results of the supercalibration analysis on the solar spectra found in the UVES archive with slit widths and settings that were also used during quasar observations. As is clearly seen, there is a fairly wide range of long-range velocity slopes across the sparsely sampled history of UVES. The range of slopes is typically between $\pm 200 \text{ m s}^{-1}$ per 1000 Å with increased divergence after 2010. Data for the King et al. (2012) were all taken in the years before 2009. The different slopes over time do not suggest any simple characterization as a function of time.

A number of hypotheses were tested in an attempt to correlate the long-range slopes and parameters in the header values of the object exposures as well as the corresponding ThAr exposures (e.g. seeing, telescope altitude/elevation, slit-width, etc.), with no clear relationship found. There are some hints that the distortions are caused by a combination of effects, with at least one potentially deterministic cause investigated in Section 4.3. Fig. 5 may also hint
that the spectrograph’s wavelength distortions might be quasi-stable for a period of time before an event (e.g. a mechanical realignment or earthquake) creates a larger change. An example of this may be the period ∼2004–2008 over which the distortion slope appears to be ∼200 m s⁻¹ per 1000 Å. However, a similar slope does not seem apparent in the asteroid observations from 2006 December in Molaro et al. (2008b). Also, Rahmani et al. (2013) found substantially different slopes in asteroid exposures from 2006, 2010, 2011 and 2012 (∼315, 150, 210 and 615 m s⁻¹ per 1000 Å, respectively) for the blue arm of UVES compared to our supercalibration results in the red arm in the same years. Therefore, the lack of slope variations seen in Fig. 5 for ∼2004–2008 may well be due to the very sparse sampling available.

Finally, in principle the supercalibration approach allows us to check for and measure any overall velocity shifts between the two arms of UVES. Obviously, such shifts might arise from misalignment of the two corresponding entrance slits, as projected on the sky, but they might also arise from the same (as yet unknown) physical effect that causes the long-range distortions. Molaro et al. (2008b) found that the UVES ‘arm shift’ was ≤30 m s⁻¹ in their asteroid observations. For the 2013 solar twin and asteroid results shown in Fig. 4, there is also no clear velocity offset between the blue and red arms of UVES. However, the archival solar twin supercalibrations provide few opportunities to measure the offset: in all but four cases, the ThAr wavelength calibration exposures for the blue and red arms were not taken simultaneously in a single dichroic setting like the stellar exposure. Wavelength setting changes between the blue- and red-arm ThAr exposures should be expected to produce velocity shifts of up to ∼300 m s⁻¹ in those cases. From the four exposures in which appropriate interarm calibration is available (in mid-2010 and mid-2013), we find velocity shifts <100 m s⁻¹ by comparing the fitted slopes at the nominal wavelength centres of the two arms.

4.1.2 Keck-HIRES

The HIRES spectrograph has had a number of upgrades throughout its life on the Keck telescope. Two significant upgrades were the installation of its image rotator at the end of 1996, and the single-chip CCD that was upgraded to a mosaic of three CCDs in mid-2004. In the Keck sample of Murphy et al. (2003, 2004), 77 of the 140 absorption system spectra were taken in the era before the image rotator was installed, while all of the spectra were taken during the ‘single-chip’ era of HIRES. There were a number of nights of available archival data of solar twins and asteroids over the past 15 yr. An example of the pre-image rotator supercalibration is shown in Fig. 4. The slope of the best-fitting line to the data is 740 m s⁻¹ per 1000 Å. While it is clear that there is a large, significant slope, it is also clear that a more elaborate model of the shape of the distortion could be fitted. However, we will fit a single straight line for the sake of simplicity.

During the three-chip era, the image rotator was always used and the wavelength coverage was significantly improved. Fig. 7 shows the relatively small 50 m s⁻¹ per 1000 Å slope across the three CCD chips in an asteroid exposure taken on 2011 October 21. The intraorder distortions are still evident as well; we do not observe any clear changes to their shape or amplitude with the transition to the three-chip era.

We find a larger range in velocity distortion slopes in the archival data of solar spectra taken with HIRES compared with those of UVES. Each of the solar twin or asteroid exposures we could identify in the HIRES archive was supercalibrated against the solar spectrum as described in Section 3.3, and a best-fitting linear slope was fit to the final supercalibration distortions. The history of this linear slope over the past 15 yr is plotted in Fig. 8. Generally, after the image rotator was installed, it appears that the long-range velocity slopes settle into a consistent range of ∼±200 m s⁻¹ with no clear difference between the single-chip and three-chip eras. However, while we could only identify two nights with useable data during the pre-image rotator era, it is clear that there are larger velocity distortions in those spectra. It is not clear at all from these pre-rotator data how well the slope we find might generalize to the rest of this era. Nevertheless, we note that, as observations were not made with the slit oriented with its spatial direction projected perpendicular to the physical horizon during this era, differential atmospheric refraction will have caused different wavelengths to fall to different positions across the slit. This would have led to velocity distortions (e.g. Murphy et al. 2001b, 2003) and may be a contributing factor to the increased slopes observed in Fig. 8 before 1996.

Figure 6. The supercalibration result for an exposure of Ceres (asteroid) taken with HIRES on 1995 July 5. The exposure was taken in the ‘pre-image rotator’ era of HIRES. The resulting supercalibration velocity shift is plotted after an arbitrary constant velocity offset was added.

Figure 7. The supercalibration result for an exposure of Ceres (asteroid) taken with HIRES on 2011 October 21. The exposure was taken with the image rotator in use during the three-chip era of HIRES, and the resulting supercalibration velocity shift is plotted after an arbitrary constant velocity offset was added. At wavelengths greater than 6000 Å, sky lines begin to dominate the spectrum. We mask these sky lines, which has the effect of producing gaps in the spectral coverage of the supercalibration results.
Figure 8. The best-fitting supercalibration slope for all archival HIRES solar twin and asteroid exposures we could identify with spectrograph setups similar to those used for the quasar spectra used by Murphy et al. (2004). The vertical lines denote two upgrades to HIRES: the installation of the image rotator in late 1996 and the three-CCD chip mosaic installation in 2004. All of the HIRES measurements used in the Murphy et al. (2004)/King et al. (2012) studies were made prior to 2004.

4.2 Quasar slit position effects

There are fundamental differences between a ThAr and quasar exposure. First, the ThAr calibration lamp light fills the slit during the calibration exposure, whereas the quasar presents a seeing disc at the slit. Secondly, the ThAr light is directed to the slit via a fold mirror, and any misalignment with respect to the quasar light path could lead to differential vignetting by the spectrograph optics. Finally, the ThAr light does not pass through the telescope optics, and any vignetting effects, for example, from the support structure of the secondary mirror, will not be present in the ThAr exposure (e.g. Valenti et al. 1995).

In addition to these inherent differences, the practical goal of keeping a quasar centred in the slit during long exposures is often difficult to maintain. The quasar often drifts within – both along and across – the slit. Drifts across the slit are particularly problematic because they translate to velocity shifts in the spectral lines and possibly higher order effects leading to velocity distortions. For example, the effective IP will change as one side of the quasar seeing disc is vignetted by the slit. If that effect has a wavelength-dependent component (e.g. seeing dependence on wavelength), a velocity distortion could be induced. Also, as discussed above (Section 4.1.2), if observations are not made at the parallactic angle, differential atmospheric refraction may cause long-range velocity distortions. However, as discussed in Murphy et al. (2001b, 2003), this is only relevant for HIRES quasar spectra taken before the image rotator was installed in 1996; all other spectra were observed with the slit held at the appropriate angle.

Here, we attempt to quantify miscalibrations due to such quasar position effects by taking several exposures of bright standard stars with the iodine cell in place and deliberately placing the quasar at different positions across the slit.

4.2.1 VLT-UVES

Two fast-rotating, bright stars, HR9087 and HR1996, were observed in 2009 with VLT-UVES with a 0.7 arcsec slit and ‘attached’ ThAr exposures. Three exposures of each star were recorded with the iodine cell in place in the following way: the star was displaced from the slit centre by about a third of the slit width and an exposure was taken. The displacement was made in the spectral direction alone, i.e. it was not moved along the slit, but only across the (short) width of the slit. The star was then placed in the centre of the slit and a second exposure was taken, followed by a third exposure with the star displaced by about a third of the slit width in the opposite direction to the first exposure. Finally, the iodine cell was removed from the light path and an ‘attached’ ThAr was taken. This entire procedure was done within a single OB, so there was a single ‘attached’ ThAr exposure for the three corresponding star exposures.

The iodine cell supercalibration was applied to each of the star exposures (each calibrated with the single ThAr exposure) and the results are shown in Fig. 9. The shifts in the star slit position appear to translate only to a constant velocity shift, as expected, and by the expected amount (i.e. ∼2 km s⁻¹). The intraorder and long-range velocity distortions are also clearly apparent. However, neither of these appear to change in a deterministic way with the star slit position. One final note is that these exposures were taken within a single night, and yet the long-range supercalibration slope is ≈400 m s⁻¹ per 1000 Å in each of the HR9087 (upper plot) spectra, while ≈100 m s⁻¹ per 1000 Å in the HR1996 (lower plot) spectra.
4.2.2 Keck-HIRES

In contrast to UVES, the gratings of the HIRES spectrograph are not automatically reset after each OB (indeed there is no OB structure or concept when using HIRES). Instead, observers leave the spectrograph’s gratings in place and take a ThAr before the telescope slewed to a new object. This allows for a more simple procedure when conducting the same slit position experiment and this was undertaken with HIRES in 2009 November using a 0.861 arcsec slit, with the star Hiltner 600, with the results shown in Fig. 10. A second test was conducted a month later using the stars HR9087 and GD 71, whose results are shown in Fig. 11. In HIRES, it appears that the intraorder distortions might change in shape systematically with the placement of the star across the slit (cf. UVES). However, this does not appear to have any effect on the long-range distortion slope which seems nearly flat for these exposures.

4.3 Stability of the VLT-UVES wavelength scale

While the supercalibration method in Section 3 was used to derive absolute velocity distortions, the relative stability of the ThAr wavelength solutions can be tested in a more direct manner: by comparing ThAr wavelength solutions from exposures taken over a short timespan to each other. As shown in Section 4.1.1, for most UVES exposures there are clear long-range velocity distortions. Here, we investigate whether there are drifts in the spectrograph over ∼20 min timescales which change these distortions.

For three science–ThAr exposure pairs (call them A, B and C) with ‘attached’ ThAr calibration exposures, taken about 10 minutes apart, we reduced science exposure B with each ThAr exposure. In other words, the ThAr exposures A and C were effectively ‘unattached’ with respect to science exposure B, while ThAr exposure B was ‘attached’ to science exposure B. We compare the ‘attached’ wavelength solutions with the ‘unattached’ ones in Fig. 12 by simply subtracting ThAr exposure B’s wavelength solution from those of ThAr exposures A and C. Fig. 12 shows that there is clearly an instability in the ThAr wavelength solution over ∼20 min timescales that can produce a relative long-range velocity distortion of several hundred m s$^{-1}$ over 1000 Å. Further, the relative slope appears to be shared between the two arms, while the relative offset between the central wavelength of each arm appears to be relatively aligned. We stress that this is the relative slope because this is a
slope only in comparison to the ‘attached’ ThAr wavelength solution. This behaviour is remarkably similar to that found in the absolute velocity distortions of Section 4.1.1, which suggests that the cause of the long-range distortions is likely a physical effect within the spectrograph.

We have identified the apparent cause of this effect by extending the same analysis to other ThAr exposures taken throughout that night and two taken the previous night. Fig. 13 shows the relationship between the slope of the best-fitting linear velocity distortion in the blue CCD against the derotator angle. The two red points are the ThAr exposures taken the previous night, and they also appear to align well with the overall slope of the trend. The tightness of the correlation suggests that these relative distortions arise due to the change in derotator angle with only a small possible contribution from other effects like mechanical and/or temperature drifts in the spectrograph. The exposures cover only a small derotator angle range and, in ongoing tests to be reported in a future paper, it appears likely that the trend does not continue linearly but rather cycles sinusoidally. It is surprising that the image rotator would itself induce a long-range velocity distortion in the ThAr spectrum, and it remains unclear whether, and in what manner, the effect would potentially propagate to the quasar spectrum as well. Again, this is only the intrinsic relative instability in the ThAr wavelength solution, and the absolute distortions in the wavelength scale of the quasar spectrum cannot be inferred from it except by a comparison method like supercalibration.

Finally, we undertook a similar analysis with Keck-HIRES, but on that spectrograph the ThAr light does not pass through the image rotator (unlike on UVES), and no relationship between rotator angle and any relative slope was found.

### 4.4 Summary and hypothesis

The distortion results of the supercalibration method can be summarized as follows. In both UVES and HIRES, tests of the effect of deliberate slit position offsets shows that the position of an astronomical object across the slit will give rise to a constant velocity shift to the spectrum, while a miscentring does not appear to induce long-range velocity slopes. These constant velocity shifts have the effect of smearing the spectrum and degrading the overall signal in co-added spectra, but will not add to a relative velocity shift between lines, except in cases where different wavelength coverages are co-added (Evans & Murphy 2013). Also, the guiding will move the object in the slit, especially during long exposures typical of quasar observations. The slit position effects will therefore be present in most quasar exposures but they will not greatly affect varying-α analyses.

Much more important are the intraorder and long-range velocity distortions, both of which are ubiquitous in both spectrographs. The long-range distortions are particularly concerning for varying-α analyses. It appears that in UVES there tends to be a ‘lightning bolt’ distortion in the wavelength scale across the blue and red arms of the spectrograph. In HIRES, it appears that, in most cases, the same distortion applies across all three chips in the single arm, albeit with some flattening in the bluest ~third of the wavelength coverage. The long-range distortions do not appear to change with the slit position of the object in either spectrograph, whereas the intraorder distortion shapes may change due to this effect in HIRES.

With these facts in mind, we may establish a working hypothesis for the cause(s) of the long-range distortions, though we do not claim to provide an ultimate explanation here. We propose that the effective IP changes across the spectrographs’ focal planes in both the spectral and spatial directions, according to some vignetting effect within the spectrographs. It has been shown previously that the HIRES IP varies across an order in iodine star studies (Valenti et al. 1995; Butler et al. 1996); we assume the UVES IP must vary by a similar magnitude. If the IP variation is significantly different for the ThAr calibration exposure, it may lead to the calibration distortions we observe. Because the long-range distortions are not noticeably sensitive to astronomical slit position, if this hypothesis is correct then the vignetting effect must be most prominent and variable in the ThAr calibration exposures. This possibility is supported by Fig. 13, which shows large changes in the distortion slope when different ThAr exposures, taken at different (de)rotator angles, are compared. Differential changes in the IP across the focal plane, between the ThAr and astronomical object exposures, will be degenerate (to first order) with apparent relative velocity shifts between transitions at different wavelengths. That is, long-range and intraorder velocity distortions will result, and cause systematic effects in Δα/α measurements.

### 5 IMPLICATIONS FOR PREVIOUS VARYING-α STUDIES

The long-range velocity distortions identified in Section 4 have direct implications for measuring Δα/α with UVES and HIRES. In this section, we analyse the potential impact of these distortions on previous studies by applying a simple model of the measured supercalibration distortions to simulated data. We then fit for Δα/α on this distorted simulated data in an attempt to quantify the effect of the velocity distortions. The absorption systems that we consider come from the VLT-UVES measurements of Webb et al. (2011) and King et al. (2012) and the Keck-HIRES measurements of Murphy et al. (2003, 2004) and King et al. (2012).

The simulated data for both UVES and HIRES were generated with the same process, and we applied the distortion model of each spectrograph to its respective absorption system sample. We used RDGEN 10.0⁵ to simulate each absorption system spectrum with a pixel-size of 1.3 km s⁻¹, an SNR of 2000 pix⁻¹ and a Gaussian IP

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⁵ Both VPFIT and RDGEN are available at http://www.ast.cam.ac.uk/~rfc/vpfit.html
FWHM of 5.0 km s\(^{-1}\). We placed each simulated absorption system at the corresponding measured redshift of each system in the HIRES or UVES sample. In contrast to the measured systems, these simulated systems were created with a single velocity component with Doppler parameter \(b = 2.5 \text{ km s}^{-1}\). We use a single component velocity structure in our simulated data instead of the multicomponent models fitted to the real data in the original analysis for the sake of simplicity and to focus attention on the effect of the distortions on \(\Delta \alpha / \alpha\) rather than possible effects of a complicated velocity structure. Finally, the column densities, \(N\), for the different ionic species were assigned in relative proportion similar to the simple model in Murphy & Berengut (2014) based on the solar abundance pattern for the singly ionized species (which will dominate in damped Lyman \(\alpha\) systems).\(^\text{10}\) To give an explicit example: consider an absorption system in the VLT-UVES analysis of King et al. (2012) at a redshift \(z = 2.7686\) in which the following transitions were used to measure \(\Delta \alpha / \alpha\): Fe \(\text{II}\) 1608, Si \(\text{II}\) 1526 and Si \(\text{II}\) 1808. Correspondingly, in our simulation, we simulated a spectrum with a single velocity-component absorption system at the same redshift, \(z = 2.7686\), with \(b = 2.5 \text{ km s}^{-1}\) and the column densities for those transitions of \(\log [N(\text{Fe } \text{II})/\text{cm}^2] = 13.00\) and \(\log [N(\text{Si } \text{II})/\text{cm}^2] = 13.06\).

We then distort this simulated spectrum by applying a simple model of the long-range velocity shift to the wavelength scale using equation (1). We fit for \(\Delta \alpha / \alpha\) on the final distorted spectrum, and since we simulated the spectrum with \(\Delta \alpha / \alpha = 0\), any non-zero \(\Delta \alpha / \alpha\) must result directly from the applied distortion model (this is why the SNR used in the simulation is very high, 2000 pixels\(^{-1}\); the statistical error on \(\Delta \alpha / \alpha\) will therefore be negligibly small). The process of fitting for \(\Delta \alpha / \alpha\) that we adopt is the same approach used in Murphy et al. (2004) and King et al. (2012): (i) use \(\text{VIFIT}\) 10.0 to fit a single component absorption feature [fixing \(\Delta \alpha / \alpha = 0\)] to create an initial fit; and (ii) run this initial fit, this time allowing \(\Delta \alpha / \alpha\) to vary to give the final fit. In all of these tests, the \(b\), \(z\) and \(\alpha\) parameters are tied together across all species, while the log \(N\) value for each species is allowed to vary. In this way, we run a simulated experiment of an ensemble of observations for a given velocity distortion model.

5.1 VLT-UVES simulation

We create the simple VLT distortion model by capturing the most striking characteristics of the VLT distortions: that each spectrograph arm tends to share a similar velocity distortion slope (both in sign and magnitude), and the central wavelengths of each arm tend to be aligned in velocity, i.e. there is no overall velocity shift between the arms. That is, there is just a single parameter required to describe the model – the distortion slope of both arms. To define this parameter, we use the supercalibration information we have for the era in which the quasar spectra used by King et al. (2012) were taken, i.e. prior to 2009 (see Fig. 5). For each night of observations in that era, we average the slopes for the supercalibration exposures of the bluer of the two chips in the red arm of UVES. The slope used in our simple model is the median of these nightly averages prior to 2009, i.e. 117 m s\(^{-1}\) per 1000 Å. While this value typifies the slopes found, it should be noted that slopes as large as 600 m s\(^{-1}\) were measured for UVES with the supercalibration method (e.g. Fig. 4).

\(^{10}\) Specifically, the log \(N\) assigned to each species was (in units of \(\text{cm}^{-2}\)): Mg \(\text{i}\) 11.28, Mg \(\text{II}\) 13.08; Al \(\text{i}\) 11.98; Al \(\text{II}\) 11.38; Si \(\text{II}\) 13.06; Cr \(\text{II}\) 11.18; Fe \(\text{II}\) 13.00; Mn \(\text{II}\) 11.03; Ni \(\text{II}\) 11.75; Ti \(\text{II}\) 11.46 and Zn \(\text{II}\) 11.18.

\(^{11}\) Available at https://github.com/jbwhit/AstroTools
\( \Delta \alpha/\alpha \) at higher redshifts is reproduced by the model, as well as the fact that the average magnitude of \( \Delta \alpha/\alpha \) is similar at the low- and high-redshift ends. The simple model also predicts that \( \Delta \alpha/\alpha \) should change markedly when the \( \text{Mg}\,\text{II} \) transitions fall in the red arm while the \( \text{Fe}\,\text{II} \) transitions fall on the blue arm, i.e. the narrow redshift range where the velocity shift between the \( \text{Mg}\,\text{II} \) and \( \text{Fe}\,\text{II} \) transitions reverses sign. It is intriguing and perhaps telling that this matches the large deviation in the mean \( \Delta \alpha/\alpha \) in the observations at \( z_{\text{abs}} \approx 0.8 \). On the other hand, the model does not reproduce the similar apparent positive deviation in \( \Delta \alpha/\alpha \) at \( z_{\text{abs}} \approx 1.6 \), nor does that deviation appear to be explained by the gap between the arms in other commonly used UVES wavelength settings we explored.

The lower panel of Fig. 15 shows the binned weighted mean results from the quasar spectra of King et al. (2012) after correcting each absorber’s \( \Delta \alpha/\alpha \) value with its corresponding simulated value from the simple distortion model. The binning and weighting followed the same procedure as the upper panel.\(^{12}\) No evidence for a deviation in \( \Delta \alpha/\alpha \) from zero remains after the correction. For example, the weighted mean \( \Delta \alpha/\alpha \) drops from +2.1 \( \pm \) 1.2 ppm reported in King et al. to +0.8 \( \pm \) 1.2 ppm. This, of course, assumes that uncertainties in the model correction are negligible, which is unlikely to be true in detail. Nevertheless, two other factors provide some additional confidence that the model broadly reflects the distortions likely to be present in the VLT-UVES quasar spectra.

(i) The individual \( \Delta \alpha/\alpha \) values from the quasar spectra and simulated spectra correlate strongly. The 153 \( \Delta \alpha/\alpha \) measurement–simulation pairs have a Spearman rank correlation coefficient of 0.25 with an associated probability of \( p = 0.2 \) per cent of by-chance correlation (i.e. \( \approx 3.1\sigma \) significance).

(ii) Correcting the quasar \( \Delta \alpha/\alpha \) values with those from the simple distortion model reduces the scatter. The root-mean-square (rms) deviation from the mean \( \Delta \alpha/\alpha \) in the quasar sample is 27.4 ppm; this reduces to 26.8 ppm after subtracting the individual simulated \( \Delta \alpha/\alpha \) values from the corresponding quasar measurements. To estimate the significance of this reduction, we constructed 10 000 realizations of the simulated sample by selecting randomly, with replacement, 153 values from the simulated sample for each realization. This randomizes the association between absorbers and the corresponding corrections to \( \Delta \alpha/\alpha \). Each realization of the simulated sample was used to correct the quasar \( \Delta \alpha/\alpha \) values and the rms was computed as before. This reveals that a reduction to an rms of \( \leq 26.8 \) ppm occurs only \( p = 0.3 \) per cent of the time. That is, the reduction in the rms we observe has a \( \approx 3.0\sigma \) significance. Recognizing that the mean \( \Delta \alpha/\alpha \) is redshift-dependent in the quasar results in Fig. 15, we conducted the same test in three redshift bins. Similar reductions in the rms were found, though with lower statistical significance: 20.5 to 19.8 ppm with \( p = 2 \) per cent for \( z_{\text{abs}} \leq 1.241 \), 32.6 to 32.0 ppm with \( p = 9 \) per cent for \( z_{\text{abs}} \geq 1.857 \), and no reduction from 27.3 ppm for the middle redshift bin with \( p = 37 \) per cent.

It is important to emphasize that we have adopted a single distortion slope to characterize our model of the distortions in the UVES
quasar spectra, whereas we do find considerable variation in this parameter in the rather sparse supercalibration information from the data archive over the period before 2009. Scaling the slope used in the model will simply scale the deviation of the model $\Delta \alpha / \alpha$ points away from zero in Fig. 15; changing its sign will reverse the deviations away from zero. A more appropriate model would have to take into account information about the distortion slope for each of the many different exposures, sometimes in different wavelength settings, for each quasar in the King et al. (2012) study, but such a rich data base of supercalibration exposures does not exist. Nevertheless, even with the sparse information at hand, and the consequently simple model used, it appears that the long-range distortions have the characteristics to adequately explain the $\Delta \alpha / \alpha$ UVES values measured in King et al. (2012).

In particular, our simple model does not incorporate any effect that should cause a correlation between the $\Delta \alpha / \alpha$ value and the quasar sky position – particularly declination – that might explain the $\sim 2\sigma$ evidence, within the UVES results alone, for the dipole-like variation in $\Delta \alpha / \alpha$ across the sky identified in King et al. (2012). Indeed, after correcting the UVES quasar results with the simulated ones from our model, and following the same dipole analysis in King et al., we find very little change to the best-fitting dipole+monopole model parameters, with the statistical significance of the dipolar variation (beyond a monopole-only model) changing only from $\approx 2.3 \text{ to } \approx 2.1\sigma$. However, the clear connection between the UVES derotator angle and changes in the ThAr lamp spectra seen in Fig. 13 may ultimately prove important. That connection, combined with the fact that almost all the King et al. quasar spectra were calibrated with subsequent, day-time ThAr spectra (i.e. at a small number of standard, fixed derotator angles), leaves open the possibility of a subtle correlation between distortion slope and quasar declination in UVES. We have not yet identified any direct evidence for such a correlation.

### 5.2 Keck-HIRES Simulation

The Keck-HIRES data used in Murphy et al. (2003, 2004) were all taken during the single CCD chip era. The single chip era is further divided into two time periods: before and after the image rotator was installed in 1996, as illustrated in Fig. 8. Of the 140 absorption systems in the Keck sample, 77 were observed during this pre-rotator era. Given that we currently have no physical explanation or model for the origin of the long-range distortions in HIRES, this leaves no reliable way to extrapolate the results of these few supercalibrations to the many quasar spectra taken in the pre-rotator era. In addition, and in contrast to VLT-UVES, the Keck-HIRES long-range velocity distortions are not as easily modelled. We find roughly linear slopes of both positive and negative sign, as well as evidence of a bend in the distortion (as seen in Fig. 6). Our search for a relationship between distortion sign and observational parameters such as seeing, telescope altitude/elevation, etc., did not yield any trend (as with UVES).

We create the simple Keck model by characterizing the supercalibration distortions as simply as possible. For each night of observation in the era where the data from Murphy et al. (2004) was observed, we average the slopes for the supercalibration exposures, and take the median of these nightly averages. The average slope is $66$ m s$^{-1}$ per 1000 Å with a standard deviation of $201$ m s$^{-1}$ per 1000 Å. We used this average value and the $1\sigma$ deviations as the slope for three simple HIRES models to apply to the simulated HIRES sample. The distortion models that we used are shown in Fig. 16. We apply these HIRES models to simulated absorption spectra corresponding to those used to measure $\Delta \alpha / \alpha$ in Murphy et al. (2004), i.e. using the information in table A1 of King et al. (2012). Following the same procedure used for the UVES sample in Section 5.1, we plot the results in Fig. 17.

The pattern of $\Delta \alpha / \alpha$ values in Fig. 17 shows that a linear model can reproduce either the lower redshift ($z < 1.5$) region, or the higher redshift ($z > 1.5$) region, but not both at the same time. A linear velocity distortion across the wavelength range corresponds to a simple compression or expansion of the wavelength scale, and Murphy et al. (2003) showed such models give opposite-signed behaviour in $\Delta \alpha / \alpha$ across the measured redshift range. Our test here confirms that a single linear velocity distortion is not a good model for the Keck results and we do not find a single model that reliably reproduces the Keck measurements. On the other hand, it is important to note that, within the $1\sigma$ range of slopes, a linear distortion produces $\Delta \alpha / \alpha$ values that encompass almost all of the measured results. Therefore, the long-range distortions observed in the Keck-HIRES supercalibration spectra have the general characteristics and magnitude to explain the possible evidence for a varying $\alpha$ from HIRES quasar spectra. However, the variability in the distortion slopes observed, combined with the uniformly negative $\Delta \alpha / \alpha$ at all redshifts in the HIRES results, is the main barrier to these being a complete explanation at this stage.

Another potential problem is the paucity of supercalibration information currently available for the pre-rotator era of HIRES (i.e. before late 1996). Indeed, we only have supercalibration for two nights in that epoch, which accounts for over half of the Keck-HIRES absorber sample – see Fig. 8. As discussed in Section 4.1.2, differential atmospheric refraction will have caused long-range distortions in the quasar and supercalibration spectra in the pre-rotator era. The possible effect of this on the Keck-HIRES $\Delta \alpha / \alpha$ results was considered in detail by Murphy et al. (2001b, 2003). Despite simulations demonstrating that the effect should be detectable in the 77 affected absorbers, no correlation between $\Delta \alpha / \alpha$ and zenith distance was observed. The pre- and post-rotator samples also gave very similar average $\Delta \alpha / \alpha$ values. Thus, despite the possibility that pre-rotator HIRES spectra may have an additional, systematic contribution to their long-range distortions, evidence for it is not
available from the very limited supercalibration information or the \( \Delta \alpha/\alpha \) results themselves.

5.2.1 High-contrast subsample

In the Keck measurements of Murphy et al. (2004), a subset of the \( \Delta \alpha/\alpha \) values were found to have a larger scatter than implied by their statistical uncertainties. This subset of systems was at \( z_{\text{abs}} > 1.8 \) and there was significant additional scatter ‘particularly around \( z_{\text{abs}} \approx 1.9 \)’. This subset was found to correspond to absorbers in which a large number of transitions were used to determine \( \Delta \alpha/\alpha \) and, importantly, where there was a large range in the optical depths of these transitions. The large difference in the optical depths led to the systems being labelled ‘high-contrast’ systems, with the remainder being labelled ‘low contrast’. An additional random error term of 20.9 ppm was added in quadrature to this ‘high-contrast’ sample in Murphy et al. (2004). King et al. (2012) revisited and re-analysed the same subsample. Using a different method of ‘least trimmed squares’, they found that the ‘high-contrast’ sample required an additional 17.4 ppm to be added in quadrature to the statistical errors for this subsample.

Fig. 18 shows the effect of the average-slope model (66 m s\(^{-1}\) per 1000 Å) velocity distortion applied to simulated data, with the red points highlighting the ‘high-contrast’ sample. The simple linear model yields \( \Delta \alpha/\alpha \) results that increase in scatter for certain systems – especially around the systems that lie at \( z_{\text{abs}} \approx 1.9 \). The extra scatter is clearly evident, and it suggests that even our simple models, constructed with a single velocity component and only a linear distortion, create significant additional scatter around that redshift. It is still possible that the explanation for the additional scatter observed, but long-range distortions may be part of the explanation as well.

6 SUMMARY AND CONCLUSIONS

We have presented a new method for testing the wavelength calibration accuracy of high-resolution spectrographs using exposures of ‘solar twin’ stars and an FTS solar reference spectrum. This ‘supercalibration’ method is similar to those based on iodine cell stellar exposures and asteroid exposures presented previously and we have improved those methods here as well. The solar twin and asteroid supercalibration techniques provide a similar density of spectral information as the iodine cell method but have the additional advantage that the solar spectral features cover the entire wavelength range of optical high-resolution spectrographs (e.g. 3000–10 000 Å). The solar twin method presented here also carries significant advantages over the asteroid method: solar twins are located at fixed sky positions, at all right ascensions, and many are brighter (\( \lesssim 9 \) mag) than most asteroids. It is therefore practical and relatively efficient to observe a solar twin immediately after the primary object of interest, in the same instrument set-up, with minimal telescope slew, and with a very short exposure. In future, this will enable more reliable checks on the standard ThAr wavelength scale ‘attached’ to the primary object exposures.

By applying the supercalibration technique to solar twin, asteroid and iodine cell star exposures from both Keck-HIRES and VLT-UVES, we find that significant distortions of the wavelength calibration are ubiquitous in both spectrographs. The distortions
are on scales of both echelle orders (∼50–100 Å, ‘intraorder’) and entire spectrograph arms (∼1000–3000 Å, ‘long range’), and seem to occur over the full variety of instrument set-ups and epochs. The intraorder distortions have peak-to-peak amplitudes of up to ∼500 m s⁻¹ in both spectrographs. We find that the long-range velocity distortions are approximately linear with wavelength in each spectrograph arm. In UVES, they usually have a very similar linear slope in each arm, with little velocity shift between the centres of the two arms. In HIRES’s single arm, many of the supercalibration exposures show evidence for a somewhat non-linear distortion, typically with a flattening in the bluest ∼third of the wavelength range. Characterizing each spectrograph arm with a linear distortion, we find similar magnitudes for the slope in both spectrographs: typically <200 m s⁻¹ per 1000 Å but up to ∼800 m s⁻¹ per 1000 Å in some exposures. The sign of the slope seems to fluctuate in both spectrographs over the 1–1.5 decades for which we have (sparse) supercalibration information. The magnitude, and possibly the sign, also fluctuates on very short (i.e. intraday) time-scales. See Figs 5 and 8.

We explored the possible physical drivers of these distortions in both spectrographs and established a working hypothesis for their cause: differential vignetting of the astronomical object and ThAr calibration light paths within the spectrograph, with the likelihood that the ThAr-vignetting dominates and is most variable. Some evidence supporting this hypothesis is that (i) the long-range and, at least for UVES, intraorder distortions do not appear to change as the position of the astronomical object within the spectrograph slit is varied; (ii) the long-range slope for UVES changes significantly when ThAr exposures taken at different (de)rotator angles are compared. If this hypothesis is correct and the ultimate, mechanical cause can be firmly established, it may be possible to accurately predict the long-range distortions expected in previous quasar exposures. However, at present, the available information is not sufficient to confirm our hypothesis. The results of ongoing, dedicated tests on UVES and HIRES will be reported in a future paper.

Finally, we estimated the approximate effect of the long-range distortions on the measurements of ∆λ/λ from large samples of archival HIRES (Webb et al. 1999, 2001; Murphy et al. 2001a, 2003, 2004) and UVES (Webb et al. 2011; King et al. 2012) using simulated quasar spectra. In the absence of a causal, physical model to predict the long-range distortions, we instead modelled them with a single, linear slope per spectrograph arm, as shown in Figs 14 and 16 for UVES (two arms) and HIRES (one arm), respectively. The slope assumed for each spectrograph was simply representative of the significantly variable but sparsely sampled information about the long-range distortions over the epochs in which the relevant quasar spectra were recorded (Figs 5 and 8). Even with these simplifying assumptions, the effect on simulated quasar spectra mimics many of the features of the UVES results obtained in King et al. (2012), including a slow change in the sign of ∆λ/λ from źabs ∼ 1 to źabs ∼ 1.8 and a sharp change at źabs ∼ 0.8. Further, the simulated ∆λ/λ values correlate strongly with the UVES quasar values, and correcting the latter with the former significantly reduces the scatter in ∆λ/λ. However, the HIRES model does not simultaneously reproduce a mean ∆λ/λ of the same sign at both low and high redshifts, as observed in the quasar results (Murphy et al. 2003, 2004).

In summary, it is clear that long-range distortions of the wavelength scale identified here have the characteristics required to adequately explain the VLT-UVES quasar measurements of ∆λ/λ, though they cannot entirely explain those from Keck-HIRES. That is, if both sets of quasar measurements are corrected with our distortion models, the VLT measurements are consistent with ∆λ/λ = 0 at all redshifts, while the Keck results deviate from zero at either ź < 1.5 or ź > 1.5 depending on the sign of the prevailing distortions. As a consequence, combining the data sets to search for subtle variations with redshift or across the sky, for example, requires a more detailed understanding of the possible systematic errors in the Keck-HIRES quasar measurements (at least). The long-range distortions therefore significantly weaken the possible evidence for variations in the fine-structure constant over cosmological time and spatial scales. Understanding the causes of the intraorder and long-range distortions, and whether they can be corrected, will also be crucial for future quasar measurements of ∆λ/λ and for avoiding them in future spectrographs. In the interim, we recommend following each quasar exposure in such campaigns with both ThAr calibration and solar twin supercalibration exposures to gauge the extent of, and allow correction for, long-range wavelength distortions in slit spectrographs.

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REFERENCES

Allende Prieto C., Garcia Lopez R. J., 1998a, A&AS, 129, 41
Allende Prieto C., Garcia Lopez R. J., 1998b, A&AS, 131, 431
Bagdonaite J., Ubachs W., Murphy M. T., Whitmore J. B., 2014, ApJ, 782, 10
Baguhl S., Jehin E., Ledoux C., Cabanac R., Melo C., Gilmozzi R. The ESO Paranal Science Operations Team, 2003, The Messenger, 114, 10
Bedding T. R. et al., 2001, ApJ, 549, L105
Butler R. P., Marcy G. W., Williams E., McCarthy C., Dosanjh P., Vogt S. S., 1996, PASP, 108, 500

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