Possible evidence for a variable fine structure constant from QSO absorption lines: motivations, analysis and results

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ABSTRACT
An experimental search for variation in the fundamental coupling constants is strongly motivated by modern high-energy physics theories. Comparison of quasar absorption line spectra with laboratory spectra provides a sensitive probe for variability of the fine structure constant, $\alpha$, over cosmological time-scales. We have previously developed and applied a new method providing an order of magnitude gain in precision over previous optical astrophysical constraints. Here we extend that work by including new quasar spectra of damped Lyman-\alpha absorption systems. We also re-analyse our previous lower redshift data and confirm our initial results. The constraints on $\alpha$ come from simultaneous fitting of absorption lines of subsets of the following species: Mg\textsc{i}, Mg\textsc{ii}, Al\textsc{ii}, Al\textsc{iii}, Si\textsc{ii}, Cr\textsc{ii}, Fe\textsc{ii}, Ni\textsc{ii} and Zn\textsc{ii}. We present a detailed description of our methods and results based on an analysis of 49 quasar absorption systems (towards 28 QSOs) covering the redshift range $0.5 < z < 3.5$. There is statistical evidence for a smaller $\alpha$ at earlier epochs: $\Delta \alpha/\alpha = (-0.72 \pm 0.18) \times 10^{-5}$. The new and original samples are independent but separately yield consistent and significant non-zero values of $\Delta \alpha/\alpha$. We summarise the results of a thorough investigation of systematic effects published in a companion paper. The value we quote above is the raw value, not corrected for any of these systematic effects. The only significant systematic effects so far identified, if removed from our data, would lead to a more significant deviation of $\Delta \alpha/\alpha$ from zero.

Key words: atomic data – line: profiles – methods: laboratory – techniques: spectroscopic – quasars: absorption lines – ultraviolet: general

1 INTRODUCTION
High resolution spectroscopy of QSO absorption systems provides a precise probe of fundamental physics. In previous papers (Dzuba, Flambaum & Webb 1999a,b; Webb et al. 1999, hereafter W99) we introduced and applied a new and highly sensitive method for constraining space-time variations of the fine structure constant, $\alpha \equiv \frac{e^2}{\hbar c}$. Using 30 Keck/HIRES absorption spectra containing Mg\textsc{ii} and Fe\textsc{ii}, we reported a tentative detection of a variation in $\alpha$: $\Delta \alpha/\alpha = (-1.09 \pm 0.36) \times 10^{-5}$, where $\Delta \alpha/\alpha$ is defined as

$$\Delta \alpha/\alpha = (\alpha_z - \alpha_0)/\alpha_0, \quad (1)$$

$\alpha_0$ is the present day value of $\alpha$ and $\alpha_z$ is the value at the absorption redshift, $z$. The absorption redshifts ranged from $\sim$0.6–1.6.

* Data presented herein were obtained at the W.M. Keck Observatory, which is operated as a scientific partnership among the California Institute of Technology, the University of California and the National Aeronautics and Space Administration. The Observatory was made possible by the generous financial support of the W.M. Keck Foundation.

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Here we continue this work, presenting new measurements of $\Delta \alpha/\alpha$ in high redshift damped Lyman-$\alpha$ systems (DLAs) over the range $0.9 < z < 3.5$, and a re-analysis of the W99 data set. Four papers present our new work on this subject. A brief summary of all results is given in Webb et al. (2001). The present paper provides a detailed description of our methods and results. A companion paper (Murphy et al. 2001b, hereafter M01b) presents a thorough examination of systematic effects. An additional paper (Murphy et al. 2001c) presents an analysis of a sample of Si IV QSO absorbers.

The present paper is organized as follows. Section 2 describes theoretical motivations for a search for varying $\alpha$. In Section 3 we summarise previous experimental constraints on varying $\alpha$. Section 4 presents the theoretical basis of the new method for determining $\Delta \alpha/\alpha$ using QSO absorbers. Section 5 describes the experimental components of our study: high-resolution QSO observations and precise laboratory rest wavelength measurements. In Section 6 we discuss our analysis technique in detail and present our results. For completeness we also summarise the systematic effects discussed in detail in M01b. Section 7 summarises our new results and outlines future work.

\section{Theoretical Background}

\subsection{Early Historical Interest}

The constancy of the fundamental constants began to be questioned when Milne (1935, 1937) and Dirac (1937) suggested that the Newtonian gravitational constant, $G$, may vary in cosmological time. Milne proposed a gravitational theory in which different physical ‘clocks’ – ‘ticking’ according to different physical processes – ‘tick’ at different rates as time progresses. The possible consequences of this hypothesis for biological and geological history were seized upon by Haldane (1937a,b) to explain aspects of their discontinuous development, whereas Kothari (1938) and Chandrasekhar (1939) pointed out some astronomical consequences of Dirac’s ‘large numbers hypothesis’ which might permit it to be tested by observation. Dirac’s Large Numbers Hypothesis attracted considerable interest (e.g. Teller 1948; Dicke 1957, 1961; Barrow 1990; Barrow & Tipler 1996) and the desire to place his idea of varying $G$ on a firmer theoretical footing led to the development of scalar-tensor generalisations of Einstein’s theory of general relativity in which the variation of $G$ was described self-consistently by the propagation of a scalar field which also acted as a source of space-time curvature (Brans & Dicke 1961).

Jordan (1937, 1939) was the first to consider how Dirac’s hypothesis might be applied to forces other than gravity, but rejected the possibility of time variations in the weak interaction or the electron-proton mass ratio (Jordan 1937, 1939). Later, Gamow (1967) showed that geological problems caused by Dirac’s proposed variation in $G$ that had been pointed out by Teller (1948) could be avoided by interpreting the large numbers hypothesis as requiring the time-variation of the charge on the electron, $e$, rather than $G$. Observational limits on possible variations of $\alpha$ or the weak and strong interactions were more restrictive than those on $G$ although no self-consistent theory permitting the variation of non-gravitational force constants was developed to make the observational limits rigorous. Landau (1955) proposed that variation in $\alpha$ could be connected to renormalization rules in quantum electrodynamics.

Current motivation for a search for a varying $\alpha$ comes from modern theories which attempt to unify gravity with other interactions.

\subsection{Modern Theoretical Motivations for Varying $\alpha$}

At present there are many theoretical motivations for a search for varying $\alpha$. However, these theories, being relatively recent, may not be widely appreciated within the context of astronomical tests of their viability. We therefore summarise recent ideas below.

\subsubsection{Multi-dimensional Unification Theories}

One of the greatest challenges facing modern theoretical physics is the quantization of the gravitational interaction. Early attempts at creating such a unification were made using a geometrization in $(4 + D)$-dimensional curved space-times in the spirit of the old Kaluza-Klein scenario to unite gravity and electromagnetism (Kaluza 1921; Klein 1926). Three-dimensional gauge couplings like $\alpha$, $\alpha_{\text{weak}}$, and $\alpha_{\text{strong}}$ then vary as the inverse square of the mean scale of the extra dimensions. Thus, the evolution of the scale size of the extra dimensions is related to variability of the low-energy coupling constants in the 4-dimensional subspace in simple Kaluza-Klein and superstring theories.

Damour & Polyakov (1994) showed that cosmological variation in $\alpha$ may proceed at different rates at different points in space-time (see also Forgás & Horváth 1979; Barrow 1987; Li & Gott 1998). Various functional forms for time variation of $\alpha/G$ have been derived using Kaluza-Klein theory and the assumption of constant masses. Chodos & Detweiler (1980) find $\alpha/G \propto t$ and Freund (1982) finds $\alpha/G \propto t^\frac{1}{4}$. Wu & Wang (1986) have found that $\alpha \propto G \sim 10^{-11}\text{yr}^{-1}$ where the proportionality constant is unknown. It is interesting to note that using a similar analysis to Wu & Wang, Maeda (1988) derived $\alpha \propto t^{-4/3}$.

Marciano (1984) discussed the self-consistency relations required if there are simultaneous variations of different constants in unified gauge theories. He also examined any possible non-monotonic variation in $\alpha$ with $t$, using the running coupling dependence of strong, weak, and electromagnetic interactions to produce self-consistent predictions for the simultaneous variation of more than one coupling or mass ratio. These were discussed in Drinkwater et al. (1998). Typically, variation in $G$ and $\alpha$ could be linked by relations of the form $\Delta \alpha \sim \Delta G$.

These features of extra dimensions mean that in all string theories (and M-theory, of which they are presumed to be limiting cases, Horava & Witten 1996a,b), any extra dimensions of space need to be held static with high accuracy in order to avoid gross conflict with observation. In the currently popular scenarios for M-theory (e.g. Antoniadis et al. 1998; Arkani-Hamed, Dimopoulos & Dvali 1998; Randall & Sundrum 1999a,b), only the gravitational force is assumed to act in all ($>3$) spatial dimensions (the ‘bulk’) whilst all other interactions act only in 3-dimensional space (the
‘brane’). Observations of the constancy of 3-dimensional non-gravitational constants governing the strengths of those interactions in three dimensions (like \( \alpha \)) could therefore be of crucial importance in testing this theoretical scenario. The scale of the extra dimensions was until recently believed to be necessarily of order the Planck scale \( \sim 10^{-33} \) cm but it is possible they could be as large as \( \sim 0.01 \) mm leading to large changes in the form of the Newtonian law of gravity on length scales below this distance. At present, this is consistent with all known experiments. The challenge of testing the law of gravity on sub-millimetre scales is considerable because other forces strongly dominate the effects of gravity on these scales.

### 2.2.2 Scalar Theories

The first self consistent theory of electromagnetism which incorporates varying \( \alpha \), and which reduces to Maxwell’s theory in the limit of constant \( \alpha \), was that developed by Bekenstein (1982). It introduces a scalar field whose variation in space and time produces effective variation in the electron charge (or, equivalently, the permittivity of free space). The form of the propagation equation for the evolution of the scalar field is strongly constrained by the natural requirements that it be second order, causal and linearly coupled to the matter density. This particular theory has been constrained by several astronomical observations (Livio & Stiavelli 1998) and used to illustrate consequences of space and time variations of constants (Barrow & O’Toole 2000).

The general structure of Bekenstein’s theory can also be applied to other couplings, and it has recently been used to investigate the problem of varying the strong coupling constant of QCD by Chamoun, Landau & Vucetich (2000). Bekenstein makes the simplifying assumption that the gravitational sector of the theory be unchanged from that of general relativity. This amounts to neglecting the contribution of the kinetic energy of the scalar field associated with \( \alpha \) variation to the expansion dynamics of the universe. This defect can be avoided in other versions of this theory (Barrow & Magueijo 2000; Magueijo 2000). It should be emphasised that there is no single self-consistent theory incorporating varying \( \alpha \) and theoretical limits need to be quoted in conjunction with the theoretical framework used to confront observational data. If different interactions are unified by electro-weak or grand unified theories then the ramifications of introducing varying \( \alpha \) will be deeper and wider and a scalar theory would need to accommodate the effects of varying \( \alpha \) on the other gauge couplings.

### 2.2.3 Varying speed of light theories

One appeal of varying speed of light theories is that they provide alternative potential solutions to a range of cosmological problems such as the flatness, horizon and monopole problems (Moffat 1993; Barrow & Magueijo 1999a,b; Albrecht & Magueijo 1999; Barrow 1999). Barrow & Magueijo (1998) have also expressed Bekenstein’s (1982) varying-\( c \) theory in terms of varying \( \alpha \).

Barrow & Magueijo (2000) developed a particular theory for varying \( c \) (or \( \alpha \)) in which the stress contributed by the cosmological constant varies through the combination \( \Lambda c^2 \). They also showed how the observed non-zero cosmological acceleration (Schmidt et al. 1998; Perlmutter et al. 1999) might be linked to a varying \( \alpha \). They examined a class of varying-c theories in which changes in \( c \) are driven by a scalar field which is coupled to the gravitational effect of pressure. Changes in \( c \) convert the \( \Lambda \) energy density into radiation, preventing \( \Lambda \) from dominating the universe in the radiation epoch. As pressureless matter begins to dominate, variations in \( c \) slow, and \( \Lambda \) begins to dominate. The very slow variation of the scalar field driving changes in \( c \) is like that of scalar fields in quintessence theories in the presence of perfect fluids. This type of theory allows the time variations in \( c \) or \( \alpha \) to be \( \sim 10^{-5} H_0 \) at \( z \sim 1 \) and yet the associated \( \Lambda \) term can be dominant today and produce acceleration (the \( 10^{-5} \) factor is created naturally in this theory by the ratio of the radiation to matter density in the universe today). We therefore expect only very small residual variation in \( \alpha \) in a \( \Lambda \) dominated universe. The existence of simple theories of this sort provides a strong motivation for studies like the present one.

### 2.2.4 Other theories

Several authors have suggested other motivations for varying \( \alpha \). For example, Hill & Ross (1988a,b) (see also Hill, Steinhardt & Turner 1990) have suggested that oscillatory variations in \( \alpha \) might be expected if there exists a soft boson field that has electromagnetic couplings to either the Maxwell scalar, \( F_{\mu \nu} F^{\mu \nu} \), or to the electron state, \( \bar{\psi} \psi \). If the boson field has a mass \( m \) then the frequency of emission and absorption of radiation will vary with a frequency \( \sim m^{-1} \). An oscillatory \( \alpha \) might also be attributable to the decaying oscillations of a scalar field that couples to \( F_{\mu \nu} F^{\mu \nu} \). Such a theory is allowed by enforcing an approximate global symmetry (Carroll 1998).

In summary, there is much current theoretical motivation for experimental searches for variability in \( \alpha \), particularly at medium to high redshifts. A detection of variation may allow us to probe the extra dimensions expected from many modern unified theories. A search for varying \( \alpha \) provides an important tool for seeking out and constraining the form of new physics.

## 3 PREVIOUS EXPERIMENTAL WORK

### 3.1 Terrestrial and laboratory constraints

Direct laboratory measurements provide interesting constraints on a time-varying \( \alpha \). Prestage, Robert & Maleki (1995) introduced a new technique comparing the rates of clocks based on ultra-stable oscillators. Relativistic corrections are order \( (Z_n \alpha)^2 \) where \( Z_n \) is the atomic number or nuclear charge. By comparing the rates of two clocks based on different atoms (H-maser and Hg\(^+\)) over a 140 day period, they were able to constrain \( |\Delta \alpha/\alpha| \leq 3.7 \times 10^{-14} \) yr\(^{-1} \) (i.e. \( |\Delta \alpha/\alpha| \leq 1.4 \times 10^{-14} \)). Model dependent upper limits on any variation have been claimed from an analysis of the Oklo phenomenon — a natural nuclear fission reactor that operated in Gabon, West Africa, \( \sim 1.8 \) billion years ago. Shlyakhter (1976) originally
constrained the energy of the nuclear resonance level in the $^{150}$Sm isotope and related this to upper bounds on $|\Delta \alpha/\alpha|$. Damour & Dyson (1996) have also analysed the problem with different model assumptions and claim $-0.9 \times 10^{-7} < \Delta \alpha/\alpha < 1.2 \times 10^{-7}$. Recently, Fujii et al. (2000) obtained somewhat tighter constraints using new samples from the Oklo reactor: $\Delta \alpha/\alpha = (-0.04 \pm 0.15) \times 10^{-7}$.

However, the Oklo limit corresponds to variations at very low ‘redshift’, $z \sim 0.1$, in a non-cosmological environment. In the absence of a detailed theory giving both time and space variations of $\alpha$, it is dangerous to compare time variations in areas of different gravitational potential (Barrow & O’Toole 2000). Also, there are considerable uncertainties regarding the complicated Oklo environment and any limits on $\alpha$ derived from it can be weakened by allowing other interaction strengths and mass ratios to vary in time as well.

3.2 Constraints from QSO spectra

Savedoff (1956) first analysed doublet separations seen in galaxy emission spectra to constrain possible time variation of $\alpha$. Absorption lines in intervening clouds along the line of sight to QSOs are substantially narrower than intrinsic emission lines and therefore provide a more precise probe of $\alpha$. This prompted Bahcall, Sargent & Schmidt (1967) to use alkali-doublet spacings seen in the absorption spectra of QSOs to arrive at firm upper limits on any variation. The appeal of this method is the huge time span probed by high-redshift observations. Wolfe, Brown & Roberts (1976) first applied the alkali-doublet (AD) method to intervening Mg $\Pi$ absorption. Varshalovich, Panchuk & Ivanchik (1996) have used the AD method for many absorbers to obtain upper limits on any variation at redshifts $z \sim 2.8-3.1$: $\Delta \alpha/\alpha = (2 \pm 7) \times 10^{-5}$.

Varshalovich, Potekhin & Ivanchik (2000) have recently analysed 16 Si $\text{iv}$ absorption systems (towards 6 QSOs) using the AD method. They find a mean $\Delta \alpha/\alpha = (-4.6 \pm 4.3 \pm 1.4) \times 10^{-5}$ using the Si $\text{iv}$ laboratory wavelengths of Morton (1991). The systematic component to the error above $(1.4 \times 10^{-5})$ allows for the relative uncertainties of the Si $\text{iv}$ laboratory wavelengths. However, Griesmann & Kling (2000) have increased the absolute precision of these wavelengths and their new values indicate that the Varshalovich et al. (2000) result should be corrected by $\approx +11.3 \times 10^{-5}$ to $\Delta \alpha/\alpha \approx (+7 \pm 4) \times 10^{-5}$ suggesting that the systematic error component added by Varshalovich et al. was significantly underestimated.

In Murphy et al. (2001c) we have used the new Griesmann & Kling laboratory wavelengths to constrain $\Delta \alpha/\alpha$ using 21 Si $\text{iv}$ doublets towards 8 QSOs. The spectral resolution and SNR are higher than for the Varshalovich et al. sample. This, and the higher precision laboratory wavelengths, provide a more stringent constraint of $\Delta \alpha/\alpha = (-0.5 \pm 1.3) \times 10^{-5}$. This result is nevertheless a factor of 7 less precise than the results we present in this paper, highlighting the strength of the methods we use.

The optical techniques above were based on the AD method: constraining $\alpha$ from the splitting of single ADs such as Si $\text{iv}$, C $\text{iv}$ and Mg $\text{ii}$. Very recently, however, Dzuba et al. (1999a) and W99 proposed a new method that allows an order of magnitude increase in precision. The method is based on measuring the wavelength separation between the resonance transitions of different ionic species with no restriction on the multiplet to which the transitions belong. We outline this many-multiplet (MM) method and discuss its advantages in Section 3 of this paper.

Radio spectra of QSO absorption clouds also provide the opportunity for tightly constraining possible variations in the fundamental constants. Wolfe et al. (1976) demonstrated that combining optical resonance and H $\text{I}21$ cm hyperfine absorption spectra could yield constraints on $\alpha^2 g_\mu m_e/m_p$. Here, $g_\mu$ is the proton g-factor and $m_e$ and $m_p$ are the mass of the electron and proton respectively; see also the discussion by Pagel (1983). Varshalovich & Potekhin (1996) used a comparison of H $\text{I}21$ cm hyperfine and molecular rotational absorption to constrain variations in $m_p$ but Drinkwater et al. (1998) showed that such a combination actually constrains $g_\mu \equiv \alpha^2 g_\mu$. In Murphy et al. (2001d) we have also made a more complete analysis of the two Drinkwater et al. radio spectra to obtain constraints on $g_\mu$. Assuming $g_\mu$ to be constant, we find $\Delta \alpha/\alpha = (-0.10 \pm 0.22) \times 10^{-5}$ and $\Delta \alpha/\alpha = (-0.08 \pm 0.27) \times 10^{-5}$ at $z = 0.25$ and 0.68 respectively. If we note the low-$z$ points in the lower panel (binned data) of Fig. 3 then we see that our results are also consistent with the two radio points. Carilli et al. (2000) have also recently analysed independent spectra of these two QSOs and find an upper limit on any variation consistent with our measurements: $|\Delta \alpha/\alpha| < 0.85 \times 10^{-5}$ (again assuming $g_\mu$ to be constant).

Cowie & Songaila (1995) have also obtained constraints at $z \approx 1.78$. They compare the observed frequencies of the H $\text{I}21$ cm and UV C $\text{i}$ absorption lines which are sensitive to variations in $g_\mu \alpha^2 m_p/\mu_p$. If one assumes that $g_\mu \alpha^2/\mu_p$ is constant then their constraint corresponds to $\Delta \alpha/\alpha = (0.35 \pm 0.55) \times 10^{-5}$.

3.3 Early universe (CMB and BBN)

A smaller value of $\alpha$ in the past would change the ionization history of the universe, postponing the recombination of electrons and protons, i.e. last-scattering would occur at lower redshift. It would also alter the ratio of baryons to photons at last-scattering, leading to changes in both the amplitudes and positions of features in the cosmic microwave background (CMB) power spectrum, primarily at angular scales $\lesssim 1^\circ$ (Hannestad 1999; Kipling, Scherrer & Turner 1999; Avelino, Martins & Rocha 2000; Battye, Crittenden & Weller 2000; Kujat & Scherrer 2000).

Kolb, Perry & Walker (1986) have discussed how limits can be placed on $\Delta \alpha/\alpha$ at the time of big bang nucleosynthesis (BBN) (corresponding to a redshift $z \sim 10^6 - 10^9$) by assuming a simple scaling between the value of $\alpha$ and the neutron-proton mass difference. Using observations of the $^4$He abundance they derive limits of $|\alpha/\alpha| < 15 \times 10^{-15} \hbar_00 \text{yr}^{-1}$, corresponding to $|\Delta \alpha/\alpha| < 9.9 \times 10^{-5}$.

Barrow (1987) and Campbell & Olive (1995) considered the simultaneous variation of weak, strong and electromagnetic couplings on primordial nucleosynthesis. However, these limits are beset by a crucial uncertainty as to the electromagnetic contributions to the neutron-proton mass difference. Much weaker limits are possible if attention is re-
restricted to the nuclear interaction effects on the nucleosynthesis of deuterium, helium-3, and lithium-7.

Bergström, Igiug & Rubinstein (1999) have re-examined all light elements up to \(^7\text{Li}\). By including elements heavier than \(^4\text{He}\) they avoid the problem of the unknown electromagnetic contributions to the neutron-proton mass difference, and argue that a more realistic limit, given the present observational uncertainties in the light element abundances is more like \(2 \times 10^{-2}\).

4 THEORETICAL BASIS OF THE MANY-MULTIPLET METHOD

The MM method allows an order of magnitude greater precision compared to the previous AD method. The full details behind this technique are presented in detail in Dzuba et al. (1999a,b, 2001) and W99 and so we present only the salient features here.

To explain the MM method, we begin with a simple analytic approach to estimate the relativistic effects in transition frequencies. If we consider a many-electron atom/ion then the relativistic correction, \(\Delta\), to the energy of the external electron can be written as

\[
\Delta \propto (Z_\alpha \alpha)^2 |E|^3/2 \left[ 1 - C(j,l) \right],
\]

where \(Z_\alpha\) is the nuclear charge, \(E\) is the electron energy \((E < 0, |E|\) is the ionization potential) and \(j\) and \(l\) are the total and orbital electron angular momenta. The contribution to the relativistic correction from many-body effects is described by \(C(j,l)\). For \(s\) and \(p\) orbitals, \(C(j,l) \approx 0.6\) and is of similar magnitude for \(d\) orbitals. Equation 2 therefore provides a general strategy for probing the relativistic corrections in resonance transitions.

For example, consider comparison of the transition energies of two \(s-p\) transitions, one in a light ion, the other in a heavy ion (i.e. low and high \(Z_\alpha\) respectively). The \(Z_\alpha^2\) term dominates so the relativistic corrections to the transition energies will differ greatly. Thus, comparison of the spectra of light and heavy species is a sensitive probe of \(\alpha\).

As a further example, consider an \(s-p\) and a \(d-p\) transition in a heavy species. The corrections will be large in each case but will be of opposite sign since the many-body corrections, \(C(j,l)\), begin to dominate with increasing \(j\). This situation also allows tight constraints to be placed on \(\alpha\).

Thus, comparing spectra of transitions from different multiplets and different atoms or ions, provides a sensitive method for probing variations in \(\alpha\). In comparison, the fine splitting of an \(s-p\) doublet will be substantially smaller than the absolute shift in the \(s-p\) transition energy since the excited \(p\) electron, with relatively small \(|E|\), will have much smaller relativistic corrections than the \(s\) electron. Therefore, the AD method is relatively insensitive to variations in \(\alpha\).

More formally, the energy equation for a transition from the ground state, within a particular multiplet, at a redshift \(z\) can be written as

\[
E_z = E_\infty + Q_1 Z_\alpha^2 \left( \frac{\alpha_\lambda}{\alpha_0} \right)^2 - 1 + K_1(LS) Z_\alpha^2 \left( \frac{\alpha_\lambda}{\alpha_0} \right)^2 + K_2(LS)^2 Z_\alpha^4 \left( \frac{\alpha_\lambda}{\alpha_0} \right)^4,
\]

where \(\alpha_\lambda\) may or may not be equal to the laboratory value, \(\alpha_0\). Here, \(L\) and \(S\) are the electron total orbital angular momentum and total spin respectively and \(E_\infty\) is the energy of the configuration centre. \(Q_1, K_1\) and \(K_2\) are relativistic coefficients which have been accurately computed in Dzuba et al. (1999a,b, 2001) using \textit{ab initio} many-body calculations. These calculations were tested by comparison with experimental data for energy levels and fine structure intervals. Equation 3 forms the basis of the MM method since it can be applied to any resonance transition observed in the QSO spectra – another advantage it has over the AD method.

For our purposes, the most convenient form of equation 3 is written as

\[
\omega_z = \omega_0 + q_1 x + q_2 y,
\]

where \(\omega_z\) is the wavenumber in the rest-frame of the cloud, at redshift \(z\), \(\omega_0\) is the wavenumber as measured on Earth and \(x\) and \(y\) contain the information about a possible non-zero \(\Delta \alpha/\alpha\):

\[
x \equiv \left( \frac{\alpha_\lambda}{\alpha_0} \right)^2 - 1 \quad \text{and} \quad y \equiv \left( \frac{\alpha_\lambda}{\alpha_0} \right)^4 - 1.
\]

The values of the relativistic corrections, \(q_1\) and \(q_2\), are presented in Table 1 for all transitions commonly seen in optical QSO spectra. The values of the \(q_1\) coefficients are typically an order of magnitude larger than the \(q_2\) coefficients. Therefore, it is the relative magnitudes of \(q_1\) for different transitions that characterize our ability to constrain \(\Delta \alpha/\alpha\). The uncertainty in the \(q_1\) co-efficients varies from ion-to-ion and is \(\sim 5\) cm\(^{-1}\) for alkali-like ions such as Mg\(\text{II}\). However, the co-efficients for the complicated Ni\(\text{II}\) transitions carry a larger uncertainty \(\sim 200\) cm\(^{-1}\) (Dzuba et al. 2001). The form of equation 3 is very convenient since the second and third terms only contribute if \(\Delta \alpha/\alpha \neq 0\); errors in the \(q_1\) and \(q_2\) coefficients cannot lead to an artificial non-zero value of \(\Delta \alpha/\alpha\).

From equation 3, we can see that \(q_1\) will be much larger in heavier ions due to the \(Z_\alpha^2\) dependence. Indeed, one can see in Table 1 several combinations of transitions from different ions, of very different mass, showing large differences between their respective \(q_1\) coefficients. The combination of the Mg\(\text{I}\) \(\lambda 2853\) line, the Mg\(\text{II}\) doublet and the five Fe\(\text{II}\) lines between \(\lambda 2344\) and \(\lambda 2600\) was used in W99 since the Fe\(\text{II}\) \(q_1\) coefficients typically differ from those of the Mg lines by almost an order of magnitude. It is this comparison of spectra from different ions that allows the order of magnitude increase in precision over previous methods. For comparison, we present the line shifts in wavenumber, wavelength and velocity space arising from a shift of \(\Delta \alpha/\alpha = +10^{-5}\) in Table 2.

Further examination of the \(q_1\) coefficients in Table 1 reveals several other very useful combinations of lines. In particular, note the large negative values for the Cr\(\text{II}\) lines. A comparison between Cr\(\text{II}\) spectra and that of Zn\(\text{II}\) – the \(\lambda 2026\) transition having the largest magnitude value of \(q_1\) – provides the most sensitive combinations for probing non-zero \(\Delta \alpha/\alpha\). Also, note the coefficients for Ni\(\text{II}\). Here, within the same species (but different multiplets), we have both positive and negative values for \(q_1\). This unique case is due to the very complicated multiplet structure of Ni\(\text{II}\) as discussed in detail in Dzuba et al. (2001).
We may summarise the advantages of the MM method over the AD method as follows:

- By including all relativistic corrections (i.e. including those for the ground state) there is a sensitivity gain of around an order of magnitude compared to the AD method.
- In principle, all transitions appearing in a QSO absorption system may be used. This provides an obvious statistical gain and a more precise constraint on $\Delta \alpha / \alpha$ compared to using a single AD alone.
- A further advantage of using many transitions is that the velocity structure is determined with much greater reliability due to the larger range of line strengths (see Section 5.1 for further explanation).
- A very important advantage is that comparison of transitions with positive and negative $q_1$ coefficients minimizes systematic effects (see Section 5.1.3 in particular).

Finally, we note that the $q_1$ and $q_2$ coefficients for Al ii λ1670 and Si ii λ1526 in Table 3 have not been presented elsewhere before. In the case of Al ii λ1670, the coefficients were calculated using the same methods described in Dzuba et al. (1999a,b). The coefficients for Si ii λ1808 do appear in Dzuba et al. (1999b) but the calculation has been re-performed to include other Si ii lines, including λ1526. Thus, there is a small ($\approx 5\%$) difference between the previous values and the one presented in Table 3. This small difference is within the precision of the Dzuba et al. (1999a,b) calculations and does not significantly affect our determination of $\Delta \alpha / \alpha$.

5 DATA REQUIREMENTS, ACQUISITION AND REDUCTION

The fitting of high-resolution (FWHM $\sim 7$ km s$^{-1}$, $R \sim 45000$), moderate signal-to-noise ratio (SNR $\sim 30$ per pixel) QSO absorption lines routinely yields redshifts of single velocity components measured to precisions of $\sigma(z) \sim 3 \times 10^{-6}$ or $\sigma(v) \sim 1$ km s$^{-1}$ in velocity space (Outram, Chaffee & Carswell 1999). By comparison with the line shifts in Table 3 and accepting that several well constrained velocity components will exist in each absorption complex, the level of precision achievable with the MM method is $\sigma(\Delta \alpha / \alpha) \sim 5\times 10^{-5}$ per absorption cloud. If systematic effects are to be avoided when using a large number (i.e. $\sim 50$) of absorption systems then, from equation 4 we require $\omega_0$ to be known to a precision of $\sigma(\omega_0) \sim 0.003$ cm$^{-1}$ – an order of magnitude more precise than available wavelength compilations (e.g. Morton 1991).
We therefore require high-resolution, moderate SNR QSO spectra and new laboratory measurements of UV resonance transition wavelengths in order to reach a precision of $\sigma(\Delta \alpha/\alpha) \sim 10^{-5}$ for each absorption system.

### 5.1 QSO Spectra

#### 5.1.1 General properties

All our QSO spectra were obtained at the Keck I 10 m telescope with the HIRES facility (Vogt et al. 1994). The spectra separate conveniently into two samples with several defining features. One sample comprises spectra of 28 Mg II/Fe II absorbers in the spectra of 17 QSOs covering a redshift range $0.5 < z_{\text{abs}} < 1.8$. The second sample comprises 18 damped Lyman-$\alpha$ systems (DLAs) in the spectra of 17 QSOs covering $1.8 < z_{\text{abs}} < 3.5$. This later sample also contains three lower redshift Mg II/Fe II systems (i.e. a total of 21 absorbers comprises this sample). Different groups observed each sample. Thus, with only a small degree of overlap, we label the samples according to the typical redshift of the absorption systems. The major difference between the low-$z$ and high-$z$ samples is that the low-$z$ sample only contains transitions of Mg II and Fe II whereas the high-$z$ sample has a more diverse range of transitions present (see Section 5.1.3).

#### 5.1.2 Low-$z$ ($0.5 < z < 1.8$, $(z) = 1.0$)

This sample comprises the same data set analysed in W99, with some differences as detailed in Section 5.1.2. The observations were taken in 1994 July, 1995 January and 1996 July. The SNR per pixel ranged from 15–50 with most spectra having SNR $\sim 30$. The FWHM was $\sim 6.6$ km s$^{-1}$ ($R = 45000$). The QSOs were generally bright ($m_V \lesssim 17.5$) and so several short ($\sim 1000$ s) exposures were taken of each object. The data were reduced with a combination of IRAF routines and personal code. Individual frames were overscan subtracted, bias frame corrected and flat-fielded. Cosmic rays were removed by median filtering and the frames were averaged to form the final image. $1\sigma$ error arrays were generated assuming Poisson counting statistics. We fitted continua to regions of each spectrum containing any of the relevant transitions by fitting Legendre polynomials to $\sim 500$ km s$^{-1}$ sections. Full details of the reduction process are given in Churchill (1995, 1997) and Churchill et al. (1999). We have also used the spectrum of Q0000–26 analysed by Lu et al. (1996).

Wavelength calibration of the frames was carried out within IRAF: Thorium–Argon (THAr) lamp exposures were taken before and after the QSO exposures and co-added to provide a calibration spectrum. THAr lines were selected and centroided to provide a wavelength solution. The solution was applied to the corresponding spectra without any resampling or linearization so that the absorption line shapes were not distorted in the process. We also note that no image rotator was installed during these observations and so the spectrograph slit was not perpendicular to the horizon in general. We make a detailed analysis of these points and their effect on our results in M01b.

The transitions used in this sample are the five Fe lines, Fe II $\lambda 2344$–$\lambda 2600$, and the Mg transitions, Mg I $\lambda 2853, 2803$ and Mg II $\lambda 2796$ and $\lambda 2803$. The Mg lines have small $q_i$ coefficients and so act as anchors against which the larger Fe II shifts can be measured. This set of lines is also very useful because it offers a range of line strengths due to the differing Fe II oscillator strengths (see Table 1) and, together with the similar ionization potentials of Fe II and Mg II, facilitates reliable determination of the velocity structure of the absorption complex. In some cases the Mg II lines are saturated and so the Mg II lines themselves provide only weak constraints on $\Delta \alpha/\alpha$. However, the weak Mg I $\lambda 2853$ then often serves to provide a good constraint on the velocity structure – a further advantage of using Mg/Fe absorption systems to probe $\Delta \alpha/\alpha$. To illustrate these points, we provide an example absorption system, together with our Voigt profile fits, in Fig. 1.

#### 5.1.3 High-$z$ ($0.9 < z < 3.5$, $(z) = 2.1$)

These observations were spread over many observing runs from 1994 to 1997. The SNR per pixel ranges from 15–40 with most spectra having SNR $\sim 30$ and FWHM $\lesssim 7.5$ km s$^{-1}$ ($R = 34000$). The QSOs themselves are at higher redshift and so appear much fainter than those of the low-$z$ sample: $m_V \lesssim 19.0$. Consequently, the total integration times were much longer than for the low-$z$ sample and many more frames were co-added during the reduction process.

\[ \text{Table 2. Shift in the rest frame wavenumber, wavelength and velocity space for } \Delta \alpha/\alpha = +10^{-5} \]

| Transition | $\Delta \omega$ $10^{-2}$ cm$^{-1}$ | $\Delta \lambda$ $10^{-3}$ Å | $\Delta v$ km s$^{-1}$ |
|------------|-----------------------------------|-----------------------------|----------------------|
| Mg I $\lambda 2853$ | 0.17 | -0.14 | -0.015 |
| Mg II $\lambda 2796$ | 0.42 | -0.33 | -0.035 |
| Mg II $\lambda 2803$ | 0.24 | -0.19 | -0.020 |
| Al III $\lambda 1670$ | 0.54 | -0.15 | -0.027 |
| Al III $\lambda 1854$ | 0.93 | -0.32 | -0.052 |
| Al III $\lambda 1862$ | 0.43 | -0.15 | -0.024 |
| Si II $\lambda 1526$ | 0.14 | -0.032 | -0.0062 |
| Si II $\lambda 1808$ | 1.06 | -0.35 | -0.058 |
| Cr II $\lambda 2056$ | -2.11 | 0.89 | 0.130 |
| Cr II $\lambda 2062$ | -2.40 | 1.02 | 0.148 |
| Cr II $\lambda 2066$ | -2.57 | 1.10 | 0.159 |
| Fe II $\lambda 1608$ | 2.57 | -0.66 | -0.124 |
| Fe II $\lambda 1611$ | 2.41 | -0.63 | -0.117 |
| Fe II $\lambda 2344$ | 2.84 | -1.56 | -0.199 |
| Fe II $\lambda 2374$ | 3.56 | -2.01 | -0.254 |
| Fe II $\lambda 2383$ | 3.28 | -1.86 | -0.234 |
| Fe II $\lambda 2557$ | 3.23 | -2.16 | -0.250 |
| Fe II $\lambda 2600$ | 2.91 | -1.97 | -0.227 |
| Ni II $\lambda 1700$ | 1.60 | -0.47 | -0.082 |
| Ni II $\lambda 1741$ | -1.40 | 0.42 | 0.073 |
| Ni II $\lambda 1751$ | -0.60 | 0.18 | 0.032 |
| Zn II $\lambda 2026$ | 4.96 | -2.04 | -0.301 |
| Zn II $\lambda 2062$ | 3.15 | -1.34 | -0.195 |

\[ \text{‡ IRAF is distributed by the National Optical Astronomy Observatories, which are operated by the Association of Universities for Research in Astronomy, Inc., under cooperative agreement with the National Science Foundation.} \]
Figure 1. Mg/Fe absorption system towards Q1213−003 at z = 1.554. The data have been normalized by a fit to the continuum and plotted as a histogram. Our Voigt profile fit (solid curve) and the residuals (i.e. [data]−[fit]), normalized to the 1σ errors (horizontal solid lines), are also shown. The tick–marks above the continuum indicate individual velocity components. Note the range of line strengths in Fe\textsc{ii}, facilitating determination of the velocity structure. The large number of Fe\textsc{ii} transitions and the large number of velocity components allows for tight constraints to be placed on ∆α/α. In this case, the Mg\textsc{i}λ2853 is also present but is sufficiently weak so as not to provide any constraint on ∆α/α. In cases where the Mg\textsc{ii} lines are more saturated, the Mg\textsc{i} line is typically stronger and can be used to constrain the velocity structure.

An image rotator was installed in 1996 August and so only about half the observations were carried out with the slit perpendicular to the horizon.

Most of the data were reduced using \textsc{makee}, the HIRES data reduction package written by T. Barlow. This package converts the two-dimensional echelle images to fully reduced, one-dimensional, wavelength calibrated spectra (calibration spectra were taken in the same way as for the low-z sample). Some of the spectra were reduced when \textsc{makee} had no wavelength calibration facility. In these cases, wavelength calibration was carried out using \textsc{iraf} routines. The remainder of the spectra were fully reduced within \textsc{iraf}. 1σ error arrays were generated assuming Poisson counting statistics. We fitted continua to regions of each spectrum containing any of the relevant transitions by fitting Legendre polynomials to ∼ 500 kms$^{-1}$ sections. Full details of the reduction procedures can be found in Prochaska & Wolfe (1996, 1997, 1999). Outram, Chaffee & Carswell (1999) have also kindly provided their spectrum of Q1759+75 which was taken in 1997 July.

We also noted a small but important difference between the \textsc{iraf} and \textsc{makee} wavelength calibration software. \textsc{iraf} makes use of an internal list of vacuum ThAr wavelengths and so spectra calibrated with \textsc{iraf} have “correct” wavelength scales. However, the \textsc{makee} package calibrates spectra with a list of air ThAr wavelengths and converts the final QSO wavelength scale to vacuum using the Cauchy formula for the refractive index (Weast 1979). However, this formula does not reproduce the experimental dispersion: it shows deviations from experiment at the level of 10$^{-6}$ in the optical range. We therefore converted the wavelength scales of the spectra reduced with \textsc{makee} back to air wavelengths using the Cauchy formula and then re-converted to vacuum wavelengths with the preferred Edlén (1966) formula. A detailed discussion of air–vacuum conversion with caveats of the above statements is given in M01b.
Possible evidence for a variable $\alpha$ from QSO absorption lines: motivations, analysis and results

Figure 2. Heavy element absorption lines from the damped Lyman-$\alpha$ system towards Q2206$-$199 at $z = 1.920$. We illustrate this system since it displays both saturated and unsaturated transitions. However, the metal lines in other DLAs generally have lower column densities. The data have been normalized by a fit to the continuum and plotted as a histogram. Our Voigt profile fit (solid curve) and the residuals (i.e. [data] − [fit]), normalized to the 1$\sigma$ errors (horizontal solid lines), are also shown. The tick–marks above the continuum indicate individual velocity components. In this case, the Fe II and Si II lines provide constraints on the velocity structure while the Ni II, Cr II, and Zn II are strong enough to provide tight constraints on $\Delta \alpha/\alpha$. Note that the Cr II and Zn II $\lambda$2062 profiles are blended together but that the constraints on the velocity structure from all other transitions allow us to make a statistically acceptable fit.

Theoretically, in damped systems such as those comprising this sample, the combination of lines providing the best constraints on $\Delta \alpha/\alpha$ are those of Zn II and Cr II. In practice, however, these lines are generally quite weak and so the parameter constraints are not optimal. Also, the Zn II and Cr II $\lambda$2062 profiles are often blended together (the transitions are only separated by 60 kms$^{-1}$), reducing the strength of the $\Delta \alpha/\alpha$ constraint. The Ni II lines are also generally weak but have the advantage of a variety of widely differing $q_1$ coefficients. Also note that the only Fe II lines available for these high-$z$ absorbers are the Fe II $\lambda$1608 and $\lambda$1611 lines. These can be used in conjunction with the two Si II lines to provide a reasonable constraint on $\Delta \alpha/\alpha$ but their main advantage is that they provide good constraints on the velocity structure. We plot a typical absorption complex in Fig. 2 to illustrate the above points and also to give the reader some idea of the relative strengths of the different transitions used in analysing this sample.

In 6 spectra we have also fitted the two lines of Al III. Variations in the incident radiation field could give rise to changes in the relative column densities when comparing species with ionization potentials above and below the Lyman edge. In our sample, the Al III velocity structures correspond well with those of the singly ionized atoms (consistent with the conclusions of Wolfe & Prochaska 2000) and the value of $\Delta \alpha/\alpha$ proved to be slightly better constrained by including the Al III lines. In some cases, however, some velocity components in the Al III profiles were much weaker or stronger relative to the other components when compared with the profiles of singly ionized species. In one case, our fitting algorithm removed many weak Al III components from the fit (see Section 6.1) and so we removed the Al III data in this instance.
Table 3. The isotopic structures of the Mg and Si transitions. The composite values are given in Table 3. The Mg isotopic spacings were measured by Hallstadius (1979) but the spacings for Si are estimates based on a scaling of the Mg ii λ2796 structure. The hyperfine structure of 25Mg is also shown (Drullinger, Wineland & Bergquist 1980). The last column shows the relative abundance not used for any heavier ions.

| Transition | m/amu | ω0/cm⁻¹ | λ0/Å | % |
|------------|-------|----------|------|---|
| Mg i λ2853 | 24    | 35051.271| 2852.9636 | 79.0 |
|           | 25    | 35051.295| 2852.9616 | 10.0 |
|           | 26    | 35051.318| 2852.9598 | 11.0 |
| Mg ii λ2803 | 24    | 35669.286| 2803.5324 | 79.0 |
|           | 25    | 35669.300| 2803.5313 | 2.7 |
|           | 26    | 35669.310| 2803.5305 | 1.5 |
|           | 25    | 35669.360| 2803.5266 | 2.8 |
|           | 26    | 35669.370| 2803.5258 | 3.0 |
| Mg ii λ2796 | 24    | 35760.937| 2796.3473 | 11.0 |
|           | 25    | 35760.913| 2796.3492 | 5.8 |
| Si ii λ1808 | 28    | 55309.330| 1808.0132 | 92.2 |
|           | 29    | 55309.390| 1808.0113 | 4.7 |
|           | 30    | 55309.446| 1808.0094 | 3.1 |
| Si ii λ1526 | 28    | 65500.442| 1526.7073 | 92.2 |
|           | 29    | 65500.517| 1526.7055 | 4.7 |
|           | 30    | 65500.583| 1526.7040 | 3.1 |

5.2 Laboratory wavelength measurements

The laboratory rest wavelengths were measured by various groups using Fourier transform spectrometry. We discuss the measurements for each ion below, concentrating on those issues most relevant to our analysis. We present the wavelengths that we have adopted in Table 3. It is interesting to note that, with the exception of the Fe i spectrum, the wavelengths presented in Table 3 are systematically longer than those compiled in Morton (1991) – a widely used list of resonance transition wavelengths. For a particular transition, the wavelengths are generally consistent but, taken altogether, a systematic trend is noted.

- Mg i and Mg ii: These spectra have recently been measured by Pickering, Thorne & Webb (1998). The spectra of Ni i and Ni ii were excited along with those of Mg i and Mg ii and several of these lines were used for calibration. The Ni i spectrum of Litzén, Brault & Thorne (1993) was used for reference which itself was calibrated from the Fe i and Fe ii lines of Nave et al. (1991). The Mg ii λ2796 wavelength has been measured previously by Drullinger, Wineland & Bergquist (1980) and Nagourney & Dehmelt (1981) and the wavenumbers are in excellent agreement. Also, a confirmation of the Pickering et al. (1998) wavenumbers has been made and is described briefly in Pickering et al. (2000).

Since Mg is a relatively light atom, the isotopic structure of the line profile must be taken into account. Pickering et al. (1998) used the isotopic spacings measured by Hallstadius (1979) to obtain absolute wavelengths for the isotopes. These values are listed in Table 3 and were used in our analysis.

- Si ii, Al ii and Al iii: These spectra have recently been measured by Griesmann & Kling (2000). The C iv and Si iv spectra were also measured and all spectra were calibrated using the Ar ii spectrum of Whaling et al. (1995). At present, there are no other similarly precise measurements of these spectra.

To our knowledge, the isotopic spacings for the Si ii transitions have not been measured. The mass shift and the specific mass shift should dominate the volume shift in such a light ion. The 1s2 3P2 → 1s1 3D1 transition is very similar to those of Mg ii and so the specific mass shift should be of the same order. Thus, to estimate the isotopic spacings in Si ii λ1526 we have scaled the spacings of Mg ii λ2796 by the mass shift: \( \Delta \omega_i \propto \omega_0/m^2 \) for \( \Delta \omega_i \), the wavenumber shift for a given isotope i where \( m \) is the atomic mass. We have used these spacings to fit a synthetic Gaussian emission line (centred at the composite wavelength) in order to estimate the absolute wavenumbers for the isotopes. We present the results in Table 3. We performed similar calculations for the Si ii λ1808 transition. However, the assumption that the specific shift for λ1808 is similar to that for the Mg ii transitions is not so justified in this case since the transitions are of quite different type (see Table 3). We discuss any effect this approximation may have on \( \Delta \alpha/\alpha \) in M01b but find that it should be negligibly small.

- Cr ii and Zn ii: These spectra have been measured independently using two different Fourier transform spectrometers: one at Imperial College (IC), and another at Lund University (LU). The two experiments are described in Pickering et al. (2000). The wavelength calibration was based on the Fe i and ii standards of Nave et al. (1991) in both cases.

- Fe ii: This spectrum, from 1750–3850 Å, is presented in Nave et al. (1991). The wavelength calibration was done by comparison with the Norlén (1973) Ar ii spectrum. No other (similarly precise) catalogues of Fe ii lines exist in the literature. We have obtained the Fe ii λ1608 and 1611 wavenumbers from S. Johansson (private communication).

- Ni ii: This spectrum was recently measured by Pickering et al. (2000). The original spectra were measured during the Mg i and ii experiments by Pickering et al. (1998). Wavenumber calibration was done using the Ni ii standards of Litzén, Brault & Thorne (1993) which cover the region down to about 2000 Å. The Ni i lines between 1750 Å and 2000 Å were calibrated with the Fe i and ii lines so as to be used as calibration lines for the Ni ii spectrum. R. Kling (private communication) has confirmed these wavenumbers, albeit with lower precision.

All wavelength calibrations above rely on the the Ar ii spectrum measured by either Norlén (1973) or Whaling et al. (1995). However, the Norlén and Whaling calibrations systematically disagree. The Whaling wavenumbers are larger and the difference between them is proportional to the wavenumber: \( \delta \omega = 7 \times 10^9 \omega \). Since this difference is linear in frequency (velocity) space, as long as we normalize all measured wavenumbers to the one calibration scale, any systematic error will be completely absorbed into the redshift parameter when we centroid corresponding velocity components in different transitions in the absorption systems (see Section 3 for further explanation). We choose to normalize all measured wavenumbers to the Norlén calibra-
tion scale and so the wavelengths of the Si II, Al I and Al III transitions in Table 2 have been scaled accordingly.

Also of note is that we only take into account the isotopic structures for the lightest two elements, Mg and Si. In the optically thin limit, the centroids of the isotopic structures described in Table 3 reduce to the composite values given in Table 2. When a line becomes optically thick, differential saturation of the isotopic components causes the centroid of the composite line to shift. This effect is discussed in detail in M01b and it is evident that we do not need to include isotopic information for the heavier ions.

6 ANALYSIS AND RESULTS

6.1 Analysis

Our analysis technique is based on a simultaneous \( \chi^2 \) minimization analysis of multiple component Voigt profile fits to the absorption features in several different transitions. Consider a QSO spectrum containing a single velocity component of a specific transition. Three parameters describe the Voigt profile fit to such a component: the column density, the Doppler width or \( b \)-parameter and the redshift \( z \) of the absorbing gas cloud. In our case, however, each absorption system contains many blended velocity components appearing in many different transitions.

The central assumption in the analysis is that the velocity structure seen in one ion corresponds exactly to that seen in any other ion. That is, we assume that there is negligible proper motion between corresponding velocity components of all ionic species. With this assumption comes a reduction in the number of free parameters to be varied in a particular fit since the redshift of corresponding velocity components in different transitions need only be specified once. We discuss this assumption and any effect it may have on \( \Delta \alpha/\alpha \) in M01b.

Further restrictions can be placed on the number of free parameters when fitting different transitions simultaneously since the \( b \)-parameters of corresponding velocity components in different ionic species are physically related. We may write

\[
\Delta \alpha_i = 2 \frac{kT_i}{M_i} + b_{i\text{urb}}^2
\]

as the \( b \)-parameter of an ion species \( i \) which has a mass \( M_i \). The first term describes the thermal broadening within a gas cloud which has a kinetic temperature, \( T_i \), and the second term describes an additional turbulent motion which affects all ions equally. If we assume that either thermal or turbulent broadening dominates for a particular component then again we reduce the number of free parameters. If we fit transitions of at least two ions with different masses then we can determine \( T \) and \( b_{\text{urb}} \) for each velocity component.

For the present case, we wish to add another free parameter to the fit: \( \Delta \alpha/\alpha \). From equation 6 we can see that \( \Delta \alpha/\alpha \) will be constrained by the difference \( \omega_z - \omega_0 \) for each transition if we fit two or more transitions simultaneously.

We have used the program \textsc{vpfit} (Webb 1987) to fit absorption profiles to the spectra. Previously, \textsc{vpfit} did not allow one to vary \( T \) and \( b_{\text{urb}} \) for each component independently, but dealt only with \( b_i \). There was also no provision for including \( \Delta \alpha/\alpha \) as a free parameter. We have therefore modified \textsc{vpfit} to include \( T \), \( b_{\text{urb}} \) and \( \Delta \alpha/\alpha \) explicitly as free parameters. This differs from the analysis in W99 where \( \Delta \alpha/\alpha \) was varied externally to \textsc{vpfit}. The main advantage is a significant gain in computational speed, allowing us to fit more complicated systems that would have taken prohibitively long using the method in W99. A minor point is that W99 presented 30 absorption systems whereas we present 28 using the same QSO spectral data due to slightly different subdivision of neighbouring absorption complexes.

Parameter errors can be calculated from the diagonal terms of the final parameter covariance matrix (Fisher 1958). The reliability of these errors has been confirmed using Monte Carlo simulations of a variety of different combinations of transitions and velocity structures.

\textsc{vpfit} imposes a cut-off point in parameter space such that very weak velocity components are removed from the fit when they no longer significantly affect the value of \( \chi^2 \). This presents a problem for our method since a given component may be weak in one transition (and so can be regarded as dispensable with respect to \( \chi^2 \)) but may be strong in another. An example of this can be seen in Fig. 2 where the two lowest velocity components do not appear in the weaker transitions. Conceivably, dropping even very weak components could affect our determination of \( \Delta \alpha/\alpha \). Therefore, in such cases we observed the trend in the values of \( \Delta \alpha/\alpha \), at each iteration \( i \) of the minimization routine to see if this trend was significantly altered due to line dropping. If components were dropped during a fit then we also re-ran the \textsc{vpfit} algorithm, keeping the dropped components by fixing their column density at the value just before they were dropped from the original fit. No cases were found where the values of \( \Delta \alpha/\alpha \) from the different runs differed significantly.

We impose several consistency checks before we accept a value of \( \Delta \alpha/\alpha \). Firstly, the value of \( \chi^2 \) per degree of freedom must be \( \sim 1 \). Secondly, to check internal consistency, we make three different fits to the data with three different conditions on the \( b \)-parameters: (i) entirely thermal broadening, (ii) entirely turbulent broadening and (iii) a fit where \( T \) and \( b_{\text{urb}} \) are determined by goodness of fit. The values of \( \Delta \alpha/\alpha \) derived from the three fits should be consistent with each other since the choice above should not greatly affect \( \Delta \alpha/\alpha \) (i.e. the redshifts of velocity components will not change systematically). If this was not the case then the data was rejected. Only 2 systems were rejected in this way. Since (iii) is the most physically realistic choice we expect \( \chi^2 \) for that fit to be less than that for cases (i) and (ii). This was indeed the case for all but a few systems. These exceptions were found to have very low average temperatures (across the velocity structure) or very small values of \( b_{\text{urb}} \). The difference between \( \chi^2 \) for the fit for case (iii) and (ii) or (i) respectively was small in these cases. We selected the final value of \( \Delta \alpha/\alpha \) from the regime which gave the lowest \( \chi^2 \) but the results were insensitive to this choice.

\$^6$ We require two or more transitions since fitting only one would render it and \( \Delta \alpha/\alpha \) degenerate for a single component and nearly degenerate for multiple components.

\[ \text{See http://www.ast.cam.ac.uk/~rfc/vpfit.html for details about obtaining \textsc{vpfit}.} \]
6.2 Results

We have analysed the low-$z$ sample in two stages. The first was motivated by the fact that we have used different techniques to those of W99. We took the final velocity structures for each absorption system found by W99, used them as first guesses for the parameters and determined $\Delta \alpha / \alpha$ with our new methods. In all cases the results were nearly identical to those of W99. The second stage was to fit the entire data set again, using no information about previous velocity structures. These are the results we present below.

Our results are presented in Table 4. We give the object, the QSO emission redshift, $z_{em}$, the absorption cloud redshift, $z_{abs}$, $\Delta \alpha / \alpha$ for that cloud and its associated 1$\sigma$ error. The transitions for each cloud are indicated with the ID letters defined in Table 4. Table 6 shows the weighted mean, $(\Delta \alpha / \alpha)_w$, the weighted mean, $(\Delta \alpha / \alpha)$ and the significance level, $\delta$, of the weighted mean for the low and high redshift samples and for the sample as a whole. We also include the value of the reduced $\chi^2$, $\chi^2_{red}$ (i.e. $\chi^2$ per degree of freedom), for each sample where the model is taken to be a constant equal to $(\Delta \alpha / \alpha)_w$.

Our results show that $\Delta \alpha / \alpha$ deviates from zero at a significance level of 4.1$\sigma$ over the redshift range 0.5 < $z$ < 3.5. We also see a general consistency between the low and high-$z$ samples. The values of $\chi^2_{red}$ in Table 6 are all less than unity. This indicates that, if we have miscalculated the error bars systematically, we have probably overestimated them rather than underestimated them. This is also reflected in a comparison of the root-mean-square deviation from the mean, RMS, and the average size of our error bars, $\langle \Delta \sigma (\Delta \alpha / \alpha) \rangle$; for the sample as a whole. RMS = 1.46 $\times$ 10$^{-5}$ and $\langle \Delta \sigma (\Delta \alpha / \alpha) \rangle$ = 2.01 $\times$ 10$^{-5}$. The RMS is also less than $\langle \sigma (\Delta \alpha / \alpha) \rangle$ for the low and high-$z$ samples taken alone. Assuming we have overestimated the errors on $\Delta \alpha / \alpha$ then we can scale them by a constant factor, $S$, so as to force $\chi^2_{red} = 1$. Column 8 in Table 6 shows the resulting increase in the significance of $(\Delta \alpha / \alpha)_w$. Note that the weighted means do not differ significantly from the unweighted means for either sample suggesting that the data error bars are reliable.

We have also conducted an F test on the $\Delta \alpha / \alpha$ parameter. We used the final velocity structures from the fitting procedure above to re-fit the absorption systems after removing the $\Delta \alpha / \alpha$ parameter. If $\Delta \alpha / \alpha$ is necessary to describe the data then we expect $\chi^2$ for each system to reduce when we include $\Delta \alpha / \alpha$. The reduction should be in accordance with the statistical significance of $\Delta \alpha / \alpha$ of each system. We denote $\chi^2$ for the fit to system $i$ with and without the $\Delta \alpha / \alpha$ parameter as $\chi^2_{\Delta \alpha}$ and $\chi^2_{\Delta \alpha}$ respectively. If the significance (in units of $\sigma$) of the value of $\Delta \alpha / \alpha$ for that system is $\delta_i$, we expect that

$$\sum_i \chi^2_{\Delta \alpha} - \chi^2_{\Delta \alpha} = \sum_i \delta_i^2$$

for $M$ absorbers.

The $\delta_i^2$ can be derived from the last column of Table 6. Direct calculation of both sides of equation (7) yields the results in the final two columns of Table 6. $\sum_i (\chi^2_{\Delta \alpha} - \chi^2_{\Delta \alpha}) \geq \sum_i \delta_i^2$ for both the low and high-$z$ samples, consistent with $\Delta \alpha / \alpha$ being a required parameter.

To illustrate the distribution of $\Delta \alpha / \alpha$ over cosmological time, we plot our results in Fig. 3. The upper panel of

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### Table 4

| Object | $z_{em}$ | $z_{abs}$ | Transition$^a$ | $\Delta \alpha / \alpha / 10^{-5}$ |
|--------|---------|---------|----------------|-----------------|
| low-$z$ sample | | | | |
| 0000–26 | 4.11 | 1.434 | bcqr | -0.732 ± 2.283 |
| 0002+05 | 1.90 | 0.851 | bcnpqcr | -0.239 ± 1.516 |
| 0117+21 | 1.49 | 0.729 | abcqqr | -0.403 ± 1.298 |
| 0420–01 | 0.915 | 0.633 | abc | -1.171 ± 1.800 |
| 0450–13 | 2.25 | 1.175 | bcpnpqqr | 0.314 ± 0.765 |
| 0454+03 | 1.34 | 0.860 | acnpqcr | -0.982 ± 0.868 |
| 0823–22 | 0.91 | 0.911 | bcnpqcr | -0.068 ± 0.661 |
| 1148+38 | 1.30 | 0.553 | bcq | -1.882 ± 1.699 |
| 1206+45 | 1.16 | 0.928 | bcnpqcr | -0.800 ± 1.578 |
| 1213–00 | 2.69 | 1.320 | abcnopqcr | -1.821 ± 0.893 |
| 1222+22 | 2.05 | 0.668 | bcnpq | -0.245 ± 1.549 |
| 1225+31 | 2.22 | 1.795 | abcnopqcr | -1.473 ± 1.521 |
| 1248+40 | 1.03 | 0.773 | bcnpqcr | 1.398 ± 1.260 |
| 1327+27 | 1.01 | 0.660 | bcnpqcr | -0.329 ± 1.301 |
| 1421+33 | 1.91 | 0.843 | bcnpqcr | -0.111 ± 0.793 |
| 1634+70 | 1.34 | 0.990 | bcnpqcr | -0.965 ± 0.968 |
| high-$z$ sample | | | | |
| 0019–15 | 4.53 | 3.439 | ghl | 0.290 ± 3.520 |
| 0149+33 | 2.43 | 2.140 | defghijklmstuvu | -3.420 ± 1.800 |
| 0201+37 | 2.49 | 1.476 | cnoqr | -0.775 ± 0.878 |
| 0227+30 | 1.02 | 0.519 | abcqqr | -4.486 ± 4.308 |
| 0254+04 | 1.02 | 0.934 | bcnpqcr | 0.530 ± 2.146 |
| 1317+27 | 1.01 | 0.660 | bcnpqcr | 0.348 ± 1.781 |
| 1421+33 | 1.91 | 0.843 | bcnpqcr | -0.111 ± 0.793 |
| 1427+22 | 1.01 | 0.660 | bcnpqcr | 0.348 ± 1.781 |
| 1634+70 | 1.34 | 0.990 | bcnpqcr | -1.586 ± 3.752 |

$^a$Transitions identified as in Table 4.

$^b$This absorber taken from Lu et al. (1996).

$^c$These QSOs are BL Lac objects and so their emission redshifts have large uncertainties. Indeed, the literature values for $z_{em}$ shown here are less than the measured absorption redshifts.

$^d$This absorber contributed by Outram, Chaffee & Carswell (1999).
Table 5. Statistics for the two subsamples and the sample as a whole. We give the average redshift, \( \bar{z} \), for each sample and the number of data points, \( N \), contributing to the weighted mean, \( \langle \Delta \alpha/\alpha \rangle_w \), and unweighted mean, \( \langle \Delta \alpha/\alpha \rangle \) (in units of \( 10^{-5} \)). We also give the significance, \( \delta \), of the deviation from zero and the reduced \( \chi^2 \) for the weighted mean. \( \delta_{\chi^2, \text{red}}=1 \) is the significance when we force \( \chi^2_{\text{red}}=1 \) by scaling all errors on \( \Delta \alpha/\alpha \) by \( S \). The final two columns contain the results of the F test.

| Sample | \( \bar{z} \) | \( N \) | \( \langle \Delta \alpha/\alpha \rangle_w \) | \( \langle \Delta \alpha/\alpha \rangle \) | \( \delta \) | \( \delta_{\chi^2, \text{red}}=1 \) | \( S \) | \( \sum_i (\chi^2_i - \chi^2_{\alpha}) \) | \( \sum_i \delta^2_i \) |
|--------|-----|---|-----------------|-----------------|-----|-----------------|-----|-----------------|-----|
| Low \( z \) | 1.02 | 28 | \(-0.70 \pm 0.23\) | \(-0.67 \pm 0.27\) | 3.0\( \sigma \) | 0.70 | 3.6\( \sigma \) | 0.84 | 55 | 28 |
| High \( z \) | 2.12 | 21 | \(-0.76 \pm 0.28\) | \(-0.67 \pm 0.33\) | 2.8\( \sigma \) | 0.68 | 3.3\( \sigma \) | 0.83 | 37 | 21 |
| Total | 1.49 | 49 | \(-0.72 \pm 0.18\) | \(-0.67 \pm 0.21\) | 4.1\( \sigma \) | 0.68 | 4.9\( \sigma \) | 0.83 | 92 | 49 |

Figure 3. \( \Delta \alpha/\alpha \) versus fractional look-back time for a currently popular cosmology. The upper panel shows our raw results and 1\( \sigma \) error bars: the dots represent the low-\( z \) sample and the crosses mark the high redshift sample. Note that the high-\( z \) sample does contain some lower redshift absorbers. The lower panel shows an arbitrary binning of our results: 7 bins \( \times \) 7 points per bin = 49 points. The redshifts of the points are taken as the mean redshift of clouds within that bin and the value of \( \Delta \alpha/\alpha \) is the weighted mean with its associated 1\( \sigma \) error bar.
Fig. 3 shows the raw values of $\Delta \alpha/\alpha$ as a function of fractional look-back time to the absorbing cloud using a flat $\Lambda$ dominated cosmology ($H_0 = 68 \text{ kms}^{-1}\text{Mpc}^{-1}$, $\Omega_M = 0.3$, $\Omega_\Lambda = 0.7$). The redshift scale is also given for comparison. The lower panel shows an arbitrary binning of the data such that all bins have equal number of points ($7 \text{ bins} \times 7 \text{ points}$ per bin $= 49 \text{ points}$). We plot the weighted mean for each bin with the associated $1\sigma$ error bars. At low redshifts we see that $\Delta \alpha/\alpha$ is consistent with zero. Also, the results are consistent with a generally monotonic evolution of $\alpha$ with redshift.

6.3 Systematic errors

The statistical error in our result is now small and our attention must turn to possible systematic errors. In the companion paper, M01b, we explore in detail a broad range of potential systematic errors, including the following: laboratory wavelength errors, wavelength mis-calibration, atmospheric dispersion effects, unidentified interloping transitions, isotopic ratio and/or hyperfine structure effects, intrinsic instrumental profile variations, spectrograph temperature variations, heliocentric velocity corrections, kinematic effects and large scale magnetic fields. All but two of these are shown to be negligible: atmospheric dispersion effects and isotopic abundance variation. In this Section we summarise these two effects, but first discuss how a general wavelength scale distortion affects the low-$z$ and high-$z$ samples alike. Generally, simple systematic effects might cause low-order distortions in the wavelength scale (relative to the ThAr calibration frames) or may lead to wavelength dependent mis-centroiding of absorption features.

The low-$z$ sample ($\text{Mg} \equiv/\text{Fe} \equiv$ systems) is most sensitive to systematic effects. The $\text{Fe} \equiv$ lines have large and positive $q_1$ coefficients and all lie at lower wavelengths than the $\text{Mg} \equiv$ anchors. Thus, a systematically negative $\Delta \alpha/\alpha$ can result from a slight ‘compression’ of the QSO spectra relative to the ThAr calibration frames for the low-$z$ sample. However, it is more difficult to understand the effect of simple systematic errors on the high-$z$ sample for several reasons:

(i) The transitions involved have a large range of $q_1$ coefficients. In effect, there are three types of transition: those with large and positive $q_1$, those with large and negative $q_1$ and those with small or intermediate values of $q_1$.

(ii) The different types of transition are mixed in wavelength space. In the low-$z$ sample, all the lines with large and positive $q_1$ (i.e. $\text{Fe} \equiv$ lines) lie to the blue of those with small $q_1$ (i.e. $\text{Mg} \equiv$ lines). This is not the case in the high-$z$ sample. For example, two lines with small $q_1$, $\text{Si} \equiv \lambda 1526$ and $\text{Al} \equiv \lambda 1670$, straddle two lines with large, positive $q_1$, $\text{Fe} \equiv \lambda 1608$ and $\lambda 1611$.

(iii) Different sets of transitions appear in each QSO spectrum. Some spectra may not contain all types of transition.

The value of $\langle \Delta \alpha/\alpha \rangle_w$ will be more resistant to systematic errors in the high-$z$ sample. To illustrate this point we have ‘compressed’ the spectrum of a low-$z$ and a high-$z$ absorption system by a factor of $1 \times 10^{-5}$ (i.e. the separation between any two wavelengths decreases by 1 part in $10^5$) and found a new value for $\Delta \alpha/\alpha$. We used the same first-guess velocity structures used to derive the results in Table 2 and Fig. 3. For the low-$z$ Mg/Fe system at $z = 0.911$ we find a significant decrease in $\Delta \alpha/\alpha$ due to the compression: $\Delta \alpha/\alpha = (-0.068 \pm 0.661) \times 10^{-5} \rightarrow (-1.106 \pm 0.692) \times 10^{-5}$. However, for the high-$z$ DLA at $z = 2.095$ we find a small, positive change: $\Delta \alpha/\alpha = (-0.946 \pm 0.601) \times 10^{-5} \rightarrow (-0.821 \pm 0.589) \times 10^{-5}$.

6.3.2 Atmospheric dispersion effects

Atmospheric dispersion across the spectral direction of the spectrograph slit can be avoided using an image rotator. However, as we noted in Sections 5.1.2 and 5.1.3, many of our objects were observed before HIRES was fitted with an image rotator. Dispersion across the slit can only lead to a ‘stretcher’ of the QSO spectrum relative to the ThAr frames. However, at least in the low-$z$ sample, a negative value of $\Delta \alpha/\alpha$ can only be mimicked by a ‘compression’ of the spectrum. The effect of the stretching on $\Delta \alpha/\alpha$ is not quite as clear for the high-$z$ sample (points (i)–(iii) above).

To illustrate this point we quantified the atmospheric dispersion effects in M01b and find that the high-$z$ sample is quite robust against this error. However, the low-$z$ results are more sensitive to this effect and may have to be reduced from the uncorrected value of $\langle \Delta \alpha/\alpha \rangle_w = (-0.70 \pm 0.23) \times 10^{-5}$ to $\langle \Delta \alpha/\alpha \rangle_w \approx (-1.52 \pm 0.23) \times 10^{-5}$. We stress that the magnitude of the correction here is an upper limit since several effects, all difficult to properly quantify, will act to reduce the effective compression. Note that since the above correction is an upper limit, we do not include any additional errors due to uncertainties in our model of atmospheric refraction.

6.3.3 Isotopic abundance evolution

We assumed terrestrial isotopic abundances in all species when fitting the QSO spectra. However, if the isotopic abundances in the QSO absorbers are different, small apparent shifts in the absorption lines would be introduced, potentially mimicking a non-zero $\Delta \alpha/\alpha$. $\Delta \alpha/\alpha$ is most sensitive to changes in the isotopic abundances of Mg$ \equiv$ and Si$ \equiv$ since these ions have large isotopic separations (see Section 5.2.2, Timmes, Woosley & Weaver (1995), Timmes & Clayton (1996) and Gay & Lambert (2000), suggest that the abundances of the isotopes $^{25,26}\text{Mg}$ and $^{28,30}\text{Si}$ decrease with decreasing metallicity. The QSO absorption clouds in our sample have low metallicity compared to solar (Prochaska & Wolfe 1999, 2000; Churchill et al. 1999). Thus, to obtain an upper limit on the effect this may have had on $\Delta \alpha/\alpha$, we have removed the $^{25,26}\text{Mg}$ and $^{28,30}\text{Si}$ isotopes from our analysis and re-calculated $\Delta \alpha/\alpha$ for all the absorption systems. Again, we find that the correction is towards more negative values, the corrected value being $\Delta \alpha/\alpha = (-0.96 \pm 0.17) \times 10^{-5}$ (as in Section 6.3.2, we do not add any additional errors due to uncertainties in our model since the correction we calculate is an upper limit).
6.3.4 Tests for unknown, simple systematic errors

We have also carried out other tests to search for any unknown, simple systematic effects. For example, it is unlikely that such an effect will be able to mimic the very specific $q_1$ dependence of the transitions in the high-$z$ sample. Thus, if we remove the transitions with large, positive $q_1$ coefficients from our fit and find a new value for $\Delta \alpha/\alpha$, we expect the two values to differ if the line shifts are caused by some simple systematic effect. Of course, if we remove transitions with large, positive $q_1$, we can only obtain useful constraints on $\Delta \alpha/\alpha$ if anchor lines and transitions with large, negative $q_1$ are available. Therefore, we have conducted such a test on a subset of the high-$z$ sample which contains at least one anchor line, at least one transition with large and positive $q_1$ and at least one with large and negative $q_1$. We find consistent weighted mean values of $\Delta \alpha/\alpha$ both before and after line removal. We conducted a similar test by removing lines with large, negative $q_1$ and another test by removing the anchor lines. We find consistent values before and after line removal in each case. Thus, the interpretation that the line shifts we observe are caused by a varying $\alpha$ seems robust.

7 DISCUSSION

We have conducted an experimental search for variability of $\alpha$ over the redshift range $0.5 < z < 3.5$ using QSO absorption lines as our probe. We used a new method for deriving constraints on $\Delta \alpha/\alpha$ from a comparison of QSO and laboratory spectra which, unlike the previous alkali-doublet (spin-orbit splitting) method, exploits the total relativistic effect in different atoms (see Section 4). Comparing the wavelengths of transitions from different multiplets and different atoms/ions leads to an order of magnitude gain in precision over the alkali-doublet (AD) method. Since the new, many-multiplet (MM) method allows us to use all transitions in principle, we also gain precision through increased statistics.

We have analysed the spectra of 49 absorption clouds (towards 28 QSOs) and compared the observed and laboratory wavelengths of those transitions listed in Table 1. Our low-$z$ results represent a re-analysis of the W99 data. We compare the W99 results with our re-analysis in Table 6 and we see that they are consistent. Our results for each absorption system are listed in Table 3. Over the entire sample we find statistical evidence for time variation of $\alpha$ at the 4.1$\sigma$ level: $\Delta \alpha/\alpha = (-0.72 \pm 0.18) \times 10^{-5}$ (see Table 3). This result is the `raw' result. Correcting for any possible systematic effects (Section 2.2 and M01b) would increase the significance of this deviation of $\Delta \alpha/\alpha$ from zero. We show the distribution of $\Delta \alpha/\alpha$ with cosmological time and redshift in Fig. 3.

From the analyses we present in this paper and in M01b, we conclude that if our results are due to some effect other than a real variation in $\alpha$, this will only be revealed by further independent observations and analyses using the MM method. Optical spectra are very useful for probing the range of redshifts we have explored here. However, a statistical sample of radio spectra of HI 21 cm and molecular absorption systems has the potential to increase our precision limit by another order of magnitude. This effort is hampered by the fact that very few such systems are known at present. A systematic observational search for these systems should clearly be made. Also, as the arsenal of 8–10 m class optical telescopes with high-resolution spectrographs grows, more observations should be devoted to obtaining carefully calibrated, high SNR spectra of absorption systems at both high and low-$z$. These will provide a crucial check on our results and will allow us to discover or rule out any further subtle or unknown systematic effects in the data.

ACKNOWLEDGMENTS

We are very grateful to Ulf Griesmann, Sveneric Johansson, Rainer Kling, Richard Learner, Ulf Litzén, Juliet Pickering and Anne Thorne for conducting laboratory wavelength measurements especially for the present work and for communicating their results prior to publication. We would also like to thank Michael Bessell, Tom Bica, Bob Carswell, Rolf Engleman Jr., Alberto Fernández-Soto, John Hearnshaw, Alexander Ivanvich, Jochen Liske, Leon Lucy, Geoff Marcy, Gillian Nave and Steve Vogt for very helpful communications.

We are grateful to the John Templeton Foundation for supporting this work. MTM and JKW are grateful for hospitality at the IoA Cambridge, where some of this work was carried out. CWC received partial support from NASA NAG5-6399 and NSF AST961785. JDB acknowledges support from PPARC, The Royal Society, and a Gordon Godfrey visiting professorship at UNSW. AMW received partial NSF support from NSF AST0071257.

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