**Atomic many-body theory and variation of constants of nature**

by

Michael Marchenko

A thesis submitted in satisfaction of

the requirements for the degree of

Doctor of Philosophy

in the Faculty of Science.

20 September 2015



Statement of Originality

I hereby declare that this submission is my own work and to the best of my knowledge it contains no materials previously published or written by another person, or substantial proportions of material which have been accepted for the award of any other degree or diploma at UNSW or any other educational institution, except where due acknowledgement is made in the thesis. Any contribution made to the research by others, with whom I have worked at UNSW or elsewhere, is explicitly acknowledged in the thesis. I also declare that the intellectual content of this thesis is the product of my own work, except to the extent that assistance from others in the project's design and conception or in style, presentation and linguistic expression is acknowledged.

(Signed)

**Abstract**

Fundamental physical constants are the only absolutes which exist at the moment. If they are not really constants then this is a serious philosophical problem. All measurements are binding to the fundamental physical constants. The cutting edge of the modern physics is high energy physics which can allow to go beyond Standard Model, to discover New Physics, and to understand better how the Universe came into existence (evolved). This may result in better sources of energy than the ones which are used now. Theories unifying gravity with other interactions (such as string theories and M- theory) allow or require variation of the fundamental physical constants. If one can determine precise enough limits for variation of fundamental physical constants it may help to choose the most adequate theory of unifying gravity with other interactions. This would be indirect theoretical verification of high energy physics. This verification is not feasible by experimental methods.

We use Big Bang Nucleosynthesis calculations and light element abundance data to constrain the relative variation of the deuteron binding energy since the universe was a few minutes old, δQ = Q(BBN ) − Q(present). Two approaches are used, first treating the baryon to photon ratio, η, as a free parameter, but with the additional freedom of varying δQ, and second using the WMAP value of η and solving only for δQ. Including varying Q yields a better fit to the observational data than imposing the present day value, rectifying the discrepancy between the 4H e abundance and the deuterium and 7Li abundances, **and** yields good agreement with the independently determined η**W M AP** . The minimal deviation consistent with the data is significant at about the 4-σ level; δQ/Q = −0.019 ± 0.005. If the primordial 4 He abundance lies towards the low end of values in the literature, this deviation is even larger and more statistically significant. Taking the light element abundance data at face-value, our result may be interpreted as variation of the dimensionless ratio X = m**s** /Λ**QCD** of the strange quark mass and strong scale: δX/X = (1.1 ± 0.3) × 10−3 . These results provide a strong motivation for a more thorough exploration of the potential systematic errors in the light element abundance data.

Key words: physical constants, high energy physics, Big Bang nucleosynthesis (nuclear synthesis), atomic clocks, Grand Unification, Standard Model, quasar spectra, signal processing, sensitivity, precision.

**Contents**

Abstract …………………………………………………………… page 2

Introduction ………………………………………………………… page 4

Chapter 1 …………………………………………………………… page 17

Chapter 2 …………………………………………………………… page 26

Chapter 3 …………………………………………………………… page 47

Chapter 4 …………………………………………………………… page 69

Chapter 5 …………………………………………………………… page 73

Chapter 6 …………………………………………………………… page 92

Chapter 7 …………………………………………………………… page 105

Chapter 8 …………………………………………………………… page 115

Chapter 9 …………………………………………………………… page 120

Chapter 10 …………………………………………………………… page 130

Computer code ……………………………………………………… page 131

Conclusions ………………………………………………………… page 135

References and bibliography ……………………………………….. page 137

List of figures ………………………………………………………... page 131

List of tables ………………………………………………………… page 132

List of formulas……………………………………………………… page 135

**Introduction**

Recently there was an intensive discussion of the possible space-time variation of the fine structure constant

* = e2/hc at the cosmological scale.

The first evidence for such variation has been reported in [1, 2, 3, 4, 5, 6] from the analysis of the astrophysical data. These results are to be compared with the number of experimental up-per bounds on this variation obtained from other astrophysical observations (see, e.g. [7, 8, 9]) and from the precision laboratory measurements [10, 11, 12]. Recently a number of new laboratory tests have been proposed (see, e.g. [13]). The analysis of the microwave back-ground radiation can also give some restrictions on time variation of α as suggested in [14, 15, 16]. Implementations of the space-time variation of the fine structure constant to the theory of the fundamental interactions are discussed e.g. in Refs. [17, 18, 19, 20, 21, 22, 23] (see also discussion and references in [3]).

The most straightforward way to look for the variation of is to measure the ratio of some fine structure interval to an optical transition frequency, such as ω(np1/2 → np3/2) and ω(n′s1/2 → np3/2) [37]. This ratio can be roughly estimated as 0.2 α2Z2, where Z is the nuclear charge [24]. Therefore, any diﬀerence in this ratio for a laboratory experiment and a measurement for some distant astrophysical object can be easily converted into the space-time variation of α. However, as it was pointed out in [25], one can gain about an order of magnitude in the sensitivity to the α-variation by comparing optical transitions for diﬀerent atoms. In this case the frequency of each transition can be expanded in a series in α2 :

α0 stands for the laboratory value of the fine structure constant. Note, that Eq.  [(1a)](#page1) corresponds to the expansion at α = 0, while Eq.  [(1b)](#page1) — to the expansion at α = α0 . In both cases parameters ωi(2) and qi appear due to relativistic corrections.

For a fine structure transition the first coeﬃcient on the right hand side of  [(1a)](#page1) turns to zero, while for the optical transitions it does not. Thus, for the case of a fine structure and an optical transition one can write:

Quite often the coeﬃcients ωi(2) for optical transitions are about an order of magnitude larger than corresponding coeﬃcients for the fine structure transitions ωfs(2) (this is because the relativistic correction to a ground state electron energy is substantially larger than the spin-orbit splitting in an excited state [25, 26]). Therefore, the ratio  [(3)](#page1) is, in general, more sensitive to the variation of α than the ratio  [(2](#page1)). It is also important that the signs of coeﬃcients ωi(2) in  [(3)](#page1) can vary. For example, for s-p transitions the relativistic corrections are positive while for d-p transitions they are negative. This allows to suppress possible systematic errors which “do not know” about the signs and magnitude of the relativistic corrections [25]. On the other hand, for many cases of interest, the underlying atomic theory is much more complicated for Eq.  [(3](#page1)). In particular, the most diﬃcult case corresponds to transitions to highly excited states of a multi-electron atom, where the spectrum is very dense. And this happens to be a typical situation for astrophysical spectra, in particular, for large cosmological red shifts. Corresponding atomic calculations have to account very accurately for the electronic correlations, which may affect such spectra quite dramatically.

TABLE I: Final results for parameters q from Eq.  [(1)](#page1) for Si II, Cr II, Fe II, Ni II, and Zn II. Estimated errors are in brackets.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Ion | Transition | | | ω0 (cm−1) | q (cm−1 ) | |
| Si II | 2P1o/2 | → | 2D3/2 | 55309.3365 | 520 | (30) |
|  |  | → | 2S1/2 | 65500.4492 | 50 | (30) |
| Cr II | 6S5/2 | → | 6P3o/2 | 48398.868 | −1360 | (150) |
|  |  | → | 6P5o/2 | 48491.053 | −1280 | (150) |
|  |  | → | 6P7o/2 | 48632.055 | −1110 | (150) |
| Fe II | 6D9/2 | → | 6D9o/2 | 38458.9871 | 1330 | (150) |
|  |  | → | 6D7o/2 | 38660.0494 | 1490 | (150) |
|  |  | → | 6F11o/2 | 41968.0642 | 1460 | (150) |
|  |  | → | 6F9o/2 | 42114.8329 | 1590 | (150) |
|  |  | → | 6P7o/2 | 42658.2404 | 1210 | (150) |
|  |  | → | 4F7o/2 | 62065.528 | 1100 | (300) |
|  |  | → | 6P7o/2 | 62171.625 | −1300 | (300) |
| Ni II | 2D5/2 | → | 2F7o/2 | 57080.373 | −700 | (250) |
|  |  | → | 2D5o/2 | 57420.013 | −1400 | (250) |
|  |  | → | 2F5o/2 | 58493.071 | −20 | (250) |
| Zn II 2S1/2 | | → | 2P1o/2 | 48481.077 | 1584 | (25) |
|  |  | → | 2P3o/2 | 49355.002 | 2490 | (25) |

The first calculations of the coeﬃcients q from Eq.  [(1](#page1)) for the transitions suitable for astronomical and laboratory measurements were done in Refs. [25, 26, 27, 28]. Here we present a new and more accurate calculations of the coeﬃcients q for the transitions, which are currently used in the analysis of the astrophysical data. A full list of these transitions was given in [3]. We have not re-calculated here the lightest and the most-simple atoms Mg and Al, for which the previous calculation [25] should be suﬃciently accurate and focused on more complicated ions Si II, Cr II, Fe II, Ni II, and Zn II. Our final results for them are given in Table I. Note, that here we use the single parameter q instead of two parameters q1 and q2 used in the earlier works and q ≡ ∂ω/∂x|x=0 = q1 + 2q2. Details of the calculations and discussion of the accuracy will be given in Sec.  [III.](#page3) Before that we briefly address few theoretical points in Sec. II.

Theories unifying gravity with other interactions suggest that fundamental constants could vary in space-time (see, e.g. [1]). Recent evidence of variation of the fine structure constant α in quasar absorption spectra [2] elevated interest to the search of variation of α in laboratory experiments. Comparing frequencies of diﬀerent atomic transitions over long period of time is a good way to do such search due to extremely high accuracy of measurements achieved for certain types of transitions. The best limit on local present-time variation of the fine structure constant published so far was obtained by comparing Hg+ microwave atomic clock vs hydrogen maser [3]. Recently this limit was further improved by more than an order of magnitude in comparing cesium and rubidium atomic clocks [4]. There are also many proposals for the search of variation of α in atomic optical transitions, some of which were analyzed in our previous works (see [5] and references therein). In the present paper we analyze three new proposals involving strontium/calcium, dual beam [6], dysprosium atom [5,7] and ytterbium positive ions Y b+ [8] and Y b2+ [9]. We perform relativistic many-body calculations to link variation of α with the variation of the frequencies of atomic transitions. Then we use this connection to find out what accuracy of measurements is needed to improve current best limit on time variation of the fine structure constant.

In the proposal suggested by S. Bergeson strontium-calcium dual beam is to be used to compare the frequencies of the 1S0 −3 P1 clock transitions in these atoms over a long period of time. Ca and Sr have similar electron structure. However, due to higher nuclear charge, relativistic eﬀects are larger for strontium. If α is changing, corresponding change in frequency of the clock transition for Sr would go considerably faster than for Ca. Precise measurements might be able to indicate this or, at least, put strong constrain on possible variation of α. Calculations of the relativistic eﬀects for Ca were done in our previous work [5]. In present paper we do similar calculations for Sr.

Experiments with ytterbium positive ion have advantages of greater relativistic eﬀects due to larger nuclear charge and the convenience of working with two diﬀerent transitions of the same element. There are two transitions in Yb+ involving metastable states for which comparison of frequencies is considered. One is quadrupole transition 4f 146s 2S1/2 − 4f 145d 2D5/2 and another is octupole transition 4f 146s 2S1/2 −4f 136s2 2F7/2. The quadrupole transition is basically a s−d transition while the octupole one is a f −s transition. According to simple analytical formula presented in Ref. [5] relativistic energy shifts for s electrons, and electrons with high total momentum j (like d and f electrons) are large but have opposite sign. This means that we should expect that two metastable states of Yb+ move in opposite directions if α is changing. This brings extra enhancement to the sensitivity of the measurements for Yb+ to the variation of α. Our accurate calculations presented below support these considerations.

The proposal for dysprosium is quite diﬀerent from what was considered so far. Instead of comparing two very stable atomic clock frequencies the authors of this proposal [5] suggest to measure very small frequency of the transition between two almost degenerate states of opposite parity in dysprosium. The states are 4f 105d6s 3[10]10 E = 19797.96cm−1 and 4f 95d26s 9K10 E = 19797.96cm−1. These states were used before for the search of parity non-conservation in Dy [11]. Small energy splitting and diﬀerent electron structure of these two states lead to very strong enhancement of the sensitivity of the frequency of transition

2

between the states to variation of α. The enhancement (about eight orders of magnitude) seems to be strong enough to overcome the disadvantage of dealing with states which are not very narrow.

In the present paper we calculate the values of relativistic energy shifts for Sr, Yb+ and Dy and discuss what accuracy of measurements is needed to improve current best constrain on local time variation of the fine structure constant.

**Chapter1 Many-Body Theory**

Standard many-body perturbation theory

The quantum-mechanical treatment of many-electron systems, based on the Schrodinger equation and the Coulomb interaction between the electrons,was developed shortly after the advent of quantum mechanics, particularlyby John Slater in the late 1920's and early 1930's [214]. Self-consistent-field(SCF) schemes were early developed by Slater, Hartree, Fock and others.1

Perturbative schemes for quantum-mechanical system, based on the Rayleigh-Schrodinger and Brillouin-Wigner schemes, were developed in the 1930's and 1940's, leading to the important linked-diagram expansion, introduced by Brueckner [37] and Goldstone [73] in the 1950's, primarily for nuclear applications. That scheme was in the 1960's and 1970's also applied to electronic systems [100] and extended to degenerate and quasi-degenerate energy levels [31, 112]. The next step in this development was the introduction of " all-order methods" of coupled-cluster type, where certain effects are taken to all orders of the perturbation expansion. This represents the last and probably major step of the development of a non-relativistic many-body perturbation theory (MBPT).2

The first step towards a relativistic treatment of many-electron systems was taken in the early 1930's by Gregory Breit [32], extending works made somewhat earlier by J. A. Gaunt [68]. Physically, the Gaunt interaction represents the magnetic interaction between the electrons, which is a purely relativistic effect. Breit augmented this treatment by including the leading retardation effect, due to the fact that the Coulomb interaction is not instantaneous, which is an effect of the same order.

A proper relativistic theory should be Lorentz covariant, like the Dirac single-electron theory.3 The Dirac equation for the individual electrons together with the instantaneous Coulomb and Breit interactions between the electrons represent for a many-electron system all effects up to order2 H(Hartree atomic units) or 4mec2.4 This procedure, however, is NOT Lorentz covariant, and the Breit interaction can only be treated to first-order in perturbation theory, unless projection operators are introduced to prevent the intermediate states from falling into the "Dirac sea" of negative-energy states, as discussed early by Brown and Ravenhall [36] and later by Joe Sucher [222]. The latter approach has been successfully employed for a long time in relativistic many-body calculations and is known as the no-virtual-pair approximation (NVPA). A fully covariant relativistic many-body theory requires a field-theoretical approach, i.e., the use of quantum-electrodynamics (QED). In principle, there is no sharp distinction between relativity and QED, but conventionally we shall refer to effects beyond the no-virtual-pair approximation as QED effects. This includes effects of retardation, virtual pairs and radiative effects (selfenergy, vacuum polarization, vertex correction). The systematic treatment of these effects requires a covariant approach, where the QED effects are included in the wave function. It is the main purpose of the present book to formulate the foundations of such a procedure.

**Quantum-electrodynamics**

Already in the 1930's deviations were observed between the results of precision spectroscopy and the Dirac theory for simple atomic systems, primarily the hydrogen atom. Originally, this deviation was expected to be due to vacuum polarization, i.e., spontaneous creation of electron-positron pairs in the vacuum, but this effect turned out to be too small and even of the wrong sign. An alternative explanation was the electron self-energy, i.e., the emission and absorption of a virtual photon on the same electron another effect that is not included in the Dirac theory. Early attempts to calculate this effect, however, were unsuccessful, due to singularities (infinities) in the mathematical expressions.

The first experimental observation of a clear-cut deviation from the Dirac theory was the detection in 1947 by Lamb and Retherford of the so-called Lamb shift [111], namely the shift between the 2 s and 2 p 1 = 2 levels in atomic hydrogen, levels that are exactly degenerate in the Dirac theory [53, 54]. In the same year Hans Bethe was able to explain the shift by a non-relativistic calculation, eliminating the singularity of the self energy by means of a renormalization process[16]. At about the same time Kusch and Foley observed that the magnetic g-factor of the free electron deviates slightly but significantly from the Dirac value -2 [105, 106]. These observations led to the development of the modern form of the quantum-electrodynamics theory by Feynman, Schwinger, Dyson, Tomanaga and others by which the deviations from the Dirac theory could be explained with good accuracy [210, 228, 64, 63, 58].5 The original theory of QED was applied to free electrons. During the last four decades several methods have been developed for numerical calculation of QED effects in bound electronic states. The scattering-matrix or S-matrix formulation, originally developed for dealing with the scattering of free particles, was made applicable also to bound states by Joe Sucher [220], and the numerical procedure was refined in the 1970's particularly by Peter Mohr [146]. During the last two decades the method has been extensively used in studies of highly charged ions in order to test the QED theory under extreme conditions, works that have been pioneered by Mohr and So (for a review, see ref. [152]).

The Green's function is one of the most important tools in mathematical physics with applications in essentially all branches of physics.6 During the1990's the method was adopted to bound-state QED problems by Shabaev et al. [211]. This procedure is referred to as the Two-times Green's function and has recently been extensively applied to highly-charged ions by the St Petersburg group. During the first decade of this century another procedure for numerical QED calculations was developed by the Gothenburg atomic theory group, termed the Covariant-evolution-operator (CEO) method [124], which has been applied to the fine structure and other energy-level separations of heliumlike ions. [1.111]

**Chapter 2**

THEORY

In order to find parameters q = ∂ω/∂x|x=0 in Eq.  [(1](#page1)) we perform atomic calculations for three values of x: x− = −1/8, x0 = 0, and x+ = 1/8. That allows us to determine q: q = 4 (ω(x+) − ω(x−)) and also estimate the second derivative ∂2ω/∂x2|x=0. The large value of the latter signals that interaction between levels is strong (level pseudo-crossing), and there is a risk of large errors. For these cases further analysis was done as described below.

1. Relativistic calculations of multi-electron ions.

In order to accurately account for the dominant relativistic eﬀects we use the Dirac-Hartree-Fock approximation as a starting point for all calculations of atomic spectra. Though most of the calculations were done for the Coulomb potential, we have also estimated Breit corrections by including the magnetic part of the Breit inter-action in the self-consistent field [1.29].

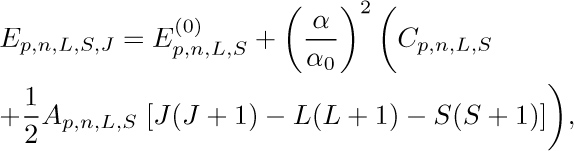
The ions we are dealing with in this paper have from one to nine electrons in the open shells. For one valence electron in Zn II the Dirac-Fock V N −1 approximation already gives rather good results. On the next step the core-valence correlations can be accounted for by means of the many-body perturbation theory (MBPT). Already the second order MBPT correction allows to reproduce the spectrum with the accuracy, better than 1%, which is more than suﬃcient for our current purposes.

Other ions of interest to us have at least three valence electrons. Here the dominant correlation correction to transition frequencies corresponds to the valence-valence correlations. This type of correlations can be accounted for with configuration interaction (CI) method. If necessary, the core-valence correlations can be included within combined CI+MBPT technique [1.30]. The latter usually provides an accuracy of the order of 1% or better for the lower part of the spectra of atoms and ions with two or three valence electrons [1.30, 31, 32]. However, the accuracy of ab initio methods decreases with the number of valence electrons and with excitation energy. Indeed, for a large number of valence electrons and/or suﬃciently high excitation energy the spectrum becomes dense and the levels with the same exact quantum numbers strongly interact with each other. The part of the spectrum of Fe II above 55000 cm−1 and, to a somewhat lesser extent, the spectrum of Ni II represent this situation. There-fore, for these ions we developed a semi-empirical fitting procedure, which is described below.

In order to have additional control of the accuracy of our CI we performed calculations for most of the ions with two diﬀerent computer packages. One package was used earlier in Refs. [30, 32, 33] and another one was used in Refs. [3, 25, 26, 27, 28, 31]. The former pack-age allows to construct flexible basis sets and optimize configuration space, while the latter allows for a larger CI space as it works with the block of the Hamiltonian matrix, which corresponds to a particular total angular momentum of atom J . When there were no significant diﬀerence between two calculations, we only give results obtained with the first package. Nevertheless, our final results presented in Table  [I](#page2) are based on both calculations.

b. Semi-empirical treatment of the strong interaction of levels: pseudo-crossing.

In the nonrelativistic limit α → 0, all multi-electron states are accurately described by the LS-coupling scheme: Eα→0 = Ep,n,L,S,J , where p = ±1 is the parity and n numerates levels with the same p, L,S, and J. For sufficiently small values of α the LS-coupling holds and the energy has the form:

 (4)

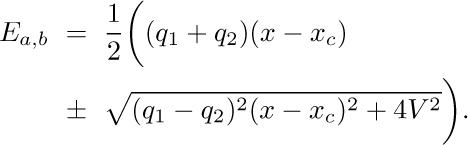
The first term in the parentheses gives the slope for the centre of the multiplet and the second term gives the fine structure. With growing α the multiplets start to overlap and when the levels with the same p and J come close, the pseudo-crossing takes place.

Near the pseudo-crossing the slope of the energy curves changes dramatically. If such crossing takes place at x ≈ 0, where x is defined by Eq.  [(1),](#page1) i.e. near the physical value of α, it can cause significant uncertainty in the values of parameters q.

Let us first analyze the behavior of the slopes q(x) in the vicinity of the pseudo-crossing in the two-level approximation. Consider two levels E1 and E2 which cross at x = xc :

|  |  |  |  |
| --- | --- | --- | --- |
| E1 | = | q1(x − xc ), | (5a) |
| E2 | = | q2(x − xc ). | (5b) |

If the interaction matrix element between these two levels is V , the exact adiabatic levels will be

 (6)

It is easy now to calculate the energy derivative in respect to x in terms of the mixing angle φ between unperturbed states 1 and 2:

 (7)

Note, that at the crossing the angle φ varies from 0 on one side through π/4 in the centre to π/2 on the other side, which leads to the change of the slope

qa(x) = ∂Ea/∂x from q1 through (q1 + q2 )/2 to q2. The narrow crossings with small V are particularly dangerous, as the slopes change very rapidly within the interval x ≈ V /|q1 − q2|. Then, even small errors in the position of the crossing point xc , or the value of V can cause large errors in qa,b. In this model we assume that non-diagonal term V = const.

For the real atom V ∝ α2. However, if the crossing region x ≪ 1, we can neglect

the dependence of V on α.

1. Semi-empirical treatment of the strong interaction of levels: multi-level case.

Eq.  [(7)](#page3) can be easily gener-alized to a multi-level case as it simply gives the slope of a physical level a as a weighted average of the mixed levels. Thus, if the level a can be expressed as a linear combination of some unperturbed LS-states ψLn ,Sn :

 (8)

the resultant slope qa is given by:

 (9)

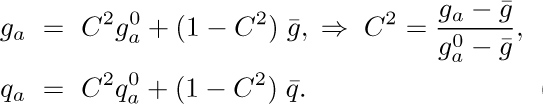
Here again we neglect weak dependence of interaction V on x in comparison to strong dependence of Cn2 on x near crossing points.

Eq.  [(9)](#page3) allows to improve ab initio coeﬃcients q if we can find the expansion coeﬃcients Cn in Eq.  [(8](#page3)). That can be done, for example, by fitting g-factors. The magnetic moment operator µ = g0(L + 2S) is diagonal in L and S and, therefore, does not mix diﬀerent LS-states. Thus, in the LS-basis the resultant g-factor for the state *a* has exactly the same form as qa:

 (10)

If the experimental g-factors are known, one can use Eq.  [(10)](#page3) to find weights Cn2 and, then find the corrected values of the slopes qa.

Sometimes, the experimental data on g-factors are in-complete. Than, one can still use a simplified version of Eqs.  [(9)](#page3) and  [(10)](#page3):

 (11a,b)

C2 here is the weight of the dominant LS-level in the experimental one, and the bar means the averaging over the admixing levels. Of course, there is some arbitrariness in calculation of averages g¯ and q¯. However, the advantage of Eqs.  [(11)](#page3) is that only one experimental g-factor is required.

1. DETAILS OF THE CALCULATION AND RESULTS

As we mentioned above, we performed calculations of energy levels for three values of the parameter x: x− = −1/8, x0 = 0, and x+ = 1/8. All three calculations were done at exactly same level of approximation, to minimize the error caused by the incompleteness of the basis sets and configuration sets. From these calculations we found two approximations for q: q− = 8(ω(x0) − ω(x−)) and q+ = 8(ω(x+) −ω(x0 )). If there were problems with level identification we performed additional calculation for x = 0.01, where the LS-coupling should be very accurate and identification is straitforward. The noticeable diﬀerence between q− and q+ signaled the possibility of the level crossing. In these cases we applied the semiempirical procedure described in Sec.  [II](#page2) to find the corrected values for q; otherwise, we simply took the average: q = (q+ + q−)/2.

1. Zn II

Zn II has the ground state configuration [1s2 . . . 3d10]4s

and we are interested in the 4s → 4pj transitions. As the theory here is much simpler than for other ions, we

TABLE II: Transition frequencies and parameters q for Zn II (in cm−1 ). Calculations were done in four diﬀerent ap-proximations: Dirac-Hartree-Fock-Coulomb (DHFC), Dirac-Hartree-Fock-Coulomb-Breit (DHFCB), Brueckner-Coulomb (BC), and Brueckner-Coulomb-Breit (BCB).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Transition | | Exper. | DHFC DHFCB | | BC | BCB |
|  |  | transition frequencies | | |  |  |
| 4s1/2 | → 4p1/2 48481.077 | | 44610.1 | 44608.1 | 48391.2 48389.4 | |
|  | → 4p3/2 | 49355.002 | 45346.9 | 45330.0 | 49263.8 49244.6 | |
|  |  | parameters q = (q+ + q−)/2 | | | |  |
| 4s1/2 | → 4p1/2 |  | 1362 | 1359 | 1594 | 1590 |
|  | → 4p3/2 |  | 2129 | 2109 | 2500 | 2479 |
|  |  |  |  |  |  |  |

used Zn II to study the importance of the core-valence correlation correction and Breit correction to the slopes q. The former correction was calculated in Brueckner approximation:

 (12)

with the self-energy operator Σ(E) calculated in the second order of MBPT (the perturbation here is the diﬀerence between the exact and Dirac-Hartree-Fock Hamiltonians, V = H − HDHF). The HDHF was calculated with the magnetic part of the Breit operator included self-consistently. The retardation part of the Breit operator is known to be significantly smaller  [[29]](#page8) and we completely neglected it here.

1. Si II

Si II has three valence electrons and the ground state configuration [1s2 . . . 2p6]3s23p. Excited configurations of interest are 3s3p2 and 3s24s. We made the CI calculation in the Coulomb approximation on the basis set, which included 1s − 8s, 2p − 8p, 3d − 8d, and 4f, 5f orbitals, which we denote as the basis set [8spd5f]. Note, that we use virtual orbitals, which are localized within the atom [34], rather than Dirac-Fock ones. This pro-vides fast convergence. CI included all single-double (SD) and partly triple excitations from three valence configurations listed above. The results of these calculations are given in Table  [III](#page4).

TABLE III: Transition frequencies ω from the ground state 2P1o/2, fine structure splitting FS , and parameters q± for Si II (in cm−1 ).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Experiment  [[35](#page8)] | |  | Theory |  |  |
|  | ω | FS | ω | FS | q− | q+ |
| 2P3o/2 | 287 | 287 | 293 | 293 | 295 | 291 |
| 4P1/2 | 44080 |  | 41643 |  | 453 | 451 |
| 4P3/2 | 44191 | 111 | 41754 | 111 | 565 | 564 |
| 4P5/2 | 44364 | 174 | 41935 | 181 | 746 | 744 |
| 2D3/2 | 55304 |  | 54655 |  | 509 | 507 |
| 2D5/2 | 55320 | 16 | 54675 | 20 | 530 | 530 |
| 2S1/2 | 65495 |  | 65148 |  | 40 | 39 |
|  |  |  |  |  |  |  |

Like in Zn, the left and write derivatives q− and q+ are close to each other, and all levels with equal exact quantum numbers are well separated. The astrophysical data exist for the levels 2S1/2 and 2D5/2. The former corresponds to the 3p → 4s, while the latter corresponds to the 3s → 3p transition and has much larger positive q.

(HDHF = EΨ, (12)

That is in agreement with the fact that relativistic corrections to the energy usually decrease with the principle quantum number n and with the orbital quantum number l. Therefore, for the ns → np transition one should expect large and positive q, while for np → (n + 1)s, there should be large cancellation of relativistic corrections to upper and to lower levels, resulting in smaller q (see discussion in [25, 26]). The dominant correction to our results should be from the core-valence correlations. In the recent calculations of Mg, which has the same core as Si II, the core-valence corrections to transition frequencies were found to be about 4% [33, 36]. We conservatively estimate corresponding correction to q to be 6% of the larger q, i.e. 30 cm−1

1. Cr II

Cr II has the ground state configuration [1s2 . . . 3p6]3d5 with five valence electrons. The astrophysical data cor-respond to the 3d → 4p transition, for which one may expect negative value of q. CI calculations here are much more complicated, than for Si II. There is strong relax-ation of the 3d shell in the discussed transition, which requires more basic d-orbitals. Therefore, we used the [6sp9d6f] basis set. In CI we included only single and double (SD) excitations. Some of the triple, quadruple, and octuple excitations were accounted for by means of the second order perturbation theory. It was found that corresponding corrections to transition frequencies were of the order of few percent, and were even smaller for parameters q. In general, these corrections did not improve the agreement with the experiment, so we present only CI results in Table  [IV](#page5).

As we mentioned above, there is strong relaxation of the 3d-shell in the 3d → 4p transition. We were not able to saturate CI space and completely account for this relaxation. Because of that, we estimate the error for q here to be close to 10%.

TABLE IV: Transition frequencies ω from the ground state 6S5/2, fine structure splitting FS, and parameters q for Cr II (in cm−1 ). CI single-double approximation was used for the Coulomb-Breit interaction.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Experiment | |  | Theory |  |
|  | ω | FS | ω | FS | q+ |
| 6D5/2 12148 | |  | 13123 |  | −2314 |
| 6D7/2 | 12304 | 156 | 13289 | 165 | −2153 |
| 6F1o/2 | 46824 |  | 47163 |  | −1798 |
| 6F3o/2 | 46906 | 82 | 47244 | 81 | −1715 |
| 6F5o/2 | 47041 | 135 | 47378 | 134 | −1579 |
| 6F7o/2 | 47228 | 187 | 47565 | 187 | −1387 |
| 6F9o/2 | 47465 | 237 | 47803 | 238 | −1148 |
| 6F11o/2 | 47752 | 287 | 48091 | 288 | −862 |
| 6P1o/2 | 48399 |  | 48684 |  | −1364 |
| 6P2o/2 | 48491 | 92 | 48790 | 106 | −1278 |
| 6P3o/2 | 48632 | 141 | 48947 | 157 | −1108 |
|  |  |  |  |  |  |

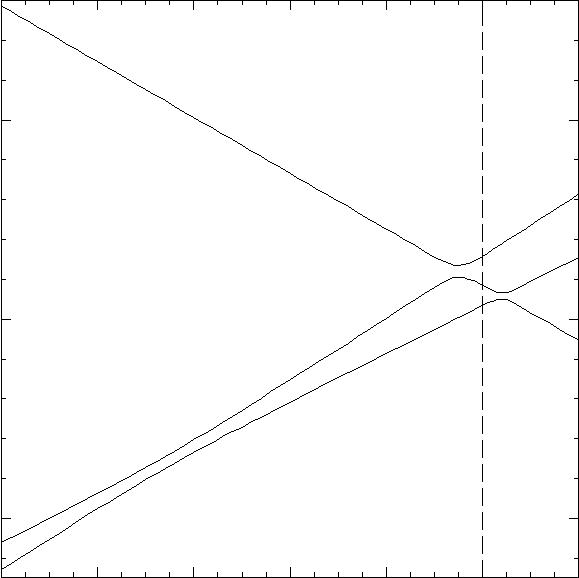
We have seen before for Zn II and Si II, that in the absence of level-crossing the diﬀerence between q+ and q− is smaller than other theoretical uncertainties. In Cr II there are no close levels which may interact with each other, so in the calculation presented in Table  [IV](#page5) we determined only the right derivative q+ . In calculations with diﬀerent basis sets we checked that the diﬀerence between q+ and q− is much smaller than the given above theoretical error (see Table I).

1. Fe II

Fe II ion has 7 valence electrons in configuration 3d64s and represents the most complicated case. The astrophysical data includes 5 lines in the band 38000 cm−1– 43000 cm−1and two lines with the frequency close to 62000 cm−1. The first band consists of three close, but separated multiplets with a regular fine structure split-tings. The 62000 cm−1 band is completely diﬀerent as the multiplets here strongly overlap and fine structure inter-vals are irregular [35]. Characteristic distance between the levels with identical exact quantum numbers is few hundred cm−1 , which is comparable to the fine structure splittings. This means that the levels strongly interact and even their identification may be a problem.

In fact, in Moore Tables [1.35] one of the multiplets of interest, namely y 6P o , is erroneously assign to the con-figuration 3d6(7S)4p. It is an obvious misprint, as there is no term 7S for configuration 3d6. This term appears, however, in the configuration 3d5 and the correct assign-ment of this multiplet should be 3d5(7S)4s4p. This as-signment is in agreement with our calculations and with the experimental g-factor of the level with J = 7/2. We checked that all close levels of the configuration 3d64p have significantly smaller g-factors.

This reassignment has dramatic consequences in terms of the corresponding parameter q as configurations 3d64p (4s − 4p transition from the ground state) and 3d54s4p (3d − 4p transition) move in the opposite directions from the ground state configuration 3d64s when x is changed. It also causes a number of pseudo-crossings to occur right in the vicinity of x = 0 (see Fig. 1).



|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 0 | 0.2 | 0.4 | 0.6 | 0.8 | 1 | 1.2 |

FIG. 1: Examples of typical interaction of levels in the upper band of Fe II. Levels are shown in arbitrary units as function of (α/α0 )2 = x + 1. Levels of configuration 3d6 4p have similar slopes and strongly interact with each other. That causes wide pseudo-crossings, similar to one shown on the left side of the plot. The level 6P7o/2 of the configuration 3d5 4s4p moves in the opposite direction. A series of sharp pseudo-crossings takes place near the physical value of α, marked by a vertical dotted line.

CI calculations for Fe II were done on the basis set [6spdf] in the SD approximation (see Table V). Triple excitations were included within second order perturbation theory and corresponding corrections were found to be relatively small. One can see from Table  [V](#page6) that for the lower band both frequencies and g-factors are reproduced rather accurately.

The first anomaly takes place at 44000 cm−1, where the levels 4D7o/2 and 4F7o/2 appear in the reverse order. Theoretical g-factors are also much further from LS values (1.429 and 1.238). That means that theoretical levels are at pseudo-crossing, while experimental levels already passed it. Indeed, calculations for x = 1/8 show that the right order of levels is restored, though the g-factors are still too far from LS values.

The second anomaly corresponds to the band above 60000 cm−1. Here the order of calculated levels diﬀers from that of the experimental ones. Note, that for this band only levels of negative parity with J = 7/2 are given in Table V. Thus, all of them can interact with each other. Let us estimate, how this interaction can aﬀect the slopes q.

TABLE V: Transition frequencies ω from the ground state 6D9/2 , g-factors, and parameters q± for Fe II (in cm−1 ).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Experiment | |  | Theory | |  |  |
|  | ω | g | ω | gg(LS) | | q− | q+ |
| 6D9o/2 | 38459 | 1.542 | 38352 |  | 1.556 | 1359 | 1363 |
| 6D7o/2 | 38660 | 1.584 | 38554 | 1.586 | 1.587 | 1522 | 1510 |
| 6F11o/2 | 41968 |  | 41864 |  | 1.455 | 1496 | 1508 |
| 6F9o/2 | 42115 | 1.43 | 42012 |  | 1.434 | 1615 | 1631 |
| 6F7o/2 | 42237 | 1.399 | 42141 | 1.396 | 1.397 | 1738 | 1737 |
| 6P7o/2 | 42658 | 1.702 | 42715 | 1.709 | 1.714 | 1241 | 1261 |
| 4D7o/2 | 44447 | 1.40 | 44600 | 1.345 | 1.429 | 1791 | 1837 |
| 4F7o/2 | 44754 | 1.29 | 44386 | 1.327 | 1.238 | 1608 | 1601 |
| 8P7o/2 | 54490 |  | 54914 | 1.936 | 1.937 | −2084 −2086 | |
| 4G7o/2 | 60957 | 0.969 | 63624 | 0.978 | 0.984 | 1640 | 1640 |
| 4H7o/2 | 61157 | 0.720 | 63498 | 0.703 | 0.667 | 1296 | 1247 |
| 4D7o/2 | 61726 | 1.411 | 66145 | 1.398 | 1.429 | 1194 | 1240 |
| 4F7o/2 | 62066 | 1.198 | 65528 | 1.252 | 1.238 | 1071 | 1052 |
| 6P7o/2 | 62172 | 1.68 | 65750 | 1.713 | 1.714 | −1524 −1514 | |
| 2G7o/2 | 62323 |  | 64798 | 0.882 | 0.889 | 1622 | 1605 |
|  |  |  |  |  |  |  |  |

Five levels from this band belong to configuration 3d64p and have close slopes with the average q¯ = 1360 cm−1. Only the level 4F7o/2 has the slope, which is 300 cm−1 smaller, than the average. The remaining level 6P7o/2 belongs to configuration 3d54s4p and has the slope of the opposite sign q1 = −1519 cm−1. Its absolute value is 500 cm−1 smaller, than for the level 8P7o/2 of the same configuration 3d54s4p. That suggests that the levels 4F7o/2 and 6P7o/2 strongly interact with each other. This is also in agreement with the fact, that these levels are the closest neighbors both experimentally and theoretically and that they cross somewhere between x− and x. There is also strong interaction be-tween the levels 2Go7/2, 4F7o/2, and 4D7o/2. That can be seen if one calculates the scalar products (overlaps) be-tween corresponding wave functions for diﬀerent values of x, such as: hi(x−)|k(x+ )i. For weekly interacting levels hi(x−)|k(x0 )i ≈ hi(x−)|k(x+ )i ≈ δi,k , so large non-diagonal matrix elements signal, that corresponding levels interact.

Interaction of levels 2Go7/2 , 4F7o/2 , and 4D7o/2 does not aﬀect the slopes q as strongly, as the interaction of 4F7o/2 and 6P7o/2 , so we can account for the former in a less accurate way, but it is important to include the latter as accurately as possible.

The level 6P7o/2 interacts with some linear combination of levels 2Go7/2, 4F7o/2 , and 4D7o/2. The slopes and g-factors of the latter are relatively close to each other, so we can simply take the average for all three:

|  |  |
| --- | --- |
| g¯ = 1.185; q¯ = 1297. | (13) |

Now we can use experimental g-factor of the state 6P7o/2

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| *58000* | |  | |  | |  | |
| *56000* | |  | |  | |  | |
| *54000* | |  | |  | |  | |
| *52000* | |  | |  | |  | |
| *50000* | |  | |  | |  | |
| 0.6 | | 0.8 | | 1.0 | | 1.2 | |

FIG. 2: Dependence of the odd levels of Ni II on (α/α0 )2 = x + 1. Solid lines correspond to J = 5/2 and dashed lines to J = 7/2. The experimental positions of the lines are shown as short horizontal lines and are all shifted by 1000 cm−1 . The order of levels from bottom up: 4D7o/2,5/2 , 4Go7/2,5/2 , 4F7o/2,5/2 , 2Go7/2 , 2F5o/2 , 2D5o/2 , and 2F5o/2 . and Eq.  [(11)](#page3) to determine the mixing:

 (14)

 (15)

Eq.  [(15)](#page6) corresponds to the correction δq = +177.

Eq. (15) corresponds to the correction \_q = +177. Therefore, for the closest level 4Fo 7/2 this model gives an estimate:

 (16)

Eqs.  [(15)](#page6) and  [(16)](#page6) show that correction for the mixing is not very large. That corresponds to the fact that experimental g-factor of the level 6P7o/2 is significantly larger than any g-factors of the levels of the configuration 3d64p. Thus, the interaction for this level is relatively small. On the contrary, the levels of the configuration 3d64p strongly interact with each other, but corresponding changes of the slopes are also relatively small (since the q values for these strongly interacting levels are approximately the same).

We estimate the accuracy of our calculations for the lower band of Fe II to be about 150 cm−1, and approximately 300 cm−1 for the values  [(15)](#page6) and  [(16](#page6)).

1. Ni II

Ni II has the ground state configuration 3d9. The spectrum is somewhat simpler, than for Fe II. There are als0 pseudo-crossings here, but they either lie far from x = 0, or are rather wide. That makes their treatment slightly easier. Nevertheless, our results significantly diﬀer from previous calculations [28].

TABLE VI: Transition frequencies ω from the ground state, g-factors, and parameters q± for Ni II (in cm−1).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Experiment | |  | Theory | |  |  |
|  | ω | g | ω | gg(LS) | | q− | q+ |
| 2D3/2 | 1507 |  | 1579 |  | 0.800 | 1559 | 1552 |
| 4D7o/2 | 51558 | 1.420 | 50415 | 1.423 | 1.429 | −2405 −2425 | |
| 4D5o/2 | 52739 | 1.356 | 51640 | 1.360 | 1.371 | −1217 −1245 | |
| 4G7o/2 | 54263 | 1.02 | 53150 | 1.016 | 0.984 | −1334 −1387 | |
| 4G5o/2 | 55019 | 0.616 | 53953 | 0.617 | 0.571 | −370 | −418 |
| 4F7o/2 | 55418 | 1.184 | 54323 | 1.183 | 1.238 | −1104 −1124 | |
| 4F5o/2 | 56075 | 0.985 | 55063 | 0.986 | 1.029 | −332 | −334 |
| 2G7o/2 | 56372 | 0.940 | 55284 | 0.933 | 0.889 | −60 | −188 |
| 2F7o/2 | 57080 | 1.154 | 56067 | 1.128 | 1.143 | −911 | −713 |
| 2D5o/2 | 57420 | 1.116 | 56520 | 1.108 | 1.200 | −1419 −1438 | |
| 2F5o/2 | 58493 | 0.946 | 57589 | 0.959 | 0.857 | −35 | −5 |
|  |  |  |  |  |  |  |  |

CI calculations were done for the Coulomb potential and included SD and partly triple excitations on the basis set [5spdf]. We calculated 5 lower odd levels with

J = 5/2 and 5 with J = 7/2 for x−, x0, and x+ , and used parabolic extrapolation for the interval −0.4 ≤ x ≤ +0.3 (see Fig. 2). It is seen that the theory accurately repro-duce relative positions of all levels. An overall agreement between the theory and the experiment becomes close to perfect if all experimental levels are shifted by 1000 cm−1 down, as it is done in Fig. 2. Note, that this shift constitutes only 2% of the average transition frequency.

Calculated g-factors are generally in agreement with the experiment [1.35] and noticeably diﬀerent from the pure LS-values (see Table VI). However, for the level 2F7o/2 theoretical g-factor is smaller than the LS value, while experimental one is larger. There are no nearby levels who may mix to this one and move g-factor closer to experiment. On the other hand, the diﬀerence with experiment is only 2% and may be within experimental accuracy.

Fig.  [2](#page6) shows that the levels 2Go7/2 and 2F7o/2 cross at x ≈ 0.3 and they already strongly interact at x = 0. Theoretical splitting for these levels is 10% larger than experimental one. Thus, they are in fact even closer to the crossing point than is predicted by the theory. The experimental splitting is equal to the theoretical one for larger value of α corresponding to x ≈ 0.15. At x = 0.15 the slopes of these levels are −265 and −590, and for x = 0 they are −124 and −812 correspondingly. Note, that the sum of the slopes at x = 0.15 diﬀers by 80 cm−1 from the sum at x = 0. According to Eq.  [(7)](#page3) for a two-level system the sum is constant. This means that these two levels repel from the lower lying level 4F7o/2 . Taking this analysis into account we suggest an average between x = 0 and x = 0.15 as our final value: q(2F7o/2 ) = −700(250).

 (1.1a)

 (1.1b)

 (1.2)

 (1.3)

 (1.4)

 (1.5a)

 (1.5b)

 (1.6)

 (1.7)

 (1.8)

 (1.9)

 (1.10)

 (1.11a)

 (1.11b)

 (1.12)

 (1.13)

 (1.14)

 (1.15)

 (1.16)

**Chapter 3**

**I. CALCULATIONS OF ENERGIES**

We use relativistic Hartree-Fock (RHF) and configuration interaction (CI) methods to do the calculations.

RHF Hamiltonian is used to generate a set of single-electron orbitals. We use a form of singe-electron wave function which explicitly depends on the fine structure constant α.

Then the RHF equation for ψ(r)n has the following form (in atomic units)

The value of relativistic eﬀects is studied by varying the value of α in (2). In particular, non-relativistic limit corresponds to α = 0.

In the CI calculations we use approach similar to what was first developed in Ref. [2.12]. Electrons occupying open shells are considered as valence electrons and all other are core electrons. Correlations between valence electrons are treated within the CI method while correlations between valence and core electrons are included by means of the many-body perturbation theory.

It describes correlations between a particular valence electron and core electrons (see Ref. [2.12] for details). Note that in contrast with Ref. [2.12] we don’t include in present work the Σ2 operator, which is a two-electron operator describing diﬀerent type of correlations between valence and core electrons. Terms with Σ2 can be considered as screening of Coulomb interaction between valence electrons by core electrons. These terms are less important than those with Σ, but much more time consuming in calculations. We either neglect them or simulate their eﬀect by introducing screening factors.

We are now going to discuss the specifics of the calculations for each atom/ion. Apart from the states of interest we also calculate energies of the other states of the same con-figurations to ensure that the accuracy is systematically good. We also calculate magnetic g-factors to ensure correct identification of states. This is particularly important for dysprosium.

**A. Strontium**

Strontium in its ground state is a closed-shell atom. It has two 5s-electrons on its outermost shell and we need to consider energy intervals between 1S0 ground state and states of the 5s5p configuration where the 3P1 metastable state is of most interest. The RHF calculations for Sr were done in V N approximation, for a closed-shell atom in its ground state. For the CI calculations we considered Sr as an atom with two valence electrons and followed the similar calculations for Ba [2.13]. Basis states for the CI+MBPT method were calculated using the B-spline technique [2.14] with 40 B-splines in a cavity of radius R = 40aB .

ˆ

The same basis functions were used to calculate Σ1 and for the CI calculations. Thirteen lowest states above core in each of the s1/2, p1/2, p3/2, d3/2 and d5/2 waves were used to construct two-electron wave function for both 5s2 and 5s5p configurations. Large number of basis functions is needed mostly for adequate description of the 5s5p configuration. This is because the V N approximation doesn’t provide us with a good 5p single-electron state. Also, the 5s single-electron state in the 5s5p configuration is diﬀerent from the 5s state in the 5s2 configuration for which Hartree-Fock calculations were done. However, with thirteen states in each wave the saturation of the basis was clearly achieved and adding more states to the basis didn’t change the energy. Two-electron basis states for the CI calculations were obtained by distributing valence electrons over 65 basis states (13 × 5) in all possible ways with a restriction of fixed parity and total momentum.

The results are presented in Table I. As one can see the accuracy for the state of the interest 3P1 is better than 1% while accuracy for other states is also good.

**B. Ytterbium**

The ground state of ytterbium positive ion is 4f 146s 2S1/2 and we need to consider transitions into the 4f 145d 2D5/2 and 4f 136s2 2F7/2 states. Therefore it is convenient to do the RHF calculations in the V N −1 approximation, for the Yb2+ ion with the 4f 14 closed-shell configuration. The 6s, 5d and other basis states for the CI method are calculated then in the field of frozen closed-shell core of Yb2+. Then, in the CI calculations, we need to consider all 4f electrons as valence ones since one of the transitions of the interest involves excitation from the 4f subshell. So, the total number of valence electrons in present CI calculations is fifteen. This is very diﬀerent from our previous calculations for Yb+ [5] in which the 4f 136s2 2F7/2 state was not considered and we were able to treat ytterbium ion as a system with one external electron above closed shells.

Our final set of single-electron states for the CI calculations consisted of 4f5/2, 4f7/2, 6s1/2, 5d3/2, 5d5/2 and few more s and f states above 4f and 6s. Note that in contrast with Sr we don’t need many basis functions here because all our single-electron wave functions correspond to the Yb+ . This makes initial approximation to be very good and leads to fast convergence of the CI calculations with respect to the basis set used.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ˆ | in calculations for Yb | + | . In a case of many valence electrons |  |
| We also don’t include Σ1 |  |  |

(fifteen for Yb+ ) correlations are dominated by correlations between them which are taken into account accurately via the CI technique. Correlations between valence electrons and core electrons mostly manifest themselves via screening of the Coulomb interaction between valence electrons. We take this eﬀect into account semi-empirically, by introducing screening factors fk . Namely, we multiply every Coulomb integral of the multi-polarity k by a numerical factor fk which is chosen to fit the energies. It turns out that good fit for Yb+ is achieved

with f2 = 0.8 and fk = 1 for all other k.

Many-electron basis states for the CI calculations were obtained by allowing all possible single and double excitations from the base configuration with the restriction of fixed parity and total momentum.

Results for energies of Yb+ are presented in Table I. The theoretical accuracy for energies as compared to the experiment is 2- 3% for the states of interest and is not worse than 5% for other states.

**C. Dysprosium**

Dysprosium atom is the most diﬃcult for calculations because of its complicated electron structure. Ground state configuration of Dy is 4f 106s2 which means that there is no realistic RHF approximation which corresponds to a closed-shell system. We do the RHF calculations for Dy in the V N approximation with an open-shell version of the RHF method. Contribution of the 4f electrons into the RHF potential is calculated as for a closed shell and then multiplied by a numerical factor to take into account its fractional occupancy. This factor is 10/14 when interaction of the 4f electrons with other core electrons is considered and 9/13 when interaction of a 4f electron with other 4f electrons is considered. When convergence is achieved we have the 4f and 6s basis states for the CI calculations. To calculate other states of valence electrons we remove one 6s electron, freeze all RHF orbitals, including 4f and 6s and calculate the 6p1/2, 6p3/2, 5d3/2, 5d5/2 and few more d-states above 5d in the field of frozen RHF core.

In the CI calculations states below 4f are considered as core states and all other as valence states. Total number of valence electrons is therefore twelve. As for the case of

|  |  |  |  |
| --- | --- | --- | --- |
|  | ˆ | and use screening factors as fitting parameters to improve agreement |  |
| Yb | we neglect Σ1 |  |

with experiment. It turns out that best fit for the 4f 106s6p configuration is achieved with f1 = 0.7 and fk = 1 for all other k. No fitting was used for other configurations.

To calculate states of the 4f 106s2, 4f 106s6p and 4f 106s5d configurations we use the 4f5/2, 4f7/2, 6s1/2, 6p1/2, 6p3/2, 5d3/2 and 5d5/2 single-electron basis functions and all possible configurations which can be obtained from these basis functions by exciting of one or two electrons from the base configuration. Same approach doesn’t work for the 4f 95d26s configuration because of huge number of many-electron basis states generated this way and as a consequence, the CI matrix is of so large size that it could not be handled by our computers. On the other hand test calculations with pairs of configurations showed that mixing of our state of interest with other configurations is small and can be neglected. We do need however to include mixing with the 4f 95d6d6s, 4f 95d7d6s and 4f 96d26s configurations. This is because our basis 5d state corresponds rather to the 4f 105d6s configuration and extra d-states are needed to correct it.

The result are presented in Table I. Note that they are considerably better than in our previous calculations [2.15]. This is because of better basis and more complete CI treatment.

**III. FREQUENCY SHIFT: RESULTS AND DISCUSSIONS**

In the vicinity of the physical value of the fine structure constant (α = α0) frequency (ω) of an atomic transition can be presented in a form

|  |  |
| --- | --- |
| ω = ω0 + qx, | (5) |

where x = (α2/α02) − 1, ω0 is the experimental value of the frequency and q is a coeﬃcient which determines the frequency dependence on the variation of α.

The results for coeﬃcients q are presented in Table II. Note that we have included in the Table the results of our old calculations for Yb+ . These calculations were done in a very diﬀerent way, assuming that Yb+ is an atom with one external electron above closed shells. Comparison of the results obtained by diﬀerent methods gives estimate of the accuracy of calculations.

Search for the time variation of the fine structure constant can be conducted by comparing two frequencies of atomic transitions over long period of time.

Current best laboratory limit on the time variation of α is α/α˙ < 10−15yr−1 [4].

In the first experiment considered in this paper a dual calcium-strontium beam is to be used to compare the frequencies of the 1S0 −3 P1 transitions in both atoms. Substituting ω1 = 15210cm−1, q1 = 230cm−1 for Ca [5], ω2 = 14504cm−1, q2 = 667cm−1 for Sr (Tables I,II) and α/α˙ = 10−15yr−1 we get are to be compared.

Δ(t)(Yb+) = 6.1 × 10−15yr−1.

Note that the width of 3P1 state in Sr may be a problem in this case. In the case of Ybfrequencies

of the 2S1/2 −2 D5/2 and 2S1/2 −2 F7/2 Substituting the numbers we get (9)

Note two orders of magnitude improvement in the magnitude in comparison with the Sr-Ca dual beam experiment.

We have also calculated q-coeﬃcient for 4f 14 1S0 - 4f 135d 3P0 (ω = 45276 cm−1) transition from YbIII ground state. This was motivated by the proposed measurements [9] of α-variation using comparison of 1S0 - 3P0 transition frequencies in In+, Tl+ and odd isotope of Yb++. The diﬀerent signs and magnitudes of relativistic corrections in In+ (q= 4414 cm−1), Tl+ (q=19745 cm−1) and Yb++ (q= -27800 cm−1) provide an excellent control of systematic errors since systematic errors are not correlated with signs and magnitudes of the frequency shifts qx, where x = (α2/α02) − 1. The same idea (combination of anchors, positive shifters and negative shifters) has been used to control systematic errors in Ref. [2.2].

In our view, a very interesting possibility is that for dysprosium. Instead of comparing frequencies of diﬀerent transitions one should measure the energy diﬀerence between two very close states of opposite parity. The corresponding q-coeﬃcient is q = 6008 + 23708 = 29716cm−1 (see Table II). The frequency of this transition ranges from few MHz to few GHz depending on isotopes and hfs components used. If we take, e.g. ω = 3.1MHz [2.10] we get

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Δ(t)(Dy) = 5.7 × 108( | α˙ | ). | (11) |  |
|  |  |
|  | α0 | |  |  |

This is an eight orders of magnitude enhancement in the relative value of the eﬀect compared to atomic clock transitions! Substituting α/α˙ = 10−15yr−1 we get

|  |  |
| --- | --- |
| Δ(t)(Dy) = 5.7 × 10−7yr−1. | (12) |

This means that to improve current best limit on local time variation of α the frequency of this transition in Dy should be measured to the accuracy of about 10−7 over about a year time interval. This seems to be feasible [2.7].

 (2.1)



 (2.2)

 (2.3)

 (2.4)

 (2.5)



 (2.6)

 (2.7)

 (2.8)

**Chapter 4**

The possibility that the fundamental constants vary is suggested by theories unifying gravity with other interactions (see, e.g. [3.1, 2, 3] and review [3.4]). The analysis of quasar absorption spectra by means of the many-multiplet method reveals anomalies which can be interpreted in terms of varying fine structure constant α [3.5, 6, 7]. The first indication that α might have been smaller at early epoch came from the analysis of magnesium and iron lines [3.5, 6]. Later inclusion of other lines belonging to many diﬀerent atoms and ions (Si, Cr, Ni, Zn, etc.) as well as many samples of data from diﬀer-ent gas clouds not only confirmed the initial claim, but made it even stronger [3.7]. However, there are some recent works in which a similar analysis indicates no variation of α in quasar absorption spectra [3.8, 9]. These works use the same many-multiplet method and the results of our calculations of the relativistic eﬀects in atoms, but analyze diﬀerent samples of data from a diﬀerent telescope. It is important to include as much data as possible into the analysis to resolve the diﬀerences, and to verify or discard the claim of a varying fine structure constant.

It is natural to analyze fine structure intervals in the search of variation of α. Indeed, initial searches of variation of α in quasar absorption spectra were based on alkali-doublet lines (alkali-doublet method) [3.10, 11, 12] and on the fine structure of O III [3.13]. However, all of the present evidence for varying fine structure constant has come from the analysis of the E1-transition frequencies (many-multiplet method) rather than fine structure intervals. These frequencies are about an order of magnitude more sensitive to the variation of α [3.6]. However, the corresponding analysis is much more complicated. One needs to perform accurate ab initio calculations of the atomic structure to reveal the dependence of transition frequencies on the fine structure constant. We have done such calculations for many atoms and ions in our previous works [3.14, 15]. In the present work we do similar calculations for some other atoms and ions for which data on quasar absorption spectra are available [3.16], and for which corresponding calculations have not previously been done.

We use the relativistic Hartree-Fock (RHF) method as a starting point of our calculations. Correlations are included by means of configuration-interaction (CI) method for many valence electron atoms, or by the many-body perturbation theory (MBPT) and Brueckner-orbital method for single valence electron atoms. The dependence of the frequencies on α is revealed by varying in computer codes.

The results are presented in the form

|  |  |
| --- | --- |
| ω = ω0 + qx, | (1) |

where x = (α2 /α20) − 1, α0 is the laboratory value of the fine structure constant, ω and ω0 are the frequencies of the transition in quasar absorption spectra and in the laboratory, respectively, and q is the relativistic energy shift that comes from the calculations. Comparing the laboratory frequencies, ω0, with those measured in the quasar absorption spectra, ω, allows one to obtain the value of α billions of years ago.

The method of calculations is described in detail in our early works [3.14, 15]. Here we only discuss the details specific for current calculations.

Some atoms and ions considered in the present work represent open-shell (many valence electron) systems. Therefore, the Hartree-Fock procedure needs to be further specified. The natural choice is to remove all open-shell electrons and start the Hartree-Fock calculations for the closed-shell core. However, this usually leads to poor convergence of the subsequent CI method. Better convergence can be achieved using the so called V N − 1 approximation in which only one valence electron is removed. Since we calculate not only the ground state but also ex-cited states of diﬀerent configurations, it is convenient to remove the electron which changes its state in the transition. Single-electron basis states for valence electrons are calculated in the V N −1 potential of the frozen-core.

The V N −1 potential corresponds to an open-shell sys-tem. We include the contribution of the open shells into the Hartree-Fock potential as if they were totally filled and then multiply them by a weighting coeﬃcient. Note that this procedure must not destroy the cancellation of the self-action (we would like to remind the reader that there is exact cancellation between direct and exchange

self-action in the Hartree-Fock equations for the closed-shell systems).

For the CI calculations we use B-splined single-electron basis set similar to those developed by Johnson et al [3.17, 18, 19]. The main diﬀerence is that we use the open-shell RHF Hamiltonian described above to calculate the B-splined states.

There are two major sources of inaccuracy in the stan-dard CI calculations. One is incompleteness of the basis set and another is core-valence correlations. We use a fitting procedure to model both eﬀects. We add an extra term into a single-electron part of the Hamiltonian for the valence electrons:

|  |  |
| --- | --- |
| αc |  |
| U (r) = −2 (r4 + a4) . | (3.2) |

Here αc is the polarizability of the atomic core and a is a cut-oﬀ parameter that is introduced to remove the singularity at r = 0. We use a = ab (Bohr radius) and treat αc as a fitting parameter. The values of αc for each partial wave (s, p, d) are chosen to fit the experimental energy levels of the many-electron atom.

The term  [(3.2)](#page2) describes polarization of the atomic core by valence electrons. It can be considered as a semi-empirical approximation to the correlation interaction of a particular valence electron with the core. It also allows us to improve the convergence of the CI calculations by modifying the single-electron basis states. Our calculations for rare-earth ions [3.20, 21] have demonstrated that using this term allows one to obtain good accuracy of calculations with the minimum number of single-electron basis states (one in each partial wave in the cited works).

Below we present the details and results of calculations for the atoms and ions considered. All transition frequencies are presented with respect to the ground state. Therefore we use the term “energy levels” instead. If a transition between excited states is needed, the corresponding relativistic energy shift q is the diﬀerence be-tween the level shifts (q2→1 = q2 − q1).

a. Manganese (Z = 25): The ground state of Mn+ is 3d54s 7 S3 and we need to consider transitions into the 3d44s4p configuration. Earlier we also considered transitions to the states of the 3d54p configuration [3.14]. Since in the present work we use diﬀerent basis set, we have repeated calculations for this configuration in order to check their accuracy.

The RHF calculations are done in the V N − 1 approximation with the 3d5 configuration of external electrons. The 4s, 4p and higher states are calculated in the same V N −1 potential. We use αc = 2.05a3B for the p-wave as a fitting parameter (see formula  [(3.2)](#page2)). The results are presented in Table I. Fitting changes both energies and q-coeﬃcients by less than 10%, and agreement with previous calculations is also within 10%. Therefore, we use 10% as a conservative estimate of the accuracy of q.

Note that the relativistic shift is positive for the s − p singe-electron transitions and negative for the d −p transitions. Having transitions with diﬀerent signs of q- coeﬃcients in the same atom (ion) helps to fight systematic errors in the search for variation of α (see Ref. [3.14] for details).

b. Titanium ( Z = 22): We perform calculations for both Ti+ and Ti2+ starting from the same RHF approximation, and using the same single-electron basis set. The ground state of Ti+ is 3d24s 4F3/2 and we need to consider transitions into states of the 3d24p configuration. The ground state of Ti2+ is 3d2 3F2 and we need to con-sider transitions into the states of the 3d4p configuration. Therefore it is convenient to do the RHF calculations for the Ti2+ ion with the 3d2 open-shell configuration. The 4s, 4p and other basis states for the CI method are calculated in the frozen-core field of Ti2+.

The fitting parameters chosen are αc = 0.38a3B for s-electrons and αc = 0.065a3B for d-electrons. The results are presented in Table II. As in the case of Mn+, there are negative and positive relativistic shifts. The eﬀects of fitting and change of basis set does not exceed 10%. The values of the q-coeﬃcients for titanium are consistent with calculations for other atoms and with semi-empirical estimations using the formulas presented in [3.14]. In particular, the values of the negative q-coeﬃcients for the d − p transitions are very close to the values for similar transitions in Cr II [3.14]. The positive coeﬃcients for Ti+ are very close to those for Mn+ after rescaling by Z 2 according to the semi-empirical formula [3.14].

TABLE I: Energies and relativistic energy shifts (q) for Mn+ (cm−1)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| State |  |  | Energy | | q |  |
|  |  | theory | | experiment |  |  |
|  |  | no fitting | fitted | [[22](#page4)] | this work | [[15](#page4)] |
| 3d5 4p | 7P2 | 36091 | 38424 | 38366 | 869 | 918 |
| 3d5 4p | 7P3 | 36252 | 38585 | 38543 | 1030 | 1110 |
| 3d5 4p | 7P4 | 36483 | 38814 | 38807 | 1276 | 1366 |
| 3d4 4s4p 7P2 | | 97323 | 83363 | 83255 | -3033 |  |
| 3d4 4s4p 7P3 | | 97554 | 83559 | 83376 | -2825 |  |
| 3d4 4s4p | 7P4 | 97858 | 83818 | 83529 | -2556 |  |
|  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |

TABLE II: Energies and relativistic energy shifts (q) for Ti+ and Ti2+ (cm−1)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | |  | Energy |  | q |
|  |  | theory |  | experiment |  |
|  |  | no fitting | fitted | [[22](#page4)] |  |
|  |  | Ti+ | |  |  |
| 3d2 4p | 4 G5/2 | 27870 | 29759 | 29544 | 396 |
| 3d2 4p | 4 F3/2 | 28845 | 30691 | 30837 | 541 |
| 3d2 4p | 4 F5/2 | 28965 | 30813 | 30959 | 673 |
| 3d2 4p | 4 D1/2 | 30582 | 32416 | 32532 | 677 |
| 3d2 4p | 4 D3/2 | 30670 | 32510 | 32603 | 791 |
| 3d4s4p | 4 D1/2 | 50651 | 52185 | 52330 | -1564 |
|  |  | Ti2+ | |  |  |
| 3d4p | 3 D1 | 80558 |  | 77000 | -1644 |
|  |  |  |  |  |  |
|  |  |  |  |  |  |

TABLE III: Energies and relativistic energy shifts (q) for Na (cm−1 )

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | State |  | Energy | q |
|  |  | theory | experiment  [[22](#page4)] |  |
| 3p | 2P1/2 | 16858 | 16956 | 45 |
| 3p | 2P3/2 | 16876 | 16973 | 63 |
| 4p | 2P1/2 | 30124 | 30267 | 53 |
| 4p | 2P3/2 | 30130 | 30273 | 59 |
|  |  |  |  |  |

TABLE IV: Energies and relativistic energy shifts (q) for the carbon atom and its ions (cm−1 )

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | State |  | Energy | q |
|  |  | theory | experiment  [[3.22](#page4)] |  |
|  |  | C |  |  |
| 2s2p3 | 3 D3 | 66722 | 64087 | 151 |
| 2s2p3 | 3 D1 | 66712 | 64090 | 141 |
| 2s2p3 | 3 D2 | 66716 | 64091 | 145 |
| 2s2p3 | 3 P1 | 75978 | 75254 | 111 |
| 2s2p3 | 3 S1 | 100170 | 105799 | 130 |
|  |  | C+ |  |  |
| 2s22p | 2 P1/2 | 74 | 63 | 63 |
| 2s2p2 | 2 D5/2 | 76506 | 74930 | 179 |
| 2s2p2 | 2 D3/2 | 76503 | 74933 | 176 |
| 2s2p2 | 2 S1/2 | 97993 | 96494 | 161 |
|  |  | C2+ |  |  |
| 2s2p | 1 P1 | 104423 | 102352 | 162 |
|  |  | C3+ |  |  |
| 2p | 2 P1/2 | 65200 | 64484 | 104 |
| 2p | 2 P3/2 | 65328 | 64592 | 232 |
|  |  |  |  |  |

c. Sodium (Z = 11): In contrast to the ions considered above, sodium is an atom with one external electron above closed shells. Its ground state is 1s22s 22p63s 2S1/2. Very accurate calculations are possible for such systems by including certain types of correlation diagrams to all orders (see, e.g. [3.23, 24]). However, since both relativistic and correlation eﬀects for sodium are small we use a simplified approach. We calculate the correlation potential ˆΣ (the average value of this operator is the correlation correction to the energy of the external electron) in the second order only. Then we use it to modify the RHF equations for the valence electron and to calculate the so called Brueckner-orbitals. Note that due to iterations of ˆΣ certain types of correlation diagrams are still included in all orders in this procedure. The final accuracy of the energy is better than 1%, and for the fine structure accuracy is 2-6% (see Table III). We believe that the accuracy for the relativistic shifts q is on the same level.

d. Carbon (Z = 6): Relativistic eﬀects for carbon and its ions are small and calculations can be done with-out fitting parameters. The ground state of neutral car-bon is 1s22s22p2 3P0 . Our RHF calculations for this atom include all electrons, however, since we need to con-sider configurations with excitations from both 2s and 2p states, we treat both as valence states in CI.

TABLE V: Energies and relativistic energy shifts (q) for oxy-gen ions (cm−1)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | State |  | Energy | q |
|  |  | theory | experiment  [[3.22](#page4)] |  |
|  |  | O+ |  |  |
| 2s2p4 | 4 P5/2 | 122620 | 119873 | 346 |
| 2s2p4 | 4 P3/2 | 122763 | 120000 | 489 |
| 2s2p4 | 4 P1/2 | 122848 | 120083 | 574 |
|  |  | O2+ |  |  |
| 2s2p3 | 3 D1 | 121299 | 120058 | 723 |
| 2s2p3 | 3 P1 | 143483 | 142382 | 726 |
|  |  | O3+ |  |  |
| 2s2p2 | 2 D3/2 | 129206 | 126950 | 840 |
|  |  | O5+ |  |  |
| 1s2 2p | 2 P1/2 | 97313 | 96375 | 340 |
| 1s2 2p | 2 P3/2 | 97913 | 96908 | 872 |
|  |  |  |  |  |

For neutral carbon we have performed the calculations for the ground state configuration as well as for excited configurations 2s22p3s, 2s2p3, 2s22p4s,2s22p3d, 2s22p4d, 2s22p5d and 2s22p6d. However, we present in Table  [IV](#page3) only results for the 2s2p3 configuration. The relativistic energy shift for all other configurations is small (q < 50 cm−1). This is smaller than uncertainty of the q-coeﬃcients for heavier atoms and ions. Since the analysis of quasar spectra is based on comparison of the relativistic eﬀects in light and heavy atoms (ions), small relativistic energy shifts in light atoms can be neglected. The q-coeﬃcients for the 2s2p3 configuration are larger because this configuration corresponds to the 2s − 2p transition from the ground state. These are the lowest valence single-electron states with the largest relativistic eﬀects. Other excited configurations correspond to the 2p − ns or 2p − nd (n ≥ 3) transitions. However, relativistic energy shifts for higher states are smaller [3.14].

The calculations for C2+ and C3+ are done in the potential of the closed-shell (helium) core. As can be seen from Table  [IV,](#page3) accuracy for the energies is within 10%. We estimate the accuracy of q-coeﬃcients at around 10-20%.

e. Oxygen (Z = 8): Relativistic eﬀects for oxygen ions are comparatively large, and become larger with in-creasing electric charge. This is in agreement with semi-empirical formulae presented in [3.14]. For neutral oxygen, however, q-coeﬃcients are approximately 20 cm−1 or less; these results are not presented here.

 (3.1)



 (3.2)

**Chapter 5**

TABLE I: High-priority lines observed in QSO spectra. The first column is the ion; the second and third columns are the rest wavelength and the transition frequency, respectively; the fourth column is the oscillator strength; the relativistic shift (q value) is shown in the fifth column, where known. Those transitions for which high-accuracy laboratory data are needed are marked with either ‘A’ (very important) or ‘B’ (mildly important). Lines for which there is no measured isotopic structure are marked ‘I’. Additionally, there are some lines for which both the transition frequency and isotope shift are known; these are marked with an ‘M’. They are included here for reference only (of course, verification would still be useful). References for precisely measured lines are given in the last column. The second set of references are for isotope shift measurements, where available. The wavelengths and oscillator strengths are taken from the compilation by Morton [4.12, 13].

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Atom/ Wavelength Frequency Oscillator | | | | | q value | | |  | Refs. |  |
|  | Ion | ˚ | ω0 (cm | −1 | ) Strength | (cm | −1 | ) |  |  |  |
|  | λ (A) |  |  |  |  |  |
|  |  |  |  | |  |  |  | |  |  |  |
|  | C I | 945.188 | 105799.1 | | 0.272600 | 130 | (60) | | M | [[20](#page7)] |  |
|  |  | 1139.793 | 87735.30 | | 0.013960 | 0 | (100) | | B |  |  |
|  |  | 1155.809 | 86519.47 | | 0.017250 | ” |  |  | B |  |  |
|  |  | 1157.186 | 86416.55 | | 0.549500 | ” |  |  | B |  |  |
|  |  | 1157.910 | 86362.52 | | 0.021780 | ” |  |  | B |  |  |
|  |  | 1188.833 | 84116.09 | | 0.016760 | ” |  |  | B |  |  |
|  |  | 1193.031 | 83820.13 | | 0.044470 | ” |  |  | B |  |  |
|  |  | 1193.996 | 83752.41 | | 0.009407 | ” |  |  | B |  |  |
|  |  | 1260.736 | 79318.78 | | 0.039370 | 30 | (10) | | A |  |  |
|  |  | 1276.483 | 78340.28 | | 0.004502 | 17 | (10) | | A |  |  |
|  |  | 1277.245 | 78293.49 | | 0.096650 | −13 | (10) | | A |  |  |
|  |  | 1280.135 | 78116.74 | | 0.024320 | −21 | (10) | | A |  |  |
|  |  | 1328.833 | 75253.97 | | 0.058040 | 117 | (10) | | A |  |  |
|  |  | 1560.309 | 64089.85 | | 0.080410 | 137 | (10) | | A |  |  |
|  |  | 1656.928 | 60352.63 | | 0.140500 | −24 | (10) | | A |  |  |
|  | C II | 1037.018 | 96430.32 | | 0.123000 | 168 | (10) | | A |  |  |
|  |  | 1335.662 | 74869.20 | | 0.012770 | 178 | (10) | | A |  |  |
|  |  | 1335.707 | 74866.68 | | 0.114900 | 181 | (10) | | A |  |  |
|  | C III | 977.020 | 102352.0 | | 0.762000 | 165 | (10) | | B |  |  |
|  | C IV | 1548.204 | 64590.99 | | 0.190800 | 232 | (20) | | A | [[4.21](#page7)] |  |
|  |  | 1550.781 | 64483.65 | | 0.095220 | 104 (20) | | | A | [[4.21](#page7)] |  |
| O I | | 1025.762 | 97488.54 | | 0.020300 | 0 (20) | | | B |  |  |
|  |  | 1026.476 | 97420.72 | | 0.002460 | ” |  |  | B |  |  |
|  |  | 1039.230 | 96225.05 | | 0.009197 | ” |  |  | B |  |  |
|  |  | 1302.168 | 76794.98 | | 0.048870 | ” |  |  | A |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |

TABLE I: (continued)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Atom/ Wavelength Frequency Oscillator | | | | | | q value | | | |  | Refs. | |  |
|  | Ion | ˚ | ω0 (cm | −1 | ) Strength | | (cm | | −1 | ) |  |  |  |  |
|  | λ (A) |  |  |  |  |  |  |
|  |  |  |  | |  |  |  |  | |  |  |  |  |  |
| Na I | | 3303.320 | 30272.58 | | 0.013400 |  | 59 | (4) | |  | B |  |  |  |
|  |  | 3303.930 | 30266.99 | | 0.006700 |  | 53 | (4) | |  | B |  |  |  |
|  |  | 5891.583 | 16973.37 | | 0.655000 |  | 63 | (4) | |  | M | [[22][23, 24](#page7)] |  |  |
|  |  | 5897.558 | 16956.17 | | 0.327000 |  | 45 | (4) | |  | M | [[4.22][25](#page7)] |  |  |
| Mg I | | 2026.477 | 49346.73 | | 0.112000 |  | 87 |  |  |  | I | [[4.26](#page7)] |  |  |
|  |  | 2852.963 | 35051.27 | | 0.181000 |  | 86 | (10) | | | M  [[26, 27][28, 29](#page7)] | | |  |
| Mg II | | 1239.925 | 80650.04 | | 0.000267 |  |  |  |  |  | B |  |  |  |
|  |  | 2796.354 | 35760.85 | | 0.612300 |  | 211 | (10) | | | M | [[26, 27][30](#page7)] |  |  |
|  |  | 2803.532 | 35669.30 | | 0.305400 |  | 120 | (10) | | | I | [[4.26, 27](#page7)] |  |  |
| Al II | | 1670.789 | 59851.97 | | 1.880000 |  | 270 | (30) | | | M | [[4.21](#page7)] |  |  |
| Al III | | 1854.718 | 53916.54 | | 0.539000 |  | 464 | (30) | | | M | [[4.21](#page7)] |  |  |
|  |  | 1862.791 | 53682.88 | | 0.268000 |  | 464 | (30) | | | M | [[4.21](#page7)] |  |  |
| Si II | | 1190.416 | 84004.26 | | 0.250200 |  |  |  |  |  | B |  |  |  |
|  |  | 1193.290 | 83801.95 | | 0.499100 |  |  |  |  |  | B |  |  |  |
|  |  | 1260.422 | 79338.50 | | 1.007000 |  |  |  |  |  | A |  |  |  |
|  |  | 1304.370 | 76665.35 | | 0.094000 |  |  |  |  |  | A |  |  |  |
|  |  | 1526.707 | 65500.45 | | 0.117094 |  | 50 | (30) | | | I | [[4.21](#page7)] |  |  |
|  |  | 1808.013 | 55309.34 | | 0.002010 |  | 520 | (30) | | | I | [[4.21](#page7)] |  |  |
| Si IV | | 1393.760 | 71748.64 | | 0.528000 |  | 862 |  |  |  | A | [[4.21](#page7)] |  |  |
|  |  | 1402.773 | 71287.54 | | 0.262000 |  | 346 |  |  |  | A | [[4.21](#page7)] |  |  |
| S II | | 1250.583 | 79962.61 | | 0.005350 |  |  |  |  |  | A |  |  |  |
|  |  | 1253.808 | 79756.83 | | 0.010700 |  |  |  |  |  | A |  |  |  |
|  |  | 1259.518 | 79395.39 | | 0.015900 |  |  |  |  |  | A |  |  |  |
| Ca II | | 3934.775 | 25414.41 | | 0.688000 |  | 452 |  |  |  | A | [[4.13](#page7)] |  |  |
|  |  | 3969.590 | 25191.52 | | 0.341000 |  | 224 |  |  |  | A | [[4.13](#page7)] |  |  |
| Ti II | | 1910.600 | 52339.58 | | 0.202000 | −1564 | | (150) | | | A |  |  |  |
|  |  | 1910.938 | 52330.32 | | 0.098000 | −1783 | | (300) | | | A |  |  |  |
|  |  | 3067.245 | 32602.55 | | 0.041500 |  | 791 | (50) | | | I | [[4.26](#page7)] |  |  |
|  |  | 3073.877 | 32532.21 | | 0.104000 |  | 677 | (50) | | | I | [[4.26](#page7)] |  |  |
|  |  | 3230.131 | 30958.50 | | 0.057300 |  | 673 | (50) | | | I | [[4.26](#page7)] |  |  |
|  |  | 3242.929 | 30836.32 | | 0.183000 |  | 541 | (50) | | | I | [[4.26](#page7)] |  |  |
|  |  | 3384.740 | 29544.37 | | 0.282000 |  | 396 | (50) | | | I | [[4.26](#page7)] |  |  |
| Cr II | | 2056.256 | 48632.06 | | 0.105000 | −1110 | | (150) | | | I | [[4.26, 31](#page7)] |  |  |
|  |  | 2062.236 | 48491.05 | | 0.078000 | −1280 | | (150) | | | I | [[4.26, 31](#page7)] |  |  |
|  |  | 2066.164 | 48398.87 | | 0.051500 | −1360 | | (150) | | | I | [[4.26, 31](#page7)] |  |  |
| Mn II | | 1197.184 | 83529.35 | | 0.156600 | −2556 | | (450) | | | B |  |  |  |
|  |  | 1199.391 | 83375.65 | | 0.105900 | −2825 | | (450) | | | B |  |  |  |
|  |  | 1201.118 | 83255.77 | | 0.088090 | −3033 | | (450) | | | B |  |  |  |
|  |  | 2576.877 | 38806.66 | | 0.288000 |  | 1420 | (150) | | | I | [[4.26](#page7)] |  |  |
|  |  | 2594.499 | 38543.08 | | 0.223000 |  | 1148 | (150) | | | I | [[4.26](#page7)] |  |  |
|  |  | 2606.462 | 38366.18 | | 0.158000 |  | 986 | (150) | | | I | [[4.26](#page7)] |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

TABLE I: (continued)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Atom/ Wavelength Frequency Oscillator | | | | | | q value | | | |  | Refs. |  |  |
|  | Ion | ˚ | ω0 (cm | −1 | ) Strength | | (cm | | −1 | ) |  |  |  |  |
|  | λ (A) |  |  |  |  |  |  |
|  |  |  |  | |  |  |  |  |  |  |  |  |  |  |
| Fe II | | 1063.176 | 94057.80 | | 0.060000 |  |  |  |  |  | B |  |  |  |
|  |  | 1063.971 | 93987.52 | | 0.003718 |  |  |  |  |  | B |  |  |  |
|  |  | 1096.877 | 91167.92 | | 0.032400 |  |  |  |  |  | B |  |  |  |
|  |  | 1121.975 | 89128.55 | | 0.020200 |  |  |  |  |  | B |  |  |  |
|  |  | 1125.448 | 88853.51 | | 0.016000 |  |  |  |  |  | B |  |  |  |
|  |  | 1143.226 | 87471.77 | | 0.017700 |  |  |  |  |  | B |  |  |  |
|  |  | 1144.939 | 87340.98 | | 0.106000 |  |  |  |  |  | B |  |  |  |
|  |  | 1260.533 | 79331.52 | | 0.025000 |  |  |  |  |  | A |  |  |  |
|  |  | 1608.450 | 62171.63 | | 0.058000 | −1300 | | (300) | | | A | [[4.32](#page7)] |  |  |
|  |  | 1611.200 | 62065.53 | | 0.001360 |  | 1100 | (300) | | | A | [[4.32](#page7)] |  |  |
|  |  | 2249.877 | 44446.88 | | 0.001821 |  |  |  |  |  | A |  |  |  |
|  |  | 2260.780 | 44232.51 | | 0.002440 |  |  |  |  |  | I | [[4.26](#page7)] |  |  |
|  |  | 2344.212 | 42658.24 | | 0.114000 |  | 1210 | (150) | | | I | [[4.26, 33](#page7)] |  |  |
|  |  | 2367.589 | 42237.06 | | 0.000212 |  | 1904 |  |  |  | A |  |  |  |
|  |  | 2374.460 | 42114.83 | | 0.031300 |  | 1590 | (150) | | | I | [[4.26, 33](#page7)] |  |  |
|  |  | 2382.764 | 41968.06 | | 0.320000 |  | 1460 | (150) | | | I | [[4.26, 33](#page7)] |  |  |
|  |  | 2586.649 | 38660.05 | | 0.069180 |  | 1490 | (150) | | | I | [[4.26, 33](#page7)] |  |  |
|  |  | 2600.172 | 38458.99 | | 0.238780 |  | 1330 | (150) | | | I | [[4.26, 33](#page7)] |  |  |
| Ni II | | 1317.217 | 75917.64 | | 0.146000 |  |  |  |  |  | A |  |  |  |
|  |  | 1370.132 | 72985.67 | | 0.076900 |  |  |  |  |  | A |  |  |  |
|  |  | 1393.324 | 71770.82 | | 0.022220 |  |  |  |  |  | A |  |  |  |
|  |  | 1454.842 | 68735.99 | | 0.032300 |  |  |  |  |  | A |  |  |  |
|  |  | 1467.259 | 68154.29 | | 0.009900 |  |  |  |  |  | A |  |  |  |
|  |  | 1467.756 | 68131.22 | | 0.006300 |  |  |  |  |  | A |  |  |  |
|  |  | 1502.148 | 66571.34 | | 0.006000 |  |  |  |  |  | A |  |  |  |
|  |  | 1703.412 | 58705.71 | | 0.012240 |  |  |  |  |  | A | [[4.31](#page7)] |  |  |
|  |  | 1709.604 | 58493.07 | | 0.032400 |  | −20 | (250) | | | A | [[4.31](#page7)] |  |  |
|  |  | 1741.553 | 57420.01 | | 0.042700 | −1400 | | (250) | | | A | [[4.31](#page7)] |  |  |
|  |  | 1751.915 | 57080.37 | | 0.027700 |  | −700 | (250) | | | A | [[4.31](#page7)] |  |  |
| Zn II | | 2026.137 | 49355.00 | | 0.489000 |  | 2479 | (25) | | | M | [[4.26, 31][34](#page7)] |  |  |
|  |  | 2062.660 | 48481.08 | | 0.256000 |  | 1584 | (25) | | | I | [[4.26, 31](#page7)] |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**Chapter 6**

**Field shift**

1. **Method**

To calculate the field shift (also called the volume shift), we add a finite perturbation due to the field shift to the nuclear potential, and then calculate the energy spectrum directly. The field shift potential is

|  |  |
| --- | --- |
| U (r) =U (R + R; r) U (R; r) | (5.1) |

where R is the nuclear radius and U (R; r) is the nuclear potential. In our codes we use a Fermi distribution for the nuclear charge density (see Fig. 5.1).

To obtain the change in energy of a state due to the field shift, we add the potential

U (r) to the nuclear potential in our Hartree-Fock calculations. By introducing a scaling factor we can increase the size of the effect and take the limit as **!** 0. To calculate the field-shift constant, we take the gradient of a level energy E vs. graph and extract F as

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| F = | E | = | 5 1 | | | lim | dE | : | (5.2) |  |
|  |  |  |  |  |  |
| **h**r2**i** | 3 2R R | | | d |  |
|  |  | **!**0 |  |  |  |

where **h**r2**i** is the mean-square radius. The nuclear charge distribution can be approximated by a uniformly charged sphere of radius R, thus **h**r2**i** = 35 R2. Note that the field-shift constant, F , is defined here as having opposite sign to the definition in some previous papers, e.g. Refs. [72] and [68].

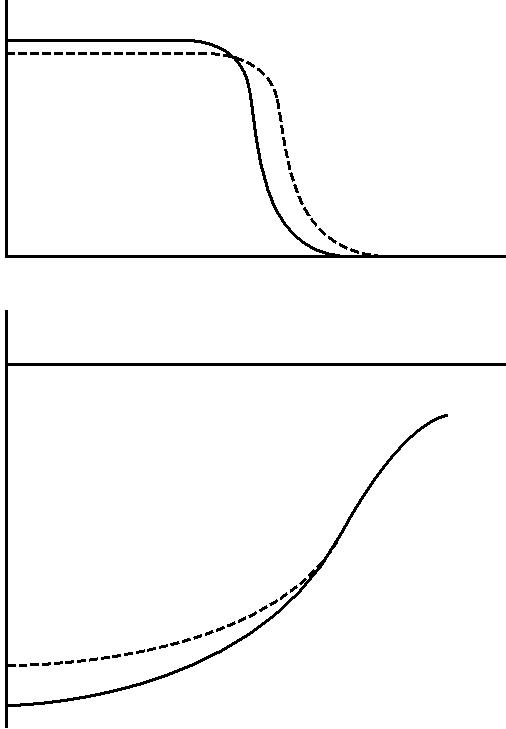
**52** **5. Field shift**

Figure 5.1: Schematic graph of the nuclear charge density distribution, , and the corresponding potential, U for two different values of the nuclear charge radius R (arbitrary units).



U 

 r R R+dR



 r

Higher-order correlation effects in the field shift are not too large, and are localised at the nucleus. For single-valence-electron atoms and ions we can include them easily by creating approximate Brueckner orbitals (solutions of the modified Hamiltonian, h = hDF + (1)) using the second-order operator, defined in Equation (3.12). The field shift is proportional in first order to the square of the wavefunction at the nucleus. Hence we can include higher-order effects quite simply by multiplying the matrix element by the square of the ratio of the Brueckner wavefunction to the Dirac-Fock wavefunction at the nucleus,

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| FDF+ | = |  | DF+ (0) |  | 2 | (5.3) |  |
| FDF | DF(0) | : |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |

|  |  |
| --- | --- |
|  |  |
|  |  |

1. **King Plots**

Using King plotsa, we can extract the ratios of field-shift constants for different transitions, provided we have experimental data for a number of different isotopes. Taking Eq. (2.7) for two transitions and , we can write

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **A;A0** | = F **h**r2**iA;A0** | + k | 1 | 1 | | ; |  |  |
|  |  |  | (5.4) |  |
| A | A**0** |  |

where k is the total mass shift constant (including normal and specific mass shifts) for transition . A similar equation can be written for transition . We wish to eliminate the **h**r2**i** and obtain useful information about the constants F and k. The two axes of our King plot are defined by

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| y(A) = |  | **A;A0** | | |  |  | =F **h**r2**iA;A0** | | | | | | | | | | | | | + k | (5.5) |  |
|  | 1 |  | 1 |  | |  |
|  |  |  |  |  | ~~1~~ |  |  |  | | | | ~~1~~ |  |  |  |  |  |
|  | **A** | **A0** |  | **A** | | **A0** | |  |  |  |
|  | **A;A0** | | |  |  | | | | | 2 |  | **A;A0** | | | | |  |  |  |
| x(A) = |  |  |  | |  |  | = F | **h**r | | | | | | **i** |  |  |  |  |  | + k : |  |  |
|  | 1 |  | 1 |  |  |  | ~~1~~ | |  |  |  |  |
|  |  |  |  | |  |  | ~~1~~ | |  | |  | | |  | |  |  |  |
|  | **A** | **A0** |  | **A** | | **A0** | |  |  |  |

x and y are often called \modi ed isotope shifts" (MIS). Plotting the points (x(A); y(A)) for several pairs of isotopes (A; A**0**) yields a straight line

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| y = | F | x + |  | k | F | k: | (5.6) |  |
| F | F |  |

This equation is useful for extracting the ratios of eld-shift constants (from the gradi-ent), but has proven less useful for extracting mass shift constants due to the generally small value of the intercept. The value of A**0** is often xed for all experiments in a partic-ular element (it usually corresponds to the leading isotope, e.g. for barium A**0** = 138), however this is not a necessary condition, and can be relaxed without changing the method.

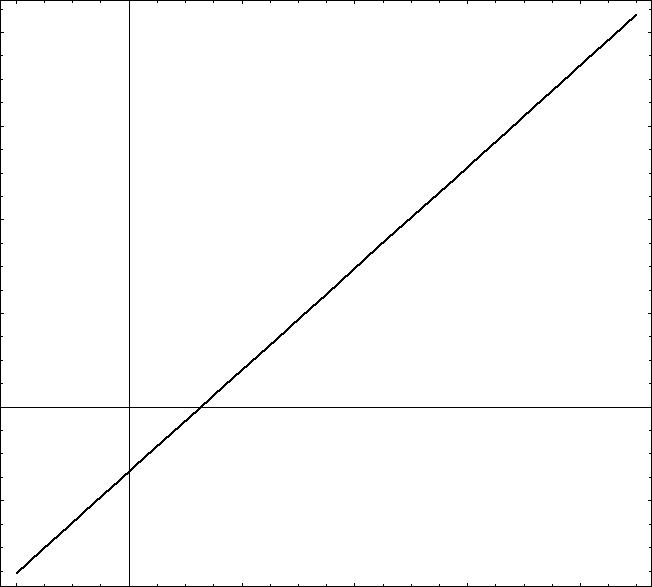
As an illustrative example, we present in Fig. 5.2 a King plot of the 6497A and 5854A lines in Ba II. The isotope shifts were taken from Villemoes **et al.**, 1993 [5.102].

**a**introduced by King, 1963 [5.57] to explain anomalies in isotope shifts of samarium; see also Hansen

**et al.**, 1965 [5.101]

**54** **5. Field shift**

Figure 5.2: King plot of the Ba II 6497 and 5854 lines. The axes are the modified isotope shifts (Eq. (5.5)) in units of GHz amu.



|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 800 |  |  |  |  | (134, 138) |  |
|  |  |  |  |  |  |
|  |  |  |  | (135, 138) | |  |
| 600 |  |  |  |  |  |  |
|  |  |  | (136, 138) | |  |  |
| 400 |  |  |  |  |  |  |
| l 6497 |  |  |  |  |  |  |
| 200 |  |  |  |  |  |  |
| 0 |  |  |  |  |  |  |
| -200 |  |  |  |  |  |  |
|  | (137, 138) |  |  |  |  |  |
| -200 | 0 | 200 | 400 | 600 | 800 |  |
|  |  |  | l 5854 |  |  |  |

1. **Results**

We tested our method for the calculation of field shift in Ba II because in barium the field shift dominates over the mass shift, and there is a lot of experimental data to compare with. We present the results of our calculations of specic-mass-shift and field-shift constants in Ba II in Table 5.2. The method for calculating SMS is discussed in Section 6.1.

Our results for field-shift constants in Ba II were found to be consistent within a few percent of the previous theoretical work by Martensson-Pendrill (Table 5.1). In the same paper, Ref. [5.68], they say that they have underestimated the 6p1**=**2 field-shift constant by around 7%, based on the difference between experimental and theoretical calculations of the hyper ne constant A. Also, their 6s constant is said to be overestimated, leading to a corrected value of F6**p3=2** 6**s** = 4:20(13) GHz/fm2. These corrected values are in better agreement with the **ab initio** values obtained in this work (F6**p3=2** 6**s** = 4:076 GHz/fm2).

|  |  |
| --- | --- |
| **5.3. Results** | **55** |
|  |  |

Table 5.1: Level field-shift constants, F , in Ba II. Due to a difference in the definition of F , the values calculated in Ref. [5.68] have been presented here with opposite sign.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| State | | Energya | F (MHz/fm2) | |
|  |  | (cm 1) | Ref. [68] | This work |
| 6s |  | 80686:87 | 4096 | 3851 |
| 6p1**=**260425:31 | | | 111:1 | 150:1 |
| 6p3**=**2 | 58734:45 | | 242:6 | 225:4 |
| 5d3**=**2 |  | 75813:02 |  | 1223 |
| 5d5**=**2 |  | 75012:05 |  | 1148 |
|  |  |  |  |  |

**a** Experimental results tabulated by Moore [98]

Table 5.2: Calculated specific-mass-shift (kSMS) and field-shift constants (F ) in Ba II transitions.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Transition | |  | kSMS (GHz amu) | F (MHz/fm | 2 | ) |  |
| (A) |  |  |
| 6p1**=**2 6s | | 4934 | 105 | -4001 |  |  |  |
| 6p3**=**2 | 6s | 4554 | 257 | -4077 |  |  |  |
| 5d5**=**2 6s | | 17622 | -550 | -4999 |  |  |  |
| 6p1**=**2 | 5d3**=**2 | 6497 | 653 | 1073 |  |  |  |
| 6p3**=**2 | 5d3**=**2 | 5854 | 805 | 997 |  |  |  |
| 6p3**=**2 | 5d5**=**2 | 6142 | 807 | 922 |  |  |  |
|  |  |  |  |  |  |  |  |

In Table 5.3 we compare our calculated values of field-shift constant ratios with

King plot data obtained by combining several different experiments and transitions.

We have used a simple weighted least squares t to obtain an experimental value for

the ratio F455=F614. A two point formula was used for ratios involving the 1762 nm

transition as experimental data exists only for the 134**;**138 and 136**;**138 isotope shifts

[5.103]. Other ratios were extracted by the groups that performed the experiments, with

much higher accuracy. Our values were found to be consistent with experimental values

to within 5%.

We have shown in this section that we can calculate field shift in heavy atoms,

where it dominates over mass shift. In the rest of this thesis we can now simply remove

its (relatively minor) contribution from the experimental data in light atoms, so that

we can compare the SMS part directly.

Table 5.3: Ratios of eld-shift constants in Ba II transitions. In the second column we list the measured values, obtained using King plots. In some cases we obtain the ratio ourselves by combining the results of two separate studies.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Transitions | | |  |  | F =F |
|  |  | ( | / | ) |  | This work | Experiment |
|  | |  |  |  | |  |  |
| 6p1**=**2 | | { 6s | / | 6p3**=**2 { 6s | | 0:982 | 0:975(3)a |
| 6p3**=**2 | | { 6s | / | 6p3**=**2 { 5d5**=**2 | | 4:42 | 4:50(6)bc |
| 6p3**=**2 | | { 6s | / | 5d5**=**2 { 6s | | 0:816 | 0:82(4)bd |
| 5d5**=**2 | | { 6s | / | 6p3**=**2 { 5d5**=**2 | | 5:42 | 5:5(3)cd |
| 6p1**=**2 | { 5d3**=**2 | | / | 6p3**=**2 { 5d3**=**2 | | 1:076 | 1:087(4)c |
| 6p3**=**2 | { 5d5**=**2 | | / | 6p3**=**2 | { 5d3**=**2 | 0:925 | 0:961(3)c |
| 6p3**=**2 | { 5d3**=**2 | | / | 6p3**=**2 | { 6s | 0:245 | 0:2312(6)c |
|  |  |  |  |  |  |  |  |

**a** Wendt **et al.** [104] **b** Wendt **et al.** [105]

**c** Villemoes **et al.** [102] **d** Zhao **et al.** [103]

**Chapter 7**

**Specific mass shift**

The specific mass shift has proven very di cult to calculate in the past (see Section 2.3). In this Chapter we describe a method of calculation which may make such calculations possible even in very di cult cases. The SMS operator is (see Eq. (2.5))

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| HSMS = | 1 |  | **pi pj** | (6.1) |  |
| M **i<j** | |  |
|  |  | **X** |  |  |  |

Using many-body perturbation theory in the residual Coulomb operator and specic mass shift (SMS) operator to calculate isotope shift shows poor convergence (see Section 2.3.1). Therefore, we are looking for an \all order" method of calculation. The finite- field scaling method is used, which reduces the task to an energy calculation, and includes the SMS in all parts of the calculation.

To calculate kSMS we include a scaled specific-mass-shift operator directly into our energy calculation from the very beginning. We add the two-body SMS operator to the

~ **j** **j** ~

Coulomb potential Q = 1= **r**1 **r**2 + **p**1 **p**2. The operator Q replaces the Coulomb

operator everywhere that it appears in an energy calculation. We recover the specific-

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| mass-shift constant as |  | =0: |  |  |
| kSMS = | d! | (6.2) |  |
| d |  |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |

~

The operator Q has the same symmetry and structure as the Coulomb operator (see Appendix A).

1. **Single-valence-electron atoms and ions**

In this section, we develop a method for calculating the isotope shift of atoms and ions that can be treated as a single electron above a closed-shell core. These include the alkali metals and singly-ionised alkaline-earths, as well as other ions such as Zn II that are fairly well approximated by a single electron above a closed-subshell core.

We test our technique by calculating the isotope shift for several light atoms. The eld shift dominates in heavy atoms, and having tested it in Ba II (Chapter 5), we can now simply remove its contribution from the experimental data in light atoms so that we can compare the SMS part directly. After obtaining good agreement with experiment in a number of species, we apply the technique to calculate isotope shift for astronomically relevant transitions in Mg II, Zn II, Ge II, Si II and Si IV.

1. **Calculation of** k**SMS**

As a zero approximation we use the Dirac-Fock (relativistic Hartree-Fock) method. At the Hartree-Fock stage we include the isotope shift in the exchange potential and iterate to obtain self-consistent \dressed" wavefunctions. In the MBPT terms explained in Ref. [6.72], the SMS matrix element at this stage is roughly equivalent to the rst-order and second-order contributions of the one-particle operator, plus higher-order corrections from the random-phase approximation (this corresponds to P (1) + S(2) in the notation of Ref. [6.72]). It is interesting to note that kSMS at this stage does not give meaningful results, and can even be of the wrong sign (it is labelled as \DF" in Table 6.1). We need to include correlation corrections in order to obtain any reasonable accuracy.

We include correlation effects to second order of MBPT; this approach gives good accuracy for energies. The perturbation is the difference between the exact and zero-order Dirac-Fock (DF) Hamiltonians, **V** = **H H**0 (see Eq. (3.18)). The many-body corrections start in second order; all first-order diagrams have been included in the self-consistent Hartree-Fock procedure. There are just four second-order diagrams, illustrated in Fig. 3.1. However, now we replace the Coulomb operator in these diagrams

Table 6.1: Level specic-mass-shift constants, kSMS, in Na I and Mg II. The Dirac-Fock (DF) value, which does not include MBPT effects, is shown separately (this is approximately equivalent to the values labelled \P (1) + S(2)" in Ref. [6.72]). This table shows that MBPT effects are very important for accurate calculation of specific mass shift in single-valence-electron atoms and ions.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Ion | State | kSMS (GHz amu) | | |  |
|  |  | Ref. [72] | | This work | |
|  |  | P (1) + S(2) | Final | DF | Final |
| Na I | 3s | -54 | 54 | -52 | 69 |
|  | 3p1**=**2 | -67 | -43 | -68 | -40 |
|  | 3p3**=**2 | -67 | -43 | -67 | -39 |
| Mg II | 3s |  | 38 | -171 | 83 |
|  | 3p1**=**2 |  | -324 | -408 | -296 |
|  | 3p3**=**2 |  | -323 | -402 | -290 |
|  |  |  |  |  |  |

~

with our two body operator Q, and use dressed Hartree-Fock wavefunctions as described

above. This gives our final value of kSMS as listed in Table 6.1.

In Table 6.1 we compare our results to those obtained by Safronova and Johnson

(Ref. [6.72]) who calculated the isotope shift to third order in standard MBPT. Our

values are significantly different, in particular the Mg II 3s level shift is more than twice

that given in Refs. [70] and [72] (Refs. [70] and [72] are broadly in agreement with each

other). However we find that this difference is not so large in the 3p { 3s transition

due to cancellation of higher-order terms between the two levels. We compare our final

results and those of Ref. [6.72] with experiment in Table 6.2. Agreement is at the level

of 1%, which is much smaller than our error estimates (see section 6.1.2).

Our method includes many-body diagrams that are different from those of Ref. [6.72],

including some chains of diagrams in all orders. It is also arguably simpler to implement

since it does not require term-by-term calculation of a large number of matrix elements.

1. **Estimation of error**

For single-valence-electron atoms and ions, an estimate of the size of neglected higher-

order diagrams can be obtained by calculating a new value of kSMS that includes

Table 6.2: Comparison of calculated values of the specific mass shift (SMS) of transitions in Na I and Mg II with experiment.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Isotopes | Transition | |  | SMS (MHz) | |  |  |  |
|  |  |  | Ref. [72] | This work | | Expt.a | |  |
| 23 22Na I | 3p1**=**2 | { 3s | 192 | 214 | (48) | 215 | (1) |  |
|  |  |  |  |  |  | 214 | (2) |  |
| 26 24Mg II | 3p3**=**2 | { 3s | 192 | 212 | (48) | 214 |  |  |
| 3p3**=**2 | { 3s | 1157 | 1196 | (18) | 1207 | (100) |  |
|  |  |  |  |  |  |  |  |  |

**a** these values are extracted from isotope shift experiments in Table 6.3

some higher-order chains of diagrams. We add the operator (1)2 (see Eq. (3.12)) to the exchange potential in the Dirac-Fock Hamiltonian (3.2) for the valence electron, h = hDF + . Thus, we calculate the single electron Brueckner orbital. We also include a scaling factor f with the operator ( **!** f ) in order to t the experimental energy. The rescaling of simulates some higher order correlation corrections that were omitted in our calculation. Including in our Hartree-Fock calculation allows us to obtain another value for kSMS, and the difference between this new value and the old second-order value gives us an estimate of the error.

1. **Comparison with experiment**

We compare our results with experimental data for alkali-metal atoms and ionised alkaline-earth metals in Table 6.3. In these systems it is more valuable to compare only the specific mass shift with those extracted from experiment than to compare the entire isotope shift. This is because the mass shift dominates strongly in these atoms and ions, and also because the SMS is generally considered more di cult to calculate. We have removed the field shift and the normal mass shift from the experimental values of the isotope shift in order to obtain an experimental value for the specific mass shift. The field shift values used in Table 6.3 were calculated using the method presented in Chapter 5. While our calculation of F has been shown to be good, the field shift also depends on having knowledge of **h**r2**i** for the relevant isotopes.

For Na I we use the value quoted in Ref. [6.72] of **h**r2**i**23**;**22 = 0:205(3) fm2. This value is only from an empirical t, and shouldn't be trusted too far. The field shift is very

Table 6.3: Comparison of calculated values of the specific mass shift (SMS) with experiment for several transitions in single-valence-electron species. The experimental values of the SMS in the final column are extracted by subtracting the normal mass shift (NMS) and field shift (FS) from the experimental isotope shift (IS).

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Isotopes | Transition | Energy | IS (expt.) | | NMS | FS | |  | SMS (MHz) | |  |  |
|  |  | (cm 1) | (MHz) | | (MHz) | (MHz) | | This work | | Expt. | |  |
| 23 22Na I | 3p1**=**2 { 3s | 16956.18 | 758:5 | (7)a | 551 | 8 |  | 214 | (48) | 215 | (1) |  |
|  |  |  | 756:9 | (1:9)b |  |  |  |  |  | 214 | (2) |  |
| 26 24Mg II | 3p3**=**2 { 3s | 16973.38 | 757:72 | (24)c | 552 | 8 |  | 212 | (48) | 214 |  |  |
| 3p3**=**2 { 3s | 35760.97 | 3050 | (100)d | 1185 | 42 |  | 1196 | (18) | 1207 | (100) |  |
| 41 39K I | 4p1**=**2 { 4s | 12985.17 | 235:25 | (75)e | 267 | 13 (5) | | 32 | (21) | 19 | (6) |  |
| 43 40Ca II | 4d1**=**2 { 4s | 27398.11 | 585 | (9)f | 564 | 13 (5) | | 20 | (30) | 34 | (13) |  |
| 4p1**=**2 { 4s | 25191.54 | 706 | (42)g | 723 | 36 (3) | | 22 | (1) | 19 | (45) |  |
|  |  |  | 672 | (9)h |  |  |  |  |  | 15 | (11) |  |
|  |  |  | 685 | (36)i |  |  |  |  |  | 2 (39) | |  |
|  | 4p3**=**2 { 4s | 25414.43 | 713 | (31)g | 729 | 36 (3) | | 5 | (1) | 20 | (34) |  |
|  |  |  | 677 | (19)h |  |  |  |  |  | 16 | (22) |  |
|  |  |  | 685 | (36)i |  |  |  |  |  | 8 (39) | |  |
|  | 3d3**=**2 { 4s | 13650.21 | 4180 | (48)g | 392 | 47 (4) | | 3502 | (217) | 3835 | (52) |  |
|  | 3d5**=**2 { 4s | 13710.90 | 4129 | (10)g | 393 | 47 (4) | | 3487 | (215) | 3783 | (14) |  |
|  | 4p1**=**2 { 3d3**=**2 | 11541.33 | 3464:3 | (3:0)j | 331 | 12 | (1) | 3479 | (218) | 3807 | (4) |  |
|  |  |  | 3483 | (40)g |  |  |  |  |  | 3826 | (41) |  |
|  | 4p3**=**2 { 3d3**=**2 | 11764.22 | 3462:4 | (2:6)j | 337 | 12 | (1) | 3507 | (217) | 3811 | (4) |  |
|  |  |  | 3446 | (20)g |  |  |  |  |  | 3795 | (21) |  |
|  | 4p3**=**2 { 3d3**=**2 | 11703.53 | 3465:4 | (3:7)j | 336 | 12 | (1) | 3492 | (216) | 3813 | (5) |  |
|  |  |  | 3427 | (33)g |  |  |  |  |  | 3774 | (34) |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |

|  |  |  |  |
| --- | --- | --- | --- |
| **a** Pescht **et al.** [106] | **e** Touchard **et al.** [110] | **h** extracted from Martensson-Pendrill **et al.** [67] | |
| **b** Huber **et al.** [107] | **f** H•orb•ack **et al.** [64] | **i** | Maleki and Goble [112] |
| **c** Gangrsky **et al.** [108] | **g** Kurth **et al.** [111] | **j** | N•ortersh•auser **et al.** [113] |
| **d** Drullinger **et al.** [109] |  |  |  |

|  |
| --- |
| **6.1. Single-valence-electron atoms and ions** |

|  |
| --- |
|  |

small in this atom, so the errors do not matter too much. For Mg II we have used the value **h**r2**i**26**;**24 = 0:33 fm2 from another empirical t, the equation Rnuc = 1:1A1**=**3 fm. This is a poor approximation, but in this case the field shift is small even in relation to the error in the experimental isotope shift. In Table 6.3 we have not included an error contribution for the field shift in either of these atoms, since we really do not know how accurate these approximations are.

The values of **h**r2**i** are known for K I and Ca II from muonic x-ray experiments, allowing us to calculate the field shift much more accurately. This is fortunate because the SMS is relatively small for the p { s transitions in these atoms, and hence the field shift plays a much larger role. We use the values **h**r2**i**41**;**39 = 0:117(40) fm2 for K I from Ref. [114], and **h**r2**i**43**;**40 = 0:1254(32) fm2 for Ca II from Ref. [6.115]. In Ca II the change in mean-square nuclear radius is given to high precision, so we have included an additional error of 5% in the field shift that comes from the constant F . This is a pessimistic estimate of error based on the accuracy we achieved calculating F for transitions in Ba II.

Table 6.3 shows that our method can reliably calculate the isotope shift in alkali-metal atoms and singly-ionised alkaline-earth metals, including those transitions with a large specific mass shift.

1. **Results**

We have shown that our method works in atoms for which we have available experimental data (Section 6.1.3). In Table 6.4 we tabulate values for the mass and field-shift constants for some astronomically useful transitions. We have not given errors for F , however we can say that they are less than 5% based on comparison of calculation with experiment in Ba II (Section 5.3).

In Table 6.5 we present the results of isotope shift calculations between common isotopes of astronomically important ions (meaning important for astronomy, rather than really ridiculously important). We have used the isotope shift constants presented in Table 6.4 with Equation (2.7) in order to calculate the isotope shift between particular

Table 6.4: Mass (kNMS and kSMS) and eld-shift constants (F ) for some useful transitions in ions that can be treated as having a single valence electron.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Ion | Transition | | F | kNMS | kSMS | |
|  |  |  | (MHz/fm2) | (GHz amu) | (GHz amu) | |
| Mg II | 3p1**=**2 { 3s | | -127 | -587 | 373 | (12) |
|  | 3p3**=**2 { 3s | | -127 | -588 | 373 | (6) |
| Si II | 4s { 3p1**=**2 | | 171 | -1077 | 1257 | (29) |
|  | 4s { 3p3**=**2 | | 171 | -1072 | 1243 | (28) |
| Si IV | 3p1**=**2 | { 3s | -484 | -1172 | 1535 | (11) |
|  | 3p3**=**2 | { 3s | -485 | -1180 | 1505 | (7) |
| Zn II | 4p1**=**2 | { 4s | -1596 | -797 | 1310 | (69) |
|  | 4p3**=**2 | { 4s | -1596 | -812 | 1266 | (69) |
| Ge II | 5s { 4p1**=**2 | | 1088 | -1026 | 1046 | (69) |
|  | 5s { 4p3**=**2 | | 1083 | -997 | 960 | (62) |
|  |  |  |  |  |  |  |

isotopes. Results of measurements for Zn II were brought to our attention [116] after

we had performed our calculations. These results matched our prediction extremely

well.

In Ge II and Si II, the specific mass shift cancels the normal mass shift entirely,

making the field shift, and hence **h**r2**i**, important. We have just used the empirical

formula Rnuc = 1:1A1**=**3 fm2 to obtain values of **h**r2**i** in these ions. This is extremely

rough, and although it seems to work in Zn II to within a 20% accuracy based on the

experimental data given, we really don't know if this holds for Si and Ge at all. In the

Si IV transitions presented, it is less important to have good values for the field shift

because there is no cancellation between the NMS and SMS.

1. **Mg I**

Magnesium is one of the simplest and well-studied two-electron atoms. Because of that

it is often used as a test ground for different methods of atomic calculations. In this

section we show that we can calculate the isotope shift of some magnesium transitions

for which experimental values are available.

Table 6.5: Total isotope shifts for some astronomically relevant transitions in single-valence-electron ions. We have presented two errors: the rst comes from our uncertainty in calculation of the specific-mass-shift constant, kSMS; and the second comes from the field shift, which is mainly due to lack of knowledge of **h**r2**i**. A negative sign means that the total shift is opposite to the normal mass shift. The experimental value for the 4p3**=**2 { 4s transition in Zn II is 676(6) MHz [6.116], in agreement with our prediction.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Isotopes | Transition | | Energya | Isotope Shift | |  |
|  |  |  | (cm 1) | (MHz) | |  |
| 30 28Si II | 4s { 3p1**=**2 | | 65495.1 | 375 | (70)(11) |  |
| 30 28Si IV | 4s { 3p3**=**2 | | 65208.1 | 351 | (67)(11) |  |
| 3p1**=**2 | { 3s | 71289.6 | 6294 | (26)(31) |  |
| 66 64Zn II | 3p3**=**2 | { 3s | 71749.9 | 6241 | (18)(31) |  |
| 4p1**=**2 | { 4s | 48480.6 | 653 | (32)(78) |  |
| 74 70Ge II | 4p3**=**2 | { 4s | 49354.4 | 632 | (33)(79) |  |
| 5s { 4p1**=**2 | | 62402.4 | 491 | (53)(101) |  |
|  | 5s { 4p3**=**2 | | 60635.3 | 533 | (48)(101) |  |
|  |  |  |  |  |  |  |

* + Moore [98]

1. **Configuration interaction**

It is interesting to examine the contribution of various parts of the CI Hamiltonian to the

SMS. We can separate the contribution of the specific mass shift from the Hamiltonian

operator of Eq. (3.7):

|  |  |
| --- | --- |
| H = H0 + HSMS = H0 +**pi pj** : | (6.3) |

**X**

**i<j**

The SMS operator for the valence electrons in the frozen core approximation can

be divided into the core, one-valence-electron and two-valence-electron parts:

|  |  |
| --- | --- |
| HSMS = HSMS(0) + HSMS(1) + HSMS(2) | (6.4) |

The rst term in Eq. (6.4) corresponds to the change of the core potential. It accounts for the change of the core orbitals when the Dirac-Fock equations are solved for the operator H . The term HSMS(1) accounts for the exchange interaction of the valence electrons with the core:

|  |  |  |  |
| --- | --- | --- | --- |
| **h**i**j**HSMS(1)**j**k**i** = | **Ncore** |  |  |
| **h**i; j**jp**1 **p**2**j**j; k**i** : | (6.5) |  |

**X**

**j**=1

|  |  |
| --- | --- |
| **6.2. Mg I** |  |
|  |  |

The last term, HSMS(2), corresponds to the specific mass shift between the two valence electrons, **p**1 **p**2.

In order to study the role of the valence correlations we made three different calculations:

1. The basic one-configurational calculation for the ground state 3s2 1S0 and for the 3s3p 1**;**3P**J** states. All core orbitals and orbitals 3s and 3p are formed in the V **N** 2 approximation (i.e. by solving Dirac-Fock equations for the core).
2. Full two-electron CI for a medium sized **r** basis set [8sp5d], which includes the orbitals 1 8s1**=**2, 2 8p**j** and 3 5d**j** . The 3s, 3p and 3d orbitals are solutions of the V **N** 2 Dirac-Fock potential. The remaining virtual orbitals are constructed by multiplying the previous orbital of the same partial wave by the simple radial

function and orthogonalizing with the other orbitals.

1. Full two-electron CI for the B-spline basis set [12spd9f ].

Below we refer to these calculations as small, medium, and large. The large calculation is already very close to the saturation of the valence CI. Here the difference between the theoretical spectrum and experiment is mostly caused by the neglect of the core-valence correlations.

Table 6.6 presents the resulting SMS level shift constants, kSMS of Eq. (2.7), in different approximations. The contributions of individual terms in Eq. (6.4) are given, as well as their sum. It is interesting to note that all of the terms are large in comparison to the total SMS. There is a large cancellation between contributions within levels, and also between different levels. This shows that high accuracy is required in each term, so that the residual SMS in transitions is still correct after cancellation.

Comparison of the different approximations shows a strong dependence on the size of the basis sets. We see that it is very important to saturate the basis as completely as possible. In some cases the SMS changes drastically even between the medium and the large basis sets. In particular, the difference between large and medium SMS calculation for the level 3s3d 3D1 is 39%. This is mostly due to the f -wave contribution, which

Table 6.6: Level specific-mass-shift constants, kSMS, in Mg I. Individual contributions from Eq. (6.4) are presented [(0), (1), (2)], as well as the total. For some levels we give medium CI (M) and one-configurational results (S) in addition to the large CI (L) ones.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | kSMS (GHz amu) | | | | | |  |  |
| Level | (0) | (1) | | (2) | | Total | | CI |  |
|  |  |  | |  |  |  | |  |  |
| 3s2 1S0 | 559 | 883 | |  | 131 | 193 | | L |  |
| " | 561 | 881 | |  | 135 | 186 | | M |  |
| " | 857 | 1125 | |  | 0 | 268 | | S |  |
| 3s4s 3S1 | 422 | 615 | |  | 44 | 149 | | L |  |
| " | 431 | 624 | |  | 52 | 142 | | M |  |
| 3s4s 1S0 | 415 | 615 | |  | 21 | 179 | | L |  |
| " | 424 | 630 | |  | 30 | 177 | | M |  |
| 3s3d 1D2 | 343 | 616 | | 267 | | 541 | | L |  |
| 3s3d 3D1 | 375 | 561 | |  | 41 | 144 | | L |  |
| " | 381 | 571 | | 10 | | 200 | | M |  |
| 3s3d 3D2 | 375 | 561 | |  | 41 | 144 | | L |  |
| 3s3d 3D3 | 375 | 561 | |  | 41 | 144 | | L |  |
| 3s3p 3P0**o** | 428 |  | 853 |  | 144 |  | 570 | L |  |
| 3 **o** | 428 |  |  |  | L |  |
| 3s3p P1 | 852 | | 145 | | 569 | |  |
| 3s3p 3P2**o** | 428 | 850 | | 145 | | 567 | | L |  |
| " | 431 | 850 | | 142 | | 561 | | M |  |
| " | 759 | 1161 | | 266 | | 668 | | S |  |
| 3s3p 1P1**o** | 408 | 698 | |  | 329 |  | 38 | L |  |
| " | 411 | 700 | |  | 341 |  | 52 | M |  |
| " | 946 | 1163 | |  | 265 |  | 49 | S |  |
| 3s4p 3P0**o** | 402 | 630 | |  | 13 | 215 | | L |  |
| 3s4p 3P1**o** | 402 | 629 | |  | 13 | 215 | | L |  |
| 3s4p 3P2**o** | 402 | 629 | |  | 13 | 214 | | L |  |
|  |  |  |  |  |  |  |  |  |  |

is absent in the medium basis set. Note that the SMS operator can only mix orbitals

with l = 1. That is why the f -wave contribution is more important for the levels of

the configuration 3s3d. On the other hand, for the same reason, the contribution of

higher partial waves to the considered levels is suppressed.

Analysis of Table 6.6 shows that valence correlations tend to decrease the contributions of the first two terms of the SMS operator. The third (two-particle) term of

the SMS operator is generally not screened. On the contrary, for some levels the two-

particle contribution grows with the size of the basis set. Note that the nal value

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **6.2. Mg I** | |  |  |  |  |  |  |  |  |  | |  |
|  |  | | | | | | | | | |  |  |
|  | Table 6.7: Speci c-mass-shift constants, kSMS, of transitions from | | | | | | | | | | |  |
|  | the ground state (3s2 1S0) in Mg I. | | | | |  |  |  |  |  |  |  |
|  |  |  |  |  |  | | | |  |  |  |  |
|  | Upper | Energya |  |  | kSMS (GHz amu) | | | |  |  |  |  |
|  | Level | (cm 1)CI | | | CI + (1) | | | CI + (1**;**2) | | |  |  |
|  | 3s3p 3P0**o** | 21850 | 378 | | 487 | | | 492 | | | |  |
|  | 3s3p 3P1**o** | 21870 |  | 377 |  | 486 | |  | 491 | |  |  |
|  | 3 **o** | 21911 |  |  |  |  |  |  |  |
|  | 3s3p P2 | 375 | | 485 | | | 489 | | | |  |
|  | 3s3p 1P1**o** | 35051 | 231 | | 120 | | | 134 | | |  |  |
|  | 3s4s 3S1 | 41197 | 43 | | 59 | | | 49 | | | |  |
|  | 3s4s 1S0 | 43503 | 13 | | 94 | | | 85 | | | |  |
|  | 3s3d 1D2 | 46403 | 345 | | 500 | | | 477 | | | |  |
|  | 3s4p 3P0**o** | 47841 | 17 | | 136 | | | 126 | | | |  |
|  | 3s4p 3P1**o** | 47844 | 16 | | 136 | | | 126 | | | |  |
|  | 3s4p 3P2**o** | 47851 | 16 | | 136 | | | 126 | | | |  |
|  | 3s3d 3D3 | 47957 | 52 | | 87 | | | 77 | | | |  |
|  | 3s3d 3D2 | 47957 | 52 | | 87 | | | 77 | | | |  |
|  | 3s3d 3D1 | 47957 | 52 | |  | | 87 |  | | 77 |  |  |
|  | 1 **o** | 49347 |  | 5 |  |  |  |  |
|  | 3s4p P1 |  | 120 | | | 108 | | | |  |
|  | 3s4d 1D2 | 53135 | 100 | | 246 | | | 239 | | | |  |
|  | 3s4d 3D1 | 54192 | 32 | | 99 | | | 88 | | | |  |
|  | 3p2 3P0 | 57813 | 225 | | 469 | | | 464 | | | |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |

**a** Experimental values tabulated by Moore [98]

of the two-particle contribution to the ground state SMS is of the same order as the other contributions (as it is for most other states), while in the one-con gurational approximation it is zero.

1. **Role of**

The B-spline basis used in this section is the same that was used to calculate energies and relativistic shift for Mg I in Section 4.1. For a comparison of energies, see Table 4.1. Agreement with experiment is within 0.4% for all considered levels. Table 6.7 presents the resulting SMS level shift constants, kSMS of Eq. (2.7). In each table we present results of the pure CI calculation (which agree with our previous calculation, Sec-tion 6.2.1), as well as calculations including (1) only, and both (1) and (2).

The core-valence e ects are very important for the SMS calculation. In particular the single-valence-electron diagrams (included in (1)) can improve accuracy drastically

in cases where the pure CI method is not very good. Although (2) is important for calculation of energy, it appears to make little difference to kSMS. This is easily understood since the most important two-body diagram (the direct diagram, Fig. 3.3.1, corresponding to the screening of the electron-electron interaction by the core electrons) makes no contribution to the SMS. The exchange diagrams in (2) do have an effect, but this is much smaller than the one-body contribution.

1. **Comparison with experiment**

In Table 6.8 we compare experimental and calculated frequency shifts between isotopes

26Mg and 24Mg ( 26**;**24). We compare the SMS part only, which is extracted from experiment by subtracting the NMS. We have ignored the eld shift for simplicity; it is approximately 20-30 MHz or 2% of the NMS, which is less than the experimental uncertainty in most cases, and is of the order of the error in our SMS calculations.

Also presented in Table 6.8, for a theoretical comparison, are the results of Veseth (Ref. [71], 1987) and Johnsson **et al.** (Ref. [79], 1999). Veseth used non-relativistic many-body perturbation theory within the algebraic approximation to calculate the isotope shift to third order for some transitions. Jonsson **et al.** used a non-relativistic multiconfigurational Hartree-Fock approach, which allowed for both core and valence excitations in the CI. These calculations are discussed in more detail in Section 2.3.

An under-studied transition that is seen in quasar absorption spectra is the 2026 A line of Mg I (3s2 1S0 **!** 3s4p 1P1**o**). From Table 6.7, we calculate the isotope shift of this line as 26**;**24 = 2950(50) MHz (the error here is based on the absence of eld shift as well as the incompleteness of saturation of the basis set used to calculate kSMS).

1. **Carbon**

The isotope shift of carbon is particularly important for testing models of chemical evolution; this is explained in Section 1.2.2. We also have one more reason to study carbon: it is a well studied atom, and we can compare the results of our method with those of other theoretical analyses, as well as a few experiments. In particular, much progress

Table 6.8: Comparison of calculated values of the specific mass shift of several transitions in Mg I with experiment. All isotope shifts are between 26Mg and 24Mg. The experimental values of the SMS are obtained by subtracting the normal mass shift (NMS) from the experimental isotope shift (IS). We have neglected the field shift; it is of the order of 20-30 MHz. Also presented are the results of Refs. [71] and [79] for theoretical comparison.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  | IS (expt.) | |  | NMS |  |  |  | SMS (MHz) | | |  |  |  |
| Transition | |  |  | (MHz) | |  | (MHz) | CI | CI + | (1) | CI + | (1**;**2) | Expt. | Ref. [71] | Ref. [79] |  |
|  | (A) |  |  |  |  |
| 3s2 1S0 **!** 3s3p 3P1**o** | | | 4572 | 2683 | (0)a |  | 1153 | 1208 | 1559 |  | 1573 | | 1530 | 1378 | 1666 |  |
| 3s2 1S0 **!** 3s3p 1P1**o** | | | 2853 | 1412 | (21)b | | 1848 | -740 | -383 |  | -428 | | -436 |  | -409 |  |
|  |  |  |  | 1390 | (31)c | |  |  |  |  |  |  | -458 |  |  |  |
| 3s3p 3P0**o** **!** | | 3s4s 3S1 | 5169 | 396 | (6)d |  | 1020 | -1347 | -1371 | | -1419 | | -1416 |  |  |  |
| 3s3p 3P1**o** **!** | | 3s4s 3S1 | 5174 | 390 | (5)d |  | 1019 | -1345 | -1369 | | -1416 | | -1409 |  |  |  |
| 3s3p 3P2**o** **!** | | 3s4s 3S1 | 5185 | 390 | (7)d |  | 1017 | -1339 | -1363 | | -1411 | | -1407 |  |  |  |
| 3s3p 3P1**o** **!** | | 3p2 3P0 | 2782 | 1810 | (80)e | | 1895 | -486 | -56 |  | -86 |  | -85 |  |  |  |
| 3s3p 3P0**o** **!** | | 3s3d 3D1 | 3830 | 60 | (15)b | | 1376 | -1377 | -1283 | | -1329 | | -1316 | -1269 |  |  |
| 3s3p 3P1**o** **!** | | 3s3d 3D1**;**2 | 3833 | 61 | (3)b |  | 1375 | -1374 | -1280 | | -1326 | | -1314 |  |  |  |
| 3s3p 3P2**o** | **!** | 3s3d 3D1**;**2**;**3 | 3839 | 58 | (4)b |  | 1373 | -1368 | -1274 | | -1321 | | -1315 |  |  |  |
| 3 **o** | 3 | 3094 | 420 | (20) | e | 1704 | -1309 | -1241 | | -1291 | | -1284 |  |  |  |
| 3s3p P1 | **!** | 3s4d D1 |  |  |  |  |
| 3s3p 1P1**o** **!** | | 3s4d 1D2 | 5530 | 2107 | (15)d | | 953 | 1059 | 1173 |  | 1195 | | 1154 |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

**a** Sterr **et al.** [117] **b** Hallstadius [118]

**c** Le Boiteux **et al.** [119]

**d** Hallstadius and Hansen [120] **e** Novero **et al.** [121]

|  |
| --- |
| **6.3. Carbon** |

|  |
| --- |
| **69** |

has been made to calculate isotope shifts using the multiconfigurational Hartree-Fock (MCHF) and configuration interaction (CI) approach [77{80]; see Section 2.3.2.

In this section we show that our CI + MBPT method has accuracy comparable to that of the MCHF calculations, and are accurate enough to be used to measure isotope abundances. We present results for each species of carbon separately, in order of increasing number of valence electrons. The basis sets used in this section are the same as those described in Section 4.2. The MBPT basis is fully saturated in the sense that the energies and isotope shifts do not change with the addition of more basis functions. The saturation achieved for the CI basis is described below.

1. **C IV**

C IV has one electron above a closed 1s2 core. It can therefore be treated as a single valence electron atom using MBPT, or as a three electron atom using CI. We have used both methods; the results are presented for comparison in Table 6.9. In each case, the calculations were done using the **B**1 basis set. The isotope shift results have also been compared with previous theoretical approaches, namely the MCHF { CI calculations presented in Ref. [77], and the combined the Hylleraas [85] and full-core plus correlation (FCPC) calculations [86] also presented in Ref. [77].

As noted previously, the MBPT basis was completely saturated, however we have only included second-order diagrams in our calculation. By contrast, the CI calculations are complete (although they do not include the Breit interaction and QED effects), but the basis is not completely saturated. We have used an effective 22spd8f basis for the CI calculation, including only single and double excitations from the leading configurations (SD-CI). We included triple excitations for a smaller basis, 14spd8f : this made a difference of less than 2 cm 1 in the transition energy, and less than 1 GHz amu for kSMS. Other f -wave and higher partial waves were also found to be unimportant.

All methods give the same value for the transition energies and SMS constants to within 0.5%.

|  |  |
| --- | --- |
| **6.3. Carbon** |  |
|  |  |

Table 6.9: Energies and speci c-mass-shift constants, kSMS of transitions from the ground state (2s 2S1**=**2) in C IV. The transi-tion energies presented do not include the addition of mass shift e ects. Note that all results presented by other groups are non-relativistic and hence do not distinguish ne-structure.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Level | Expt.a | DF + (1) | Full CI | Other works |
|  |  | Energy (cm 1) | | |
| 2p 2P1**o=**2 | 64484 | 64551 | 64594 | 64564b |
| 2p 2P3**o=**2 | 64592 | 64681 | 64725 | 64399c |
|  |  |  |  | 64449d |
|  |  | kSMS (GHz amu) | | |
| 2p 2P1**o=**2 |  | -4511 | -4521 | -4526b |
| 2p 2P3**o=**2 |  | -4504 | -4514 | -4527c |
|  |  |  |  | -4528d |
|  |  |  |  |  |

**a** Moore [98]

**b** MCHF-CI: Carlsson **et al.** [77] **c** MCHF: Godefroid **et al.** [80]

* + Hylleraas + FCPC: Results of King [85], and Wang **et al.** [86], combined and presented in Ref. [77]

1. **C III**

The ground state for C III is 1s22s2 1S0. We have done our calculations both as a four-electron CI problem (full CI) and by combining two-valence-electron CI with MBPT, considering 1s2 as the frozen core (CI + (1**;**2)). All results are presented in Table 6.10. Also included are CI results (the pure two-electron CI method) and CI + (1) results (that do not include (2)). This allows us to examine the roles of the different parts of the core-correlation. The CI and CI + (1) results are calculated with the **B**2 basis set; the complete CI + (1**;**2) results have been calculated using both the **B**1 and **B**2 sets. Additionally we have presented the MCHF results of Ref. [79].

For the full four-electron CI method we used a very large basis 16spdf , in the SD-CI approximation. This was not enough to saturate the basis entirely, and we could go no further because the Hamiltonian matrix became too large. The error in kSMS from the full CI calculation could be as large as 100 GHz amu. Nonetheless, they are in agreement with the calculations of Ref. [79], as well as the results of our own CI + MBPT.

Table 6.10: Energies and specific-mass-shift constants, kSMS, of transitions from the ground state (2s2 1S0) in C III. Note that the MCHF results are non-relativistic and hence do not distinguish ne-structure.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Level | Expt.a | CI | CI + (1) | CI + (1**;**2) | | Full CI | MCHFb |  |
|  |  |  |  | **B**2 | **B**1 |  |  |  |
| 2s2p 3P0**o** |  |  | Energy (cm 1) | | |  |  |  |
| 52367 | 52750 | 52322 | 52349 | 52383 | 52506 | 52280 |  |
| 2s2p 3P1**o** | 52391 | 52784 | 52357 | 52383 | 52418 | 52534 |  |  |
| 2s2p 3P2**o** | 52447 | 52852 | 52427 | 52453 | 52488 | 52592 |  |  |
| 2s2p 1P1**o** | 102352 | 103719 | 103365 | 102725 | 102775 | 103109 | 102598 |  |
| 2s2p 3P0**o** |  |  | kSMS (GHz amu) | | |  |  |  |
|  | -3439 | -3478 | -3473 | -3470 | -3483 | -3475 |  |
| 2s2p 3P1**o** |  | -3438 | -3476 | -3472 | -3468 | -3480 |  |  |
| 2s2p 3P2**o** |  | -3434 | -3473 | -3468 | -3465 | -3474 |  |  |
| 2s2p 1P1**o** |  | -2688 | -2759 | -2790 | -2784 | -2882 | -2817 |  |
|  |  |  |  |  |  |  |  |  |

**a** Moore [98]

**b** J•onsson **et al.** [79]

In Ref. [79] the MCHF results were given an error of 1%; our CI + MBPT results

are within this range, and so we believe that we have obtained a similar accuracy. It is

also worth noting again that we have excluded the extra box diagrams with \wrong"

parity from the results presented. The inclusion of these diagrams in (2) makes a

difference of around 0.1% to the kSMS constants.

1. **C II**

We have treated C II as a three-valence-electron ion; its ground state is 2s22p 2P1**o=**2. We have used the **B**2 basis 20spdf , which corresponds to the V **N** 1 potential, and we

have restricted ourselves in the CI problem to single and double excitations from the

leading configurations 2s22p and 2s2p2.

In Table 6.11 we present all results for C II. Again we have presented the breakdown

of the various parts of the CI + MBPT method. We have also performed our calculations using the **B**1 basis: this changed the results by less than 1% for all results except

for the 2S1**=**2 transition, in which the difference was around 3%. For this transition,

neither basis set was enough to completely saturate kSMS. Furthermore, the difference

|  |  |
| --- | --- |
| **6.3. Carbon** |  |
|  |  |

Table 6.11: Specific-mass-shift constants, kSMS, of transitions from the ground state (2s22p 2P1**o=**2) in C II. Note that the MCHF-CI results are non-relativistic and hence do not distinguish ne-structure.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Level |  | Energya |  | kSMS (GHz amu) | |  |
|  |  | (cm 1) | CI | CI + (1) | CI + (1**;**2) | MCHF-CIb |
| 2s2p2 4P1**=**2 | | 43003 | -2913 | -2956 | -2960 |  |
| 2s2p2 4P3**=**2 | | 43025 | -2912 | -2954 | -2958 |  |
| 2s2p2 4P5**=**2 | | 43054 | -2910 | -2952 | -2956 |  |
| 2s2p2 2D5**=**2 | | 74930 | -2604 | -2666 | -2672 | -2672 |
| 2s2p2 2D3**=**2 | | 74933 | -2604 | -2666 | -2671 |  |
| 2s2p2 | 2S1**=**2 | 96494 | -1204 | -1301 | -1321 | -1411 |
| 2s2p2 | 2P1**=**2 | 110624 | -1323 | -1410 | -1471 | -1531 |
| 2s2p2 | 2P3**=**2 | 110666 | -1320 | -1407 | -1468 |  |
|  |  |  |  |  |  |  |

**a** Experimental results tabulated by Moore [98] **b** J•onsson **et al.** [78]

between the results of CI + MBPT and MCHF-CI is fairly large for this transition

(around 7%). Adding the next most important configuration, 2s23s, to the leading set

changes the energy of the 2S1**=**2 transition by 30 cm 1 (0.03%) and kSMS by 14 GHz amu

(around 1%). The e ect on all other transitions was much smaller.

1. **C I**

Transition energies in neutral carbon were presented in Table 4.7. The ground state of

C I is 2s22p2 3P0. A discussion of the calculations and their limitations for this atom is

given in Section 4.2.4. In particular, being restricted to taking excitations from only a

few leading configurations leads to an error of up to 80 GHz amu in kSMS.

In Table 6.12 we present the SMS constants for C I. We are within 1% of the values

obtained using the MCHF-CI method (Refs. [77] and [78]). For most transitions the

e ect of core-correlations on kSMS is around 1 or 2%, however in some cases they are

larger (for example, in 2s2p3 3P **o** the core correlations are 8% of the total).

**6. Speci c mass shift**

Table 6.12: Specific-mass-shift constants, kSMS, of transitions from the ground state (2s22p2 3P0) in C I. Note that the MCHF-CI results are non-relativistic and hence do not distinguish ne-structure.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Level | Energya |  | kSMS (GHz amu) | |  |
|  | (cm 1) | CI | CI + (1) | CI + (1**;**2) | MCHF-CI |
| 2s22p2 1S0 | 21648 | 186 | 180 | 191 | 152b |
| 2s2p3 5S2**o** | 33735 | -2540 | -2579 | -2588 | -2583b |
| 2s22p3s 3P0**o** | 60333 | 1405 | 1405 | 1419 |  |
| 2s22p3s 3P1**o** | 60353 | 1406 | 1406 | 1420 |  |
| 2s22p3s 3P2**o** | 60393 | 1408 | 1408 | 1422 |  |
| 2s22p3s 1P1**o** | 61982 | 1549 | 1551 | 1559 | 1553b |
| 2s2p3 3D3**o** | 64087 | -2165 | -2224 | -2227 |  |
| 2s2p3 3D1**o** | 64090 | -2165 | -2224 | -2227 | -2222c |
| 2s2p3 3D2**o** | 64091 | -2165 | -2224 | -2227 |  |
| 2s2p3 3P1**o** | 75254 | -1272 | -1390 | -1392 |  |
| 2s2p3 3P2**o** | 75255 | -1272 | -1389 | -1391 |  |
| 2s2p3 3P0**o** | 75256 | -1271 | -1390 | -1392 |  |
| 2s22p3d 1D2**o** | 77680 | 1334 | 1320 | 1331 |  |
| 2s22p4s 3P0**o** | 78105 | 1398 | 1392 | 1407 |  |
| 2s22p4s 3P1**o** | 78117 | 1404 | 1397 | 1412 |  |
| 2s22p4s 3P2**o** | 78148 | 1415 | 1408 | 1422 |  |
| 2s22p3d 3F2**o** | 78199 | 1378 | 1368 | 1381 |  |
| 2s22p3d 3F3**o** | 78216 | 1381 | 1372 | 1384 |  |
| 2s22p3d 3D1**o** | 78293 | 1430 | 1422 | 1434 |  |
| 2s22p3d 3D2**o** | 78308 | 1429 | 1421 | 1432 |  |
| 2s22p3d 3D3**o** | 78318 | 1430 | 1420 | 1432 |  |
| 2s22p4s 1P1**o** | 78340 | 1443 | 1435 | 1446 |  |
| 2s22p3d 1F3**o** | 78530 | 1451 | 1440 | 1452 |  |
| 2s22p3d 1P1**o** | 78731 | 1436 | 1426 | 1438 |  |
| 2s22p3d 3P2**o** | 79311 | 948 | 998 | 1010 |  |
| 2s22p3d 3P1**o** | 79319 | 956 | 1006 | 1018 |  |
| 2s22p3d 3P0**o** | 79323 | 960 | 1009 | 1021 |  |
| 2s22p4d 1D2**o** | 83498 | 1277 | 1258 | 1268 |  |
|  |  |  |  |  |  |

**a** Experimental results tabulated by Moore [98] **b** Carlsson **et al.** [77]

**c** J•onsson **et al.** [78]

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **6.3. Carbon** | |  |  |  |  |  | |  |
|  |  | | | | | |  |  |
|  | Table 6.13: Comparison of calculated 13C { 12C isotope shifts, | | | | | | |  |
|  | 13**;**12, with experiment. | |  |  |  |  |  |  |
|  |  | |  |  | | |  |  |
|  | Transition | |  | 13**;**12 (cm 1) | | |  |
|  | Lower Level | Upper Level |  | Expt. | | This work | |  |
|  | (A) |  |
|  | C I |  |  |  |  |  |  |  |
|  | 2s22p2 3P2 | 2s2p3 5S2**o** | 2967 | 0:670 (5)a | | 0:674b | |  |
|  | 2s22p2 1S0 | 2s22p3s 1P1**o** | 2479 | 0:156 | (3)c | 0:151 | |  |
|  | C II |  |  | 0:156 | (2)d |  |  |  |
|  |  |  |  |  |  |  |  |
|  | 2s2p2 2S1**=**2 | 2s23p 2P3**o=**2 | 2837 | 0:612 | (2)c | 0:617 | |  |
|  | 2s2p2 2S1**=**2 | 2s23p 2P1**o=**2 | 2838 | 0:623 | (3)c | 0:617 | |  |
|  |  |  |  |  |  |  |  |  |

**a** Bernheim and Kittrell [122]

**b** Actually, the 2s**2**2p**2 3**P**0** { 2s2p**3 5**S**2o** transition was calculated. **c** Burnett [123]

* + Holmes [124]

1. **Comparison with experiment**

In Table 6.13 we compare our calculations with the few experiments that exist for carbon ions; in all cases agreement is within around 0.005 cm 1, which corresponds to an error in kSMS of around 20 GHz amu.

In Table 6.14 we present total isotope shifts for some important transitions. These transitions can be observed in quasar absorption spectra, and can therefore be used to probe variation of and isotope abundance evolution. The results are presented both in MHz and km/s: the latter is the preferred form for use in astronomy.

Table 6.14: Total calculated 13C { 12C ( 13**;**12) and 14C { 12C ( 14**;**12) isotope shifts for important transitions. We believe the errors are of the order of 0.1 GHz.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Transition | |  | 13**;**12 | |  | 14**;**12 | |  |  |
| Ground State | Upper Level |  | (GHz) | (km/s) | a | (GHz) | (km/s) | a |  |
| (A) |  |  |  |
| C I |  |  |  |  |  |  |  |  |  |
| 2s22p2 3P0 | 2s22p3s 3P1**o** | 1657 | -2.75 | 0.46 |  | -5.09 | 0.84 |  |  |
|  | 2s2p3 3D1**o** | 1560 | 21.10 | -3.29 |  | 39.12 | -6.10 |  |  |
|  | 2s2p3 3P1**o** | 1329 | 16.91 | -2.25 |  | 31.34 | -4.17 |  |  |
|  | 2s22p4s 3P1**o** | 1280 | -0.82 | 0.10 |  | -1.51 | 0.19 |  |  |
|  | 2s22p3d 3D1**o** | 1277 | -0.94 | 0.12 |  | -1.75 | 0.22 |  |  |
|  | 2s22p4s 1P1**o** | 1276 | -1.01 | 0.13 |  | -1.88 | 0.24 |  |  |
|  | 2s22p3d 3P1**o** | 1261 | 1.84 | -0.23 |  | 3.42 | -0.43 |  |  |
| C II |  |  |  |  |  |  |  |  |  |
| 2s22p 2P1**o=**2 | 2s2p2 2D3**=**2 | 1336 | 25.10 | -3.35 |  | 46.53 | -6.21 |  |  |
|  | 2s2p2 2D5**=**2 | 1336 | 25.10 | -3.35 |  | 46.54 | -6.21 |  |  |
|  | 2s2p2 2S1**=**2 | 1037 | 18.70 | -1.94 |  | 34.66 | -3.59 |  |  |
| C III |  |  |  |  |  |  |  |  |  |
| 2s2 1S0 | 2s2p 1P1**o** | 977 | 28.76 | -2.81 |  | 53.33 | -5.21 |  |  |
| C IV |  |  |  |  |  |  |  |  |  |
| 2s 2S1**=**2 | 2p 2P1**o=**2 | 1551 | 35.89 | -5.57 |  | 66.54 | -10.32 |  |  |
|  | 2p 2P3**o=**2 | 1548 | 35.79 | -5.54 |  | 66.35 | -10.27 |  |  |
|  |  |  |  |  |  |  |  |  |  |

* = = c (km/s). A negative velocity means that **14**C (and **13**C) are at lower wavelength than **12**C.

Chapter 8

Cosmological variation of deuteron binding energy, strong interaction and quark masses from big bang

nucleosynthesis

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 8 |  |  |  |  | 8 |  |
| 6 |  |  |  |  |  |  |
|  |  |  |  |  | 7 |  |
| 10 |  |  |  |  |  |  |
| 4 |  |  |  |  |  |  |
| 10Η‰ |  |  |  | 10 |  |  |
|  |  |  |  |  |  |
|  |  |  |  | 10 | 6 |  |
|  |  |  |  | Η‰ |  |  |
| 2 |  |  |  |  |  |  |
|  |  |  |  |  | 5 |  |
| 0 |  |  |  |  |  |  |
| 23 | 24 | 25 | 26 | 27 |  |  |
|  |  | Q‰109 HKL |  |  |  |  |

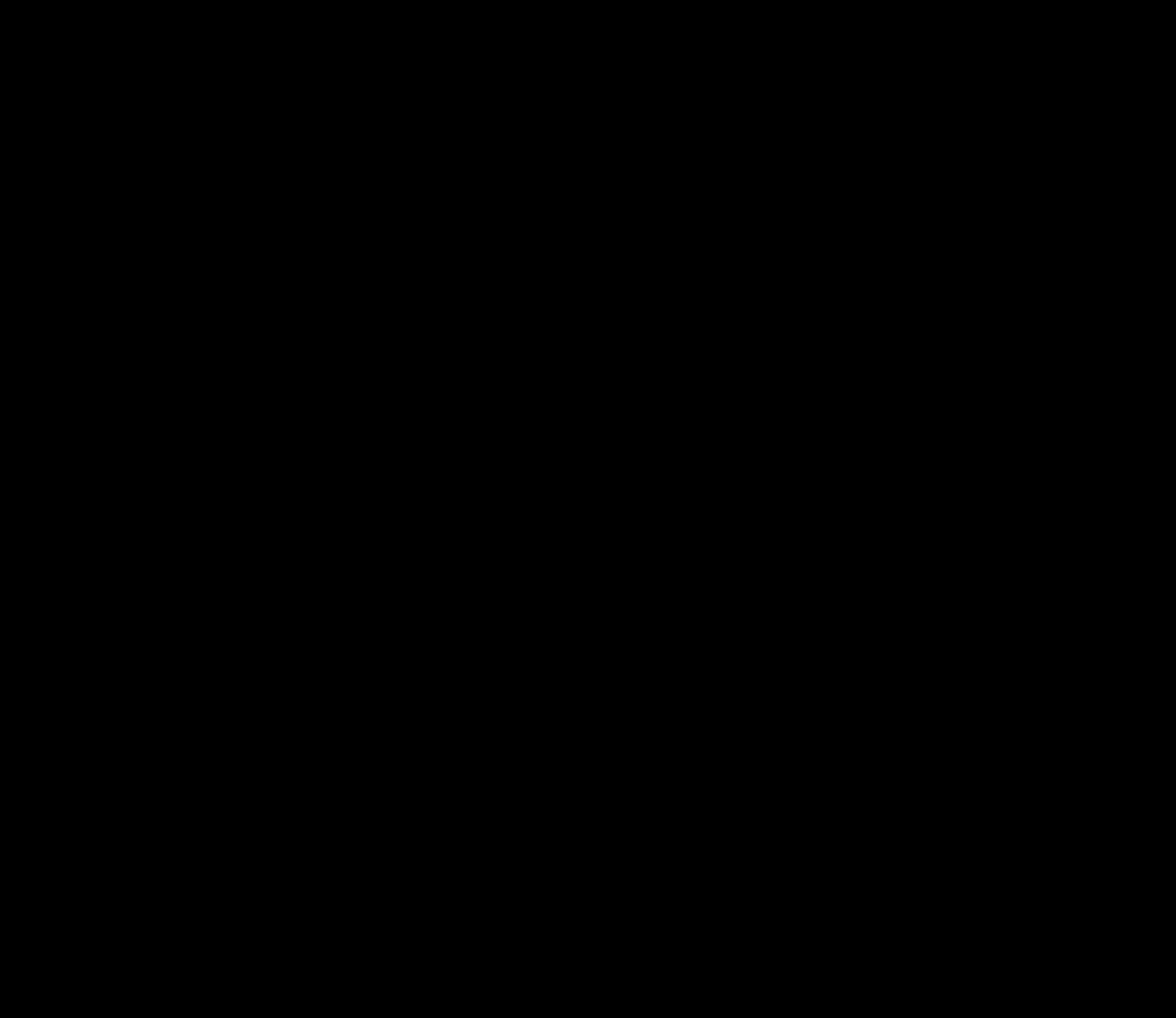


FIG. 2: 1σ-ranges around the maxima of individual likelihood functions. The solid lines show 1σ-ranges for D, the dashed lines are for 4 He (using Y**p** from  [Eq.5),](#page2) and the dot-dashed lines are for 7Li. For lithium, there are 2 solutions for η and Q, hence the shape of the error contours is more complicated.

1. Constraint from CMB anisotropy measurements

The value of η found from CMB anisotropy measurements

η0 = (6.14 ± 0.25) × 10−10

has rather high accuracy. It is natural to use the constraint from this measurement in our study of the deuteron binding energy eﬀects. To do this we construct another likelihood function which is a function of Q only.

If we neglect nondiagonal elements in wij we can con-struct the individual likelihood functions for D, 4 He, and

24 24.5 25 25.5 26 Q‰109 HKL

FIG. 3: 1σ-range about the maximum of Lf (η, Q) (again us-ing Y**p** from  [Eq.5](#page2)). The lighter shaded region shows CMB-WMAP data for η. The darker shaded region is the 1σ-range for η from BBN calculations using the present-day value of the deuteron binding energy, Q = 25.82. A lower value of Y**p** will produce a larger deviation between the η**W M AP** and η**BBN** .

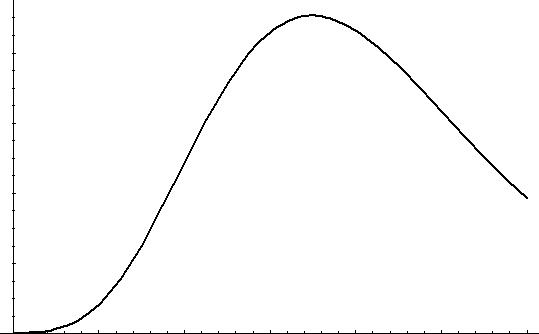
7Li. They are constructed in the same way as  [(7.23)](#page5) using instead of general function Lf (η, Q) the individual ones

LfD (η, Q), LfHe(η, Q) , LfLi(η, Q). These functions are plotted in Fig. 4 together with the general likelihood function  [(7.23](#page5))

From the deuterium likelihood function we found the position of the maximum and 1σ deviations:

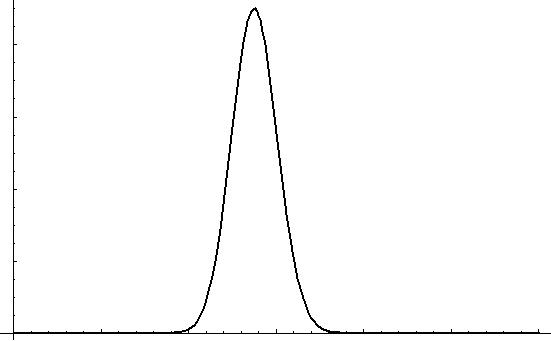
|  |  |
| --- | --- |
| QD = (25.74 + 0.92 − 0.68) × 109. | (7.24) |

LfD



|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 80 |  |  |  |  |  |  |
| 60 |  |  |  |  |  |  |
| 40 |  |  |  |  |  |  |
| 20 |  |  |  |  |  |  |
| 24.5 | 25 | 25.5 | 26 | 26.5 | Q |  |
| 27 |  |

LfHe



|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 80 |  |  |  |  |  |  |
| 60 |  |  |  |  |  |  |
| 40 |  |  |  |  |  |  |
| 20 |  |  |  |  |  |  |
| 24.5 | 25 | 25.5 | 26 | 26.5 | Q |  |
| 27 |  |
| LfLi |  |  |  |  |  |  |
| 100 |  |  |  |  |  |  |
| 80 |  |  |  |  |  |  |
| 60 |  |  |  |  |  |  |
| 40 |  |  |  |  |  |  |
| 20 |  |  |  |  |  |  |
| 24 |  | 25 | 26 | 27 | Q |  |
|  |  |  |
| LHQL |  |  |  |  |  |  |
| 150 |  |  |  |  |  |  |
| 125 |  |  |  |  |  |  |
| 100 |  |  |  |  |  |  |
| 75 |  |  |  |  |  |  |
| 50 |  |  |  |  |  |  |
| 25 |  |  |  |  |  |  |
| 24.5 | 25 | 25.5 | 26 | 26.5 | Q |  |
| 27 |  |

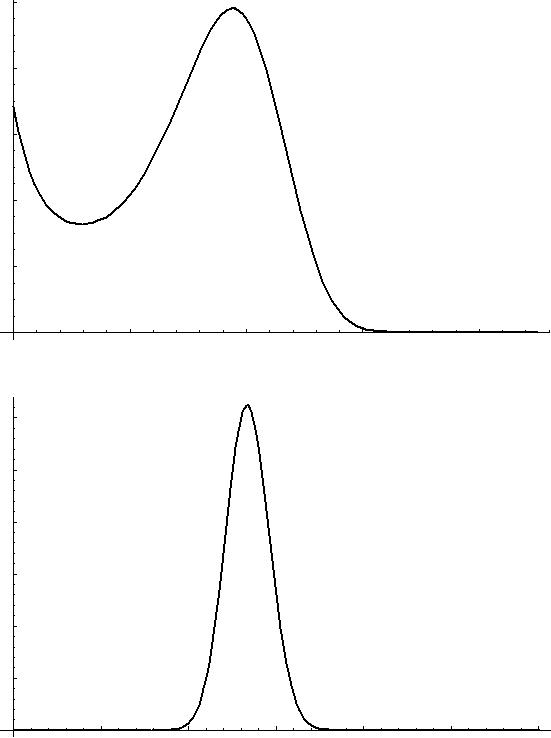


FIG. 4: Individual likelihood functions  [(7.23)](#page5) for the light el-ements. From top to bottom: D, 4 He  [(Eq.5),](#page2) Li, and the combined datset.

The shape near the maximum is apparently non-symmetric. The position of the maximum is fully com-patible with the present value of Q = 25.82 ×109 K. The helium likelihood function is much narrower (see the sec-ond panel from the top). It gives for the maximum and

6

for the 1σ the values

|  |  |
| --- | --- |
| QHe = (25.37 ± 0.13) × 109. | (7.25) |

This value lies below the present value of the binding energy. Finally, the lithium likelihood function has the maximum at

|  |  |
| --- | --- |
| QLi = (24.88 + 0.43 − 0.59) × 109. | (7.26) |

The position of this maximum is compatible with the helium result.

The general likelihood function  [(7.23)](#page5) is plotted in the lower panel in Fig. 4 The position of its maximum dif-fers only slightly from the position given by the helium likelihood function.

|  |  |
| --- | --- |
| QBBN = (25.34 ± 0.12) × 109 | (7.27) |

It is interesting to compare the light element abun-dances for two values of the deuterium binding energies. In Fig. 5 we plotted the traditional curves for the light element abundances as a functions of η for two values of Q. The dotted lines in the figures correspond to a

present value of Qpresent = 25.82 ×109 K, while the solid curves correspond to a new value QBBN = 25.34 × 109 K. Clearly, the new value QBBN moves the curves closer

to the data.

The result which we obtained may be presented as

|  |  |
| --- | --- |
| δQ/Q = −0.019 ± 0.005, | (7.28) |

where δQ = QBBN − Qpresent. If we do not fix η and try to fit it simulaneously with Q we obtain

δQ/Q = −0.022 ±0.008, η = (6.51 + 0.77 −0.66) ×10−10. (29)

The obtained η is fully compatible with the one measured by WMAP.

These values of δQ/Q and η were obtained for high value of the helium mass fraction Yp . If we use as an input the low value of Yp from  [(6)](#page2) we obtain

|  |  |
| --- | --- |
| δQ/Q = −0.048 ± 0.004, | (7.30) |

If we fit both δQ/Q and η we obtain

δQ/Q = −0.059 ±0.007, η = (7.55 + 0.91 −0.75) ×10−10. (31)

Finally if we use the value of Yp for 4He obtained using the whole sample of 14 points, with increased error bars, from  [Eq.(1),](#page2) we obtain

|  |  |
| --- | --- |
| δQ/Q = −0.033 ± 0.006, | (7.32) |

and for δQ/Q and η

δQ/Q = −0.042 ±0.009, η = (7.00 + 0.85 −0.72) ×10−10. (33)

The results given in  [eqs.(28)](#page6) and  [(30)](#page6) therefore represent an estimate of the plausible range in δQ/Q. Despite the

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | 0.00005 |  |  |  |  |  |
|  | 0.00004 |  |  |  |  |  |
| D | 0.00003 |  |  |  |  |  |
| Y |  |  |  |  |  |
|  | 0.00002 |  |  |  |  |  |
|  | 0 | 2 | 4 | 6 | 8 |  |
|  | 0.255 |  |  |  |  |  |
|  | 0.25 |  |  |  |  |  |
|  | 0.245 |  |  |  |  |  |
| p |  |  |  |  |  |  |
| Y |  |  |  |  |  |  |
|  | 0.24 |  |  |  |  |  |
|  | 0.235 |  |  |  |  |  |
|  | 0 | 2 | 4 | 6 | 8 |  |
|  | 6·10-10 |  |  |  |  |  |
|  | 5·10-10 |  |  |  |  |  |
|  | 4·10-10 |  |  |  |  |  |
| Li |  |  |  |  |  |  |
| Y |  |  |  |  |  |  |
|  | 3·10-10 |  |  |  |  |  |
|  | 2·10-10 |  |  |  |  |  |
|  | 0 | 2 | 4 | 6 | 8 |  |
|  |  |  | Η‰10-10 |  |  |  |

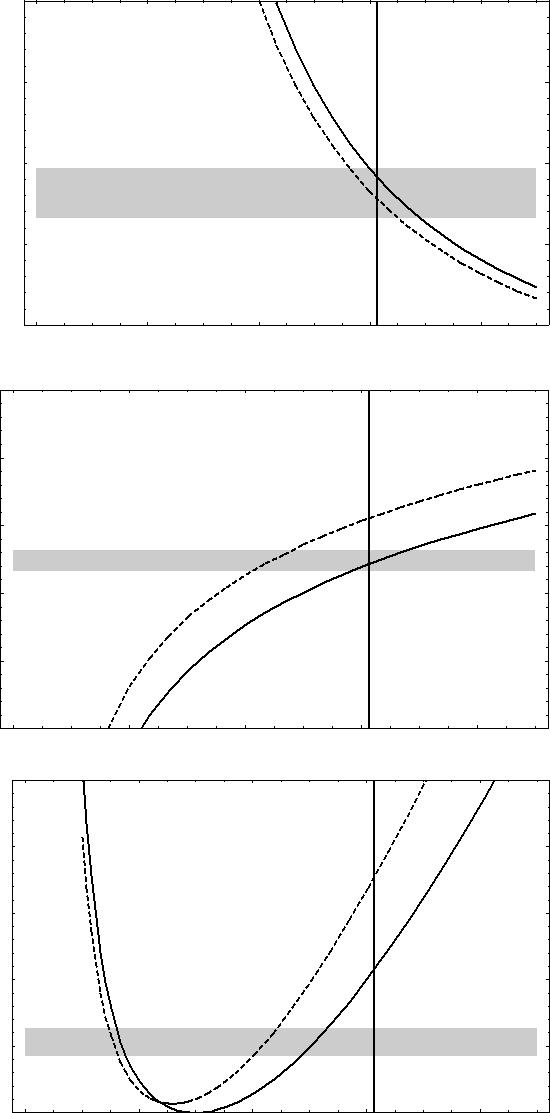


FIG. 5: The predicted light element abundance yields as a function of η, for two values of the deuteron binding energy, Q. The dotted curve corresponds to the present value of Q**present** = 25.82 × 109 K. The solid curve corresponds to the new value of Q = Q**BBN** = 25.34 × 109 K. The vertical line corresponds to η = 6.14 (WMAP value). The shaded regions is the 1σ-ranges for the observed light element abundances, where Y**p** is from  [eq.5](#page2).

7

Combining eqs.  [(32)](#page6) and  [(34)](#page7) we obtain

|  |  |  |  |
| --- | --- | --- | --- |
| δ(ms/ΛQC D ) | = (1.1 ± 0.3) × 10−3 | (7.35) |  |
| (ms/ΛQC D ) |  |

This equation may contain an additional factor (close to one) reflecting unknown theoretical uncertainty in eq.  [(7.34](#page7)). Note that we obtain here variation at the level 10−3 while the limits on variation of α [7.2, 48] and ΛQC D /Mplank [7.2, 3] are an order of magnitude weaker. This may serve as a justification of our approach.

 (BBN4DFW.1)

 (BBN4DFW.2)

 (BBN4DFW.3)

 (BBN4DFW.4)

 (BBN4DFW.5)

 (BBN4DFW.6)

--

 (BBN4DFW.7)

 (BBN4DFW.8)

 (BBN4DFW.9)

 (BBN4DFW.10)

 (BBN4DFW.11)

 (BBN4DFW.12)

 (BBN4DFW.13)

 (BBN4DFW.14)

 (BBN4DFW.15)

 (BBN4DFW.15.2)

 (BBN4DFW.16)

 (BBN4DFW.17)

--

 (BBN4DFW.18)

 (BBN4DFW.18.2)

-

 (BBN4DFW.19)

 (BBN4DFW.20)

 (BBN4DFW.20.2)

 (BBN4DFW.21)

 (BBN4DFW.22)

--

 (BBN4DFW.22.2)

 (BBN4DFW.23)

 (BBN4DFW.24)

--

 (BBN4DFW.25)

 (BBN4DFW.26)

 (BBN4DFW.27)

 (BBN4DFW.28)

 (BBN4DFW.29)

 (BBN4DFW.30)

 (BBN4DFW.31)

 (BBN4DFW.32)

 (BBN4DFW.33)

--

 (BBN4DFW.34)

-

 (BBN4DFW.35)

--

 (BBN4DFW.35.2)

 (BBN4DFW.36)

 (BBN4DFW.37)

 (BBN4DFW.38)

-

 (BBN4DFW.39)

 (BBN4DFW.40)

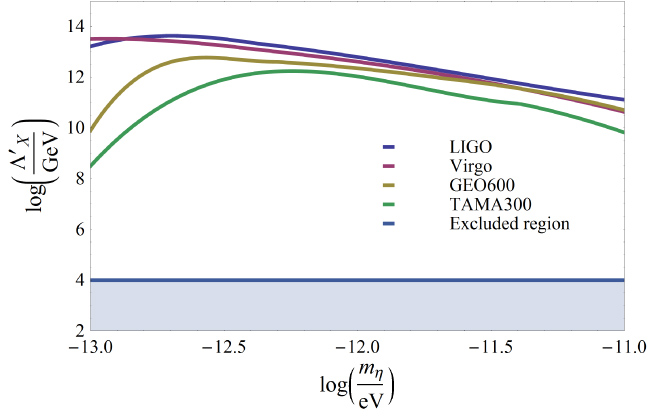
 (BBN4DFW.41)

Chapter 9

Searching for dark matter and variation of fundamental constants with laser and maser interferometry

Any slight variations in the fundamental constants of Nature, which may be induced by dark matter or some yet-to-be-discovered cosmic field, would characteristically alter the phase of a light beam inside an interferometer, which can be measured extremely precisely. Laser and maser interferometry may be applied to searches for the linear-in-time drift of the fundamental constants, detection of topological defect dark matter through transient-in-time effects and for a relic, coherently oscillating condensate, which consists of scalar dark matter fields, through oscillating effects.

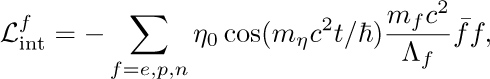
Our proposed experiments require either minor or no modifications of existing apparatus, and offer extensive reach into important and unconstrained spaces of physical parameters.

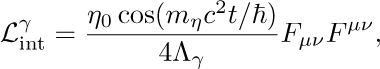


The idea that the fundamental constants of Nature might vary with time can be traced as far back as the large numbers hypothesis of Dirac, who hypothesized that the gravitational constant G might be proportional to the reciprocal of the age of the Universe [8.1]. More contemporary theories predict that the fundamental constants vary on cosmological timescales (see e.g. [8.2{4]). Astronomical observations of quasar absorption spectra hint at the existence of a spatial gradient in the value

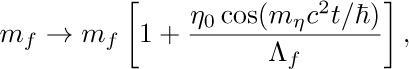
of the \_ne-structure constant, \_ = e2=~c [8.5, 6]. Data samples from the Keck Telescope and Very Large Telescope [8.7, 8] independently agree on the direction and magnitude of this gradient, which is significant at the 4:2\_ level. A consequence of this astronomical result is that, since the solar system is moving along this spatial gradient, there should exist a corresponding temporal shift in \_ in Earth's frame of reference at the level \_\_=\_ \_ 10^-19/yr [8.9]. Finding this variation with laboratory experiments could independently corroborate the astronomical result. To date, atomic clocks have provided the most sensitive laboratory limit on annual variations

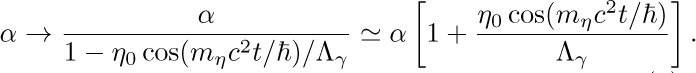
in \_: \_\_=\_ . 10^-17/yr [8.10]. The question of dark matter (DM), namely its identity, properties and non-gravitational interactions, remains one of the most important unsolved problems in physics. Various DM candidates and searches therefor have been proposed over the years [8.11]. One such candidate is the axion, a pseudoscalar particle which was originally introduced in order to resolve the strong CP problem of Quantum Chromodynamics (QCD) [12, 13] (see also [8.14{17]). The axion is believed to have formed a condensate in the early Universe [8.18]. This relic axion condensate can be sought for through a variety of distinctive signatures (see e.g. [8.19{26]). Likewise, a condensate consisting of a scalar DM particle may also have formed. The scalar field \_ comprising this condensate oscillates with frequency ! \_ m\_c2=~ and may couple to the fermion fields:

 (1)

 (2)

F is the electromagnetic \_eld tensor. \_X is a large energy scale, which from gravitational tests is constrained to be \_X \_ 1021 GeV [8.27]. Eqs. (8.1) and (8.2) alter the fundamental constants in an oscillating manner as follows, respectively:

 (3)

 (4)

Quadratic couplings in \_, with the replacement X is a less strongly constrained energy scale, with constraints from laboratory and astrophysical observations given by \_0 X \_ 10^4 GeV [8.28]. We note that the quadratic portal gives rise to not only oscillating effects, but may also lead to non-oscillating space-time variation of the fundamental constants: \_X=X = \_2 0=2(\_0X)2, which arises due to space-time variations in. These effects may be sought for using terrestrial experiments (atomic clocks, Oklo natural nuclear reactor, and laser/maser interferometry as suggested in this paper) and astrophysical observations (quasars, white dwarves, Big Bang Nucleosynthesis, Cosmic Microwave Background measurements). Another possible DM candidate is topological defect DM, which is a stable non-trivial form of DM that consists of light DM fields and is stabilised by a self-interaction potential [8.29] (self-gravitating DM fields can also form solitons, see e.g. Ref. [8.30]). These objects

may have various dimensionalities: 0D (monopoles), 1D (strings) or 2D (domain walls). The transverse size of a topological defect depends on the mass of the particle comprising the defect, d \_ ~=m\_c, which may be large (macroscopic or galactic) for a sufficiently light DM particle. The light DM particle comprising a topological defect can be either a scalar, pseudoscalar or vector particle. Recent proposals for pseudoscalar-type defect searches include using a global network of magnetometers to search for correlated transient spin preces-sion effects [8.31] and electric dipole moments [8.32] that arise from the coupling of the scalar field derivative to

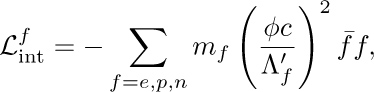
the fermion axial vector currents. Recent proposals for scalar-type defect searches include using a global net-work of atomic clocks [8.27], and Earth rotation and pul-

sar timing [8.32], to search for transient-in-time alterations of the system frequencies due to transient-in-time variation of the fundamental constants that arise from the

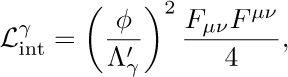
couplings of the scalar field to the fermion and photon fields. The best current sensitivities for transient-in-time variations of the fundamental constants on the

time scale of t \_ 1 􀀀 100 s with terrestrial experiments are offered by atomic clocks, with an optical/optical clock combination [33, 34] sensitive to variations in \_:

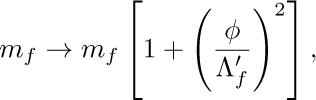
\_\_=\_ \_ 10􀀀15􀀀10􀀀16 and a hyperfine/optical clock combination [35] to variations in the electron-to-proton mass ratio me=mp: \_(me=mp)=(me=mp) \_ 10􀀀13 􀀀 10􀀀14. There are many possibilities for the interactions of topological defect DM particles with the Standard Model particles. Here we consider couplings with a quadratic dependence on the scalar field, which were considered previously in Refs. [8.27, 32]. A scalar dark matter \_field \_ may interact with fermions via the coupling:

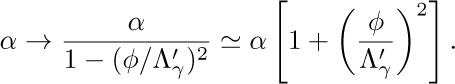
 (5)

and with photons via the coupling:

 (6)

Eqs. (8.5) and (8.6) alter the fundamental constants in a transient manner as follows, respectively:

 (7)

 (8)

In the present work, we point out that laser and maser interferometry may be used as particularly sensitive probes to search for linear-in-time, oscillating and transient variations of the fundamental constants of Nature, including \_ and me=mp. Laser and maser interferometry are very well established techniques and have already proven to be extremely sensitive probes for exotic new physics, including searches for the aether, tests of Lorentz symmetry [8.36] and gravitational wave detection [8.37]. Laser interferometry has also recently been proposed for the detection of dilaton dark matter [8.38]. We consider the use of an interferometer with two arms of lengths L1 and L2, for which the observable is the phase difference \_\_ = !\_L=c between the two split beams, where ! is the reference frequency and \_L = L1 􀀀L2. In the absence of any variation of fundamental constants, the two split beams interfere destructively (\_\_ = (2N + 1)\_, where N is an integer). In the presence of variation of the fundamental constants, the reference frequency changes, as do the arm lengths, due to changes in the sizes of the atoms, which make up the arms. Depending on the type of laser or maser, as well as the arm lengths and materials used, the net result may be a change in the phase difference, \_(\_\_). Consider the simpler case when a laser/maser with-out a resonator is used, for example, the nitrogen laser operating on the 3\_u ! 3\_g electronic transition and superradiant Raman lasers [8.39{41]. In this case, ! is determined entirely by the specific atomic/molecular transition, the simplest archetypes of which are the electronic Rydberg me=mpMr) and rotational (! \_(e2=aB~)(me=mpMr)) transitions, where \_ is the relevant nuclear magnetic dipole moment, Krel is the derivative of the hyperfine relativistic (Casimir) correction fac-tor with respect to \_, and mpMr is the relevant reduced mass. The sensitivity coefficients KX are defined by:

 (9)

where mq is the quark mass and Ʌ\_QCD is the QCD scale, and are given in Table I for several archetypal transitions,

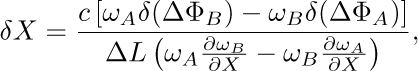
where we have made use of the relation \_(\_L)=\_L \_ \_aB=aB for \_L 6= 0 (aB is the Bohr radius). Since \_(\_\_) is proportional to \_\_, a higher laser frequency gives a

larger effect. Note that, unlike atomic clock experiments [8.10, 45, 46] and astrophysical observations [8.5, 7, 47] that search for a variation in the fundamental constants, in which two di\_erent transition lines are required to form the dimensionless ratio !A=!B, laser/maser interferometry can in principle be performed with only a single line, since the observable \_\_ is a dimensionless parameter by itself.

TABLE I. Sensitivity coe\_cients for \_, me=mp and mq=\_QCD for a laser or maser without a resonator and operating on typical atomic and molecular transitions. The values of Krel and Kmq=\_QCD for 87Rb and 133Cs have been taken from [8.42]

(see also Refs. [8.43, 44]).

Treating variations in frequencies (which depend only on the fundamental constants) and lengths independently (for variations in the latter may also arise due to undesired effects), we find

 (10)

X is a particular fundamental constant. In particular, we note that shifts in the arm lengths do not ap-pear in Eq. (8.10), meaning that undesirable e\_ects, such as seismic noise or tidal e\_ects, are not observed with this

setup and high precision may in principle be attained for low-frequency (large timescale) e\_ects. This is quite dis-tinct from conventional interferometer searches for gravi-tational waves, which have comparatively low sensitivity to low-frequency e\_ects, since in this case deviations in arm lengths are sought explicitly and low-frequency sys-tematic e\_ects greatly reduce the sensitivity of the appa-ratus in this region. Consider now the case when a laser/maser containing a resonator is used, for instance, the Nd:YAG solid-state laser. In this case, ! is determined by the length of the resonator, which changes if the fundamental constants change. In the non-relativistic limit, the wavelength and \_L (as well as the size of Earth) have the same depen-dence on the Bohr radius and so there are no observ-able e\_ects if changes of the fundamental constants are slow (adiabatic). Indeed, this may be viewed as a sim-

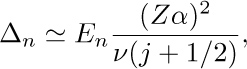
ple change in the measurement units. Transient e\_ects due to topological defect DM passage may still produce e\_ects, since changes in ! and \_L may occur at dif-ferent times. We note that a global terrestrial network (LIGO, Virgo, GEO600 and TAMA300) or a space-based network of interferometers (LISA) are particularly well

suited to search for topological defects through the cor-related e\_ects induced by defects. Likewise, temporal correlations of homogeneous e\_ects (including linear-in-

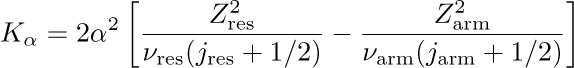
time and oscillating e\_ects) produced in several di\_erent interferomers can also be sought for. The sensitivity of interferometry to non-transient ef-fects is determined by relativistic corrections, which we estimate as follows. The size of an atom R is determined by the classical turning point of an external atomic elec-tron. Assuming that the centrifugal term \_ 1=R2 is small at large distances, we obtain (Zi + 1)e2=R = jEj.

E is the energy of the external electron and Zi is the net charge of the atomic species (for a neutral atom Zi = 0). This gives the relation: \_R=R = 􀀀\_jEj=jEj. The single-

particle relativistic correction to the energy in a many-electron atomic species is given by [8.48]:

 (11)

where En = 􀀀mee4(Zi + 1)2=2~2\_2 is the energy of the external atomic electron, j is its angular momentum, Z is the nuclear charge, and \_ \_ 1 is the e\_ective principal quantum number. The corresponding sensitivity coefficient in this case is

 (12)

Note that the sensitivity coe\_cient depends particularly

strongly on the factor Z2. jK\_j \_ 1 for light atoms and may be of the order of unity in heavy atoms. Further-more, the arms of di\_erent length can also be replaced by two arms (of the same length) made from di\_erent materials, for which the coe\_cients Z2=\_(j + 1=2) are di\_erent. We estimate the sensitivity to variations in me=mp from the di\_erences in the internuclear separations in molecular H2 and D2, which are 0:74144 \_A and 0:74152 \_A, respectively [49]. These data give: \_R=R \_ 􀀀10􀀀4 \_(me=mp)=(me=mp). Since only di\_erences in the coe\_cients of proportionality for the arm and resonator are observable in principle, the corresponding sensitivity coe\_cient is therefore Kme=mp.

Note that for a slow variation of fundamental constants (which includes linear-in-time e\_ects, transient e\_ects due to a slowly moving and/or large topological defect, and low-frequency oscillating e\_ects), the laser/maser resonator may be locked to an atomic/molecular fre-quency. In these cases, the sensitivity coe\_cients will be the same as those for the case in which a laser/maser without a resonator is used. We estimate the sensitivity of laser and maser interfer-ometry to e\_ects stemming from a relic, coherently os-cillating condensate, which consists of scalar DM \_elds. The typical spread in the oscillation frequencies of the scalar DM particles, which make up the condensate, is given by 2m\_v2=m\_c2) \_ (v2=c2), where a virial velocity of v \_ 10􀀀3c would be typical in our local Galactic neighbourhood. From the strain sensi-tivity curves of various interferometers [50{52], and as-suming that the condensate consisting of a scalar DM particle saturates the known local cold DM content, \_c2=2~2 \_ 0:4 GeV/cm3, we arrive at the accessi-ble region of parameter space shown in Fig. 1, in which we assume the use of a laser without a resonator. The region of parameter space accessible by the recently con-structed Fermilab Holometer (L = 40 m) [53] is expected to be similar to those accessible by the interferometers as shown in Fig. 1, but shifted toward higher scalar DM masses by several orders of magnitude.

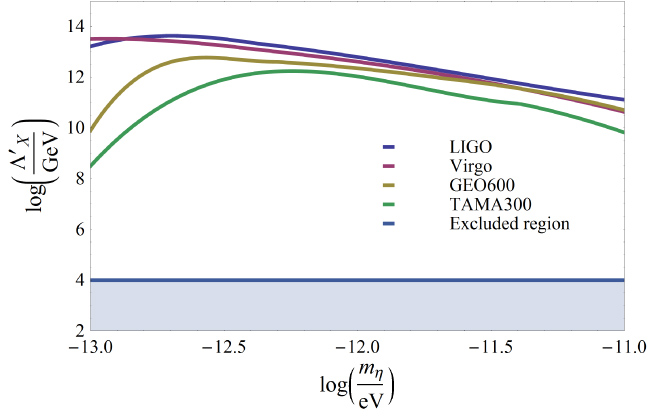
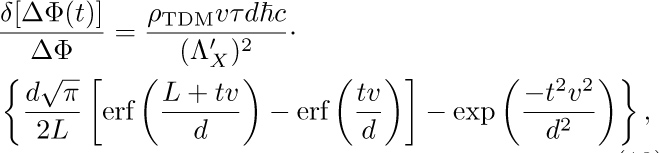
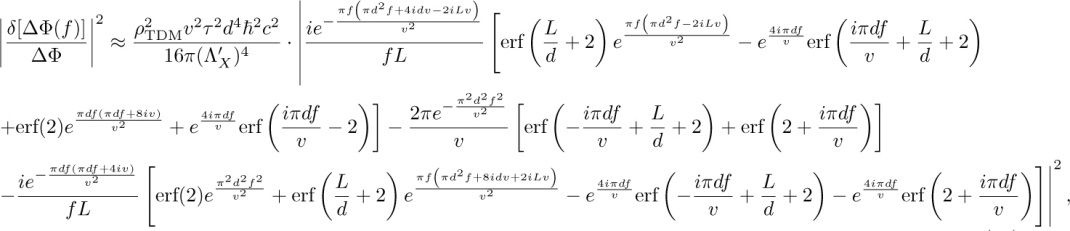


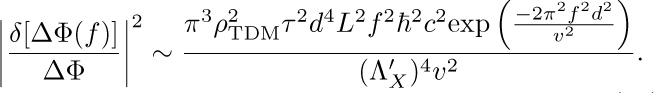
FIG. 1. (Color online) Region of dark matter parameter space accessible by various interferometers. The shaded blue region corresponds to the region of parameter space excluded by ex-isting laboratory and astrophysical observations [8.28]. Finally, we estimate the sensitivity of laser and maser interferometry to e\_ects stemming from topological de-fects, which consist of scalar DM \_elds, using the simple model of a domain wall with a Gaussian cross-sectional pro\_le of root-mean-square width d. The simplest do-main wall direction of incidence to consider (which pro duces non-zero e\_ects) is directly along one of the inter-ferometer arms (towards the laser ource, without loss of generality). Neglecting relativistic e\_ects and assuming the use of a resonator-based laser, the time-domain signal is given by

 (13)

\_TDM is the energy density associated with a topological defect network, v is the typical speed of a defect, \_ is the average time between encounters of a system with defect objects, and erf is the standard er-ror function. Cosmological models of topological defect DM have su\_cient exibility for topological defects to be the dominant contributor to the total DM content of the universe [8.27]. For the purposes of estimating the sensi-tivity of laser interferometers to topological defects, we may hence assume \_TDM \_ 0:4 GeV/cm3. Also, from hints o\_ered by pulsar timing data in relation to the pul-sar glitch phenomenon [8.32], we assume \_ \_ 1 year. The power spectrum corresponding to the time-domain signal in Eq. (8.13) is given by

 (14)

with the following asymptotic limit when d \_ L:

 (15)

From the power spectrum in (14), the plots for which are presented for interferometers of various sizes in the Supplemental Material, and the strain sensitivity curves of these interferometers [50{52], we arrive at the accessible region of parameter space shown in Fig. 2. We note that the sensitivity of interferometers drops rapidly with increasing values of d when d & L. For instance, for a LIGO interferometer (L = 4 km), the sensitivity to de-fects with d = 40 km is \_0 X . 10􀀀4 GeV. The region of parameter space accessible by the Fermilab Holometer [53] is expected to be similar to those accessible by the interferometers as shown in Fig. 2, but with a rapid drop in sensitivity occurring for d & 100 m. We hence suggest the use of laser and maser in-terferometry as particularly sensitive probes to search for linear-in-time, oscillating and transient variations of the fundamental constants of Nature, including \_ and me=mp. Our proposed experiments require either minor or no modifications of existing apparatus, and offer extensive reach into important and unconstrained spaces of physical parameters. We note that oscillating variation of fundamental constants due to a scalar condensate may also be sought for using tomic clocks.

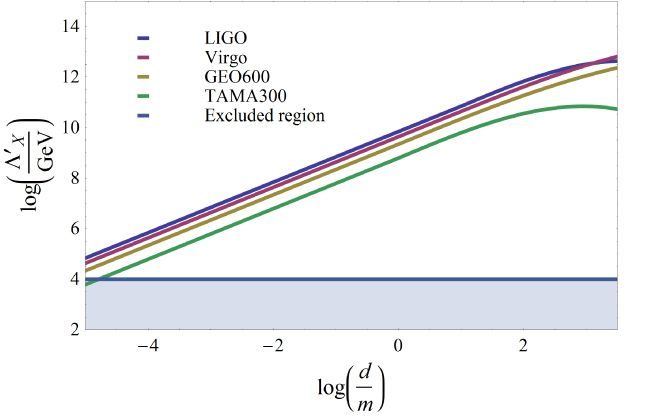


FIG. 2. (Color online) Region of dark matter parameter space accessible by various interferometers. The shaded blue region corresponds to the region of parameter space excluded by ex-isting laboratory and astrophysical observations [8.28].

SUPPLEMENTAL MATERIAL

We present the power spectra produced by a domain wall with a Gaussian cross-sectional pro\_le of root-mean-square width d, passing directly along one of the arms of a Michelson Morley interferometer. The asymptotic case d \_ L can be summarised by a single plot in the

combined variable fd (Fig. 3). The plots in the general case d . L are shown for the LIGO, Virgo, GEO600,TAMA300 and Fermilab Holometer interferometers in Figs. 4, 5, 6, 7 and 8, respectively. FIG. 3. (Color online) Power spectrum [in units\_2 TDML2\_ 2d2~2c2\_3=(\_0X)4v2\_(m/s)2] versus fd, produced by a domain wall with a Gaussian cross-sectional pro\_le passing directly along one of the arms of a Michelson-Morley interferometer with arms of equal length L.

7

FIG. 4. (Color online) Power spectra [in units \_2TDM\_ 2v2d2~2c2=(\_0X)4\_s2] versus frequency, produced by a domain wall with a Gaussian cross-sectional pro\_le passing directly along one of the arms of a LIGO interferometer (L = 4 km). From left to right: d = 1 m, d = 10 m, d = 100 m, d = 1000 m, d = 4000 m. FIG. 5. (Color online) Power spectra [in units \_2TDM\_ 2v2d2~2c2=(\_0X)4\_s2] versus frequency, produced by a domain wall with a Gaussian cross-sectional pro\_le passing directly along one of the arms of a Virgo interferometer (L = 3 km). From left to right: d = 1 m, d = 10 m, d = 100 m, d = 1000 m, d = 3000 m.

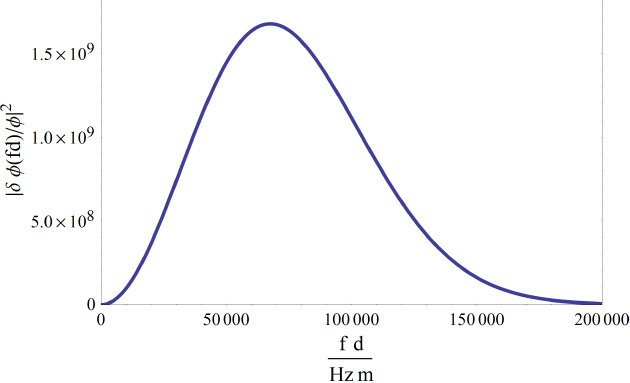
8

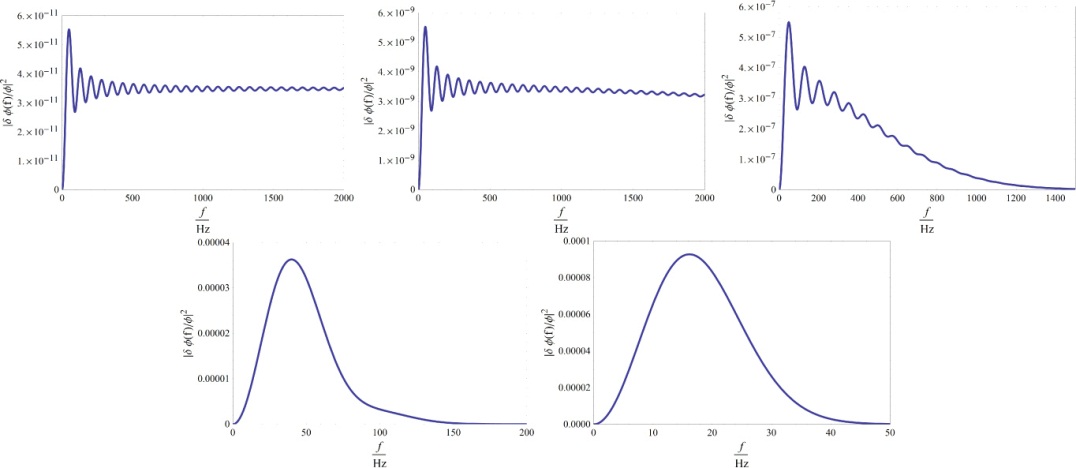
FIG. 6. (Color online) Power spectra [in units \_2TDM\_ 2v2d2~2c2=(\_0X)4\_s2] versus frequency, produced by a domain wall with a Gaussian cross-sectional pro\_le passing directly along one of the arms of a GEO600 interferometer (L = 600 m). From left to right: d = 1 m, d = 10 m, d = 100 m, d = 600 m.

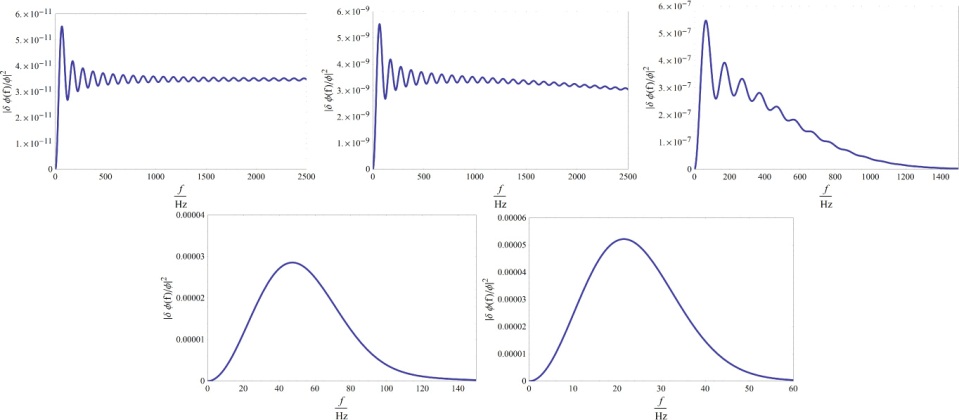
FIG. 7. (Color online) Power spectra [in units \_2TDM\_ 2v2d2~2c2=(\_0X)4\_s2] versus frequency, produced by a domain wall with a Gaussian cross-sectional pro\_le passing directly along one of the arms of a TAMA300 interferometer (L = 300 m). From left to right: d = 1 m, d = 10 m, d = 100 m, d = 300 m.

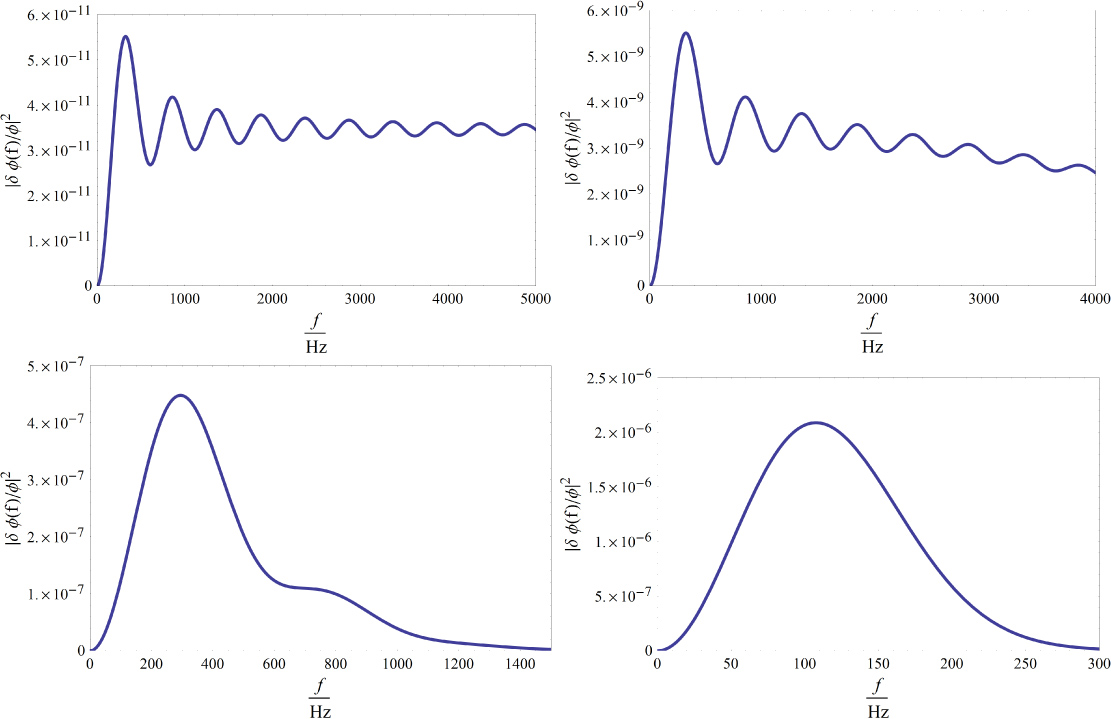
9

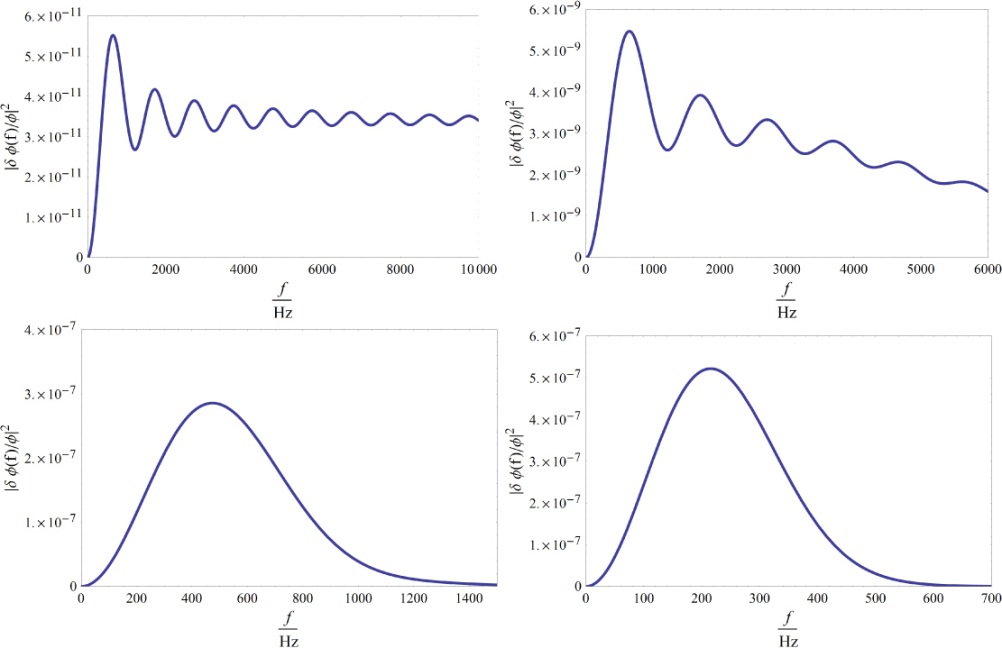
FIG. 8. (Color online) Power spectra [in units \_2TDM\_ 2v2d2~2c2=(\_0X)4\_s2] versus frequency, produced by a domain wall with a Gaussian cross-sectional pro\_le passing directly along one of the arms of a Fermilab Holometer interferometer (L = 40 m). From left to right: d = 0:1 m, d = 1 m, d = 10 m, d = 40 m.

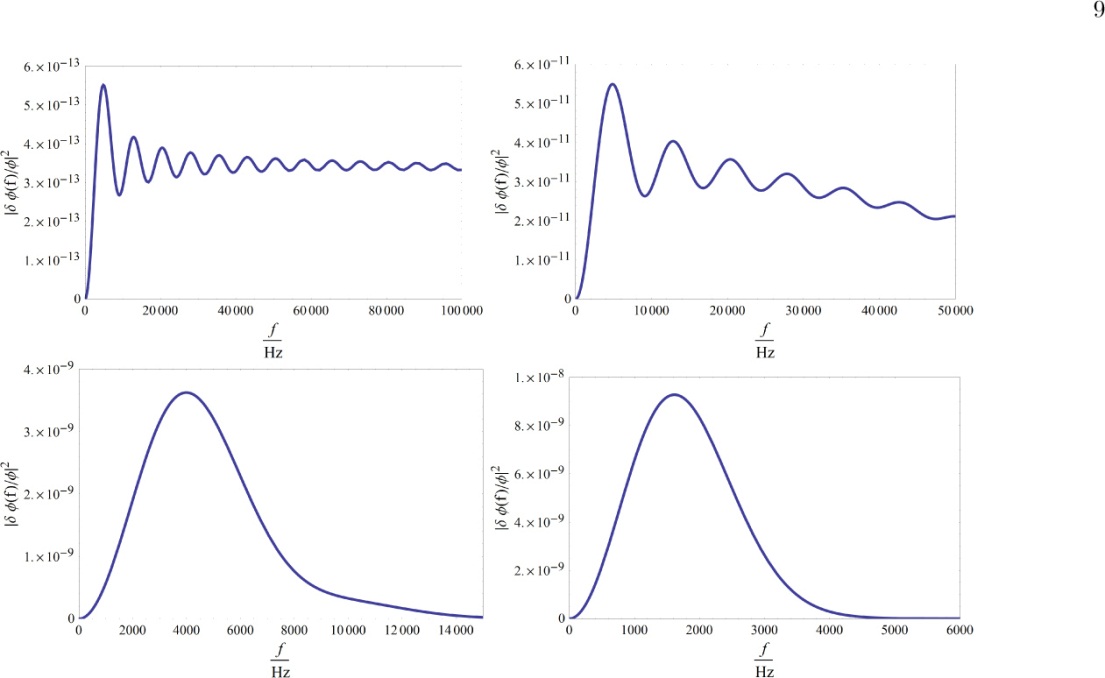








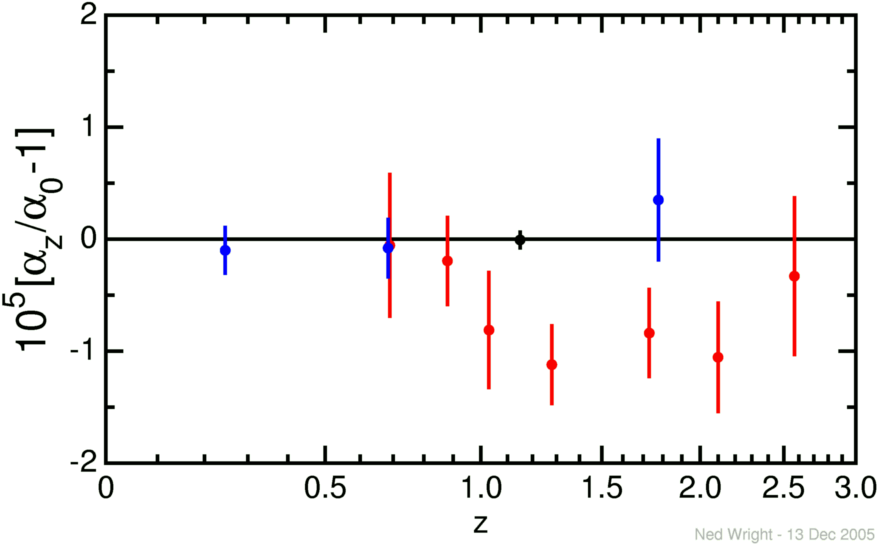




Chapter 10

Observations

Thee Sigma Rule



**Keck/HIRES spectra**

The data used here were kindly provided in reduced form by Jason X. Prochaska and Arthur M. Wolfe and are detailed in Prochaska & Wolfe (1996, 1997, 1999).

Outram et al. (1999) have also kindly contributed their spectrum of Q 1759+75 taken in July 1997. Here we provide only a brief description of the observations and data reduction, deferring a more detailed discussion to Section 3-3.1.2.

All the QSO spectra were obtained at the Keck I 10-m telescope on Mauna Kea with the HIRES facility (Vogt et al. 1994) over several observing runs from 1994 to 1997. The QSOs were generally quite faint (mV 19:0) so several ∼1-2 hour exposures were co-added for each object. Most of the data were reduced using the HIRES data reduction package written by T. Barlow, MAKEE. This package converts the two-dimensional echelle images to fully reduced, one-dimensional, wavelength-calibrated spectra.

Thorium-argon (ThAr) spectra were taken before and after the QSO exposures

and co-added to provide a calibration spectrum. ThAr lines were selected and centroided to form the wavelength solution. Some of the QSO spectra were reduced

when MAKEE had no wavelength calibration facility. In these cases, wavelength calibration was carried out using IRAF routines. Spectra not reduced in MAKEE were fully reduced within IRAF. 1 error arrays were generated assuming Poisson counting statistics. We fitted continua to regions of each spectrum containing either or both of the Si IV doublet transitions by fitting Legendre polynomials to ∼500 kms-1 sections

The sample comprises 21 Si IV absorption systems (towards 8 QSOs) over a redshift

range *z* = 2.0-3.1 (mean redshift (*Z*abs) = 2.6). The S/N per pixel ranges from

15-40 with most spectra having S=N ∼ 30 and FWHM 7:5 kms-1 (*R* = 34000).

We provide an example absorption system in Fig. 2.1. We plot all 21 absorption

systems in the Appendix.

**Analysis**

Although equation 2.1 is a simple approach to the specific case of an alkali doublet,

a more general approach is to write down the energy equation for any individual

transition, within any multiplet and for any species. Dzuba et al. (1999a,b) and

Webb et al. (1999) suggested the convenient formulation

z = 0 + *q*1xz + *q*2yz, (2.3)

where z is the wavenumber in the rest-frame of the cloud, at redshift *z*, in which

z/0 may not equal unity. 0 is the wavenumber as measured in the laboratory

and *x*z and *y*z contain the information about /:

*xz (*z/0)2 – 1 and yz  *(*z/0)4 – 1 (2.4)

The *q*1 and *q*2 coefficients represent the relativistic corrections to the energy for

a particular transition. The *q1* coefficients are typically an order of magnitude

larger than the *q2* coefficients and so it is the relative magnitudes of *q1* for different

transitions.

**Conclusions**

In this paper we present new refined calculations of the parameters q, which determine α-dependence of the transition frequencies for a number of ions used in the astrophysical search for α-variation. These ions appear to be very diﬀerent from the theoretical point of view. Because of that we had to use diﬀerent methods and dif-ferent levels of approximation for them. The final accu-racy of our results diﬀers not only for diﬀerent ions, but also for diﬀerent transitions.

The simplest system is Zn II, which has one valence electron. On the other hand, this is the heaviest ion and it has the largest core, which includes 3d10-shell. That gave us the opportunity to study corrections to q from the core-valence correlations and from Breit interaction. We found the former to be about 17% and the latter to be less than 1%. For lighter ions Breit interaction should be even smaller and can be safely neglected. Other ions also have much smaller and more rigid cores, so one might expect that core-valence correlations are few times weaker there in comparison to Zn. That allows us to neglect core-valence correlations for all other ions discussed in this paper.

Si II has the smallest core 1s2 . . . 2p 6 and three valence electrons. For neutral Mg, which has the same core, the core-valence corrections to the 3s → 3p transition frequencies were found to be about 4% [33, 36]. CI calculation for Si II is relatively simple and the errors associated with incompleteness of CI space are small. Thus, our estimate of the accuracy for Si on 6% level seems to be rather conservative.

Cr, Fe, and Ni have the core 1s2 . . . 3p6 and the core excitation energy varies from 2 a.u. for Cr II to 2.6 a.u. for Ni II. In comparison, the core excitation energy for Zn II is 0.9 a.u. Therefore, we estimate the core-valence correlation corrections for these ions to be at least two times smaller, than for Zn II.

Additional error here is associated with incomplete-ness of the CI space. These ions have from 5 to 9 valence electrons and CI space cannot be saturated. To estimate corresponding uncertainty we performed several calculations for each ion using diﬀerent basis sets and two different computer packages described in Sec. II. The basic Dirac-Hartree-Fock orbitals were calculated for diﬀerent configurations (for example, for the ground state configuration and for excited state configuration, etc.).

Supplementary information on the accuracy of our calculations can be obtained from comparison of calculated spectra and g-factors with experimental values. The later appear to be very important as they give information about electron coupling, which depends on relativistic corrections and on interaction between LS-multiplets. Our results for Cr II appear to be very close for different calculations and are in good agreement with the experiment both in terms of the gross level structure and spin-orbit splittings (see Table IV), so we estimate our final error here to be about 10 – 12%.

In this paper we present new refined calculations of the parameters q, which determine α-dependence of the transition frequencies for a number of ions used in the astrophysical search for α-variation. These ions appear to be very diﬀerent from the theoretical point of view. Because of that we had to use diﬀerent methods and dif-ferent levels of approximation for them. The final accu-racy of our results diﬀers not only for diﬀerent ions, but also for diﬀerent transitions.

The simplest system is Zn II, which has one valence electron. On the other hand, this is the heaviest ion and it has the largest core, which includes 3d10-shell. That gave us the opportunity to study corrections to q from the core-valence correlations and from Breit interaction. We found the former to be about 17% and the latter to be less than 1%. For lighter ions Breit interaction should be even smaller and can be safely neglected. Other ions also have much smaller and more rigid cores, so one might expect that core-valence correlations are few times weaker there in comparison to Zn. That allows us to neglect core-valence correlations for all other ions discussed in this paper.

Si II has the smallest core 1s2 . . . 2p 6 and three valence electrons. For neutral Mg, which has the same core, the core-valence corrections to the 3s → 3p transition frequencies were found to be about 4% [33, 36]. CI calculation for Si II is relatively simple and the errors associated with incompleteness of CI space are small. Thus, our estimate of the accuracy for Si on 6% level seems to be rather conservative.

Cr, Fe, and Ni have the core 1s2 . . . 3p6 and the core excitation energy varies from 2 a.u. for Cr II to 2.6 a.u. for Ni II. In comparison, the core excitation energy for Zn II is 0.9 a.u. Therefore, we estimate the core-valence correlation corrections for these ions to be at least two times smaller, than for Zn II.

Additional error here is associated with incomplete-ness of the CI space. These ions have from 5 to 9 valence electrons and CI space cannot be saturated. To estimate corresponding uncertainty we performed several calculations for each ion using diﬀerent basis sets and two different computer packages described in Sec. II. The basic Dirac-Hartree-Fock orbitals were calculated for diﬀerent configurations (for example, for the ground state configuration and for excited state configuration, etc.).

Supplementary information on the accuracy of our calculations can be obtained from comparison of calculated spectra and g-factors with experimental values. The later appear to be very important as they give information about electron coupling, which depends on relativistic corrections and on interaction between LS-multiplets. Our results for Cr II appear to be very close for different calculations and are in good agreement with the experiment both in terms of the gross level structure and spin-orbit splittings (see Table IV), so we estimate our final error here to be about 10 – 12%.

Allowing the deuteron binding energy, Q, to vary in BBN appears to provide a better fit to the observational light element abundance data. Varying Q simultaneously does two things; it resolves the internal inconsistency between 4He and the other light elements, and it also results in excellent independent agreement with the baryon to photon ratio determined from WMAP. (Fig. 5). However, the magnitude of the variation is sensitive primarily to the observed 4He abundance, which has the smallest relative statistical error. A systematic error in the abundance of 4He could imitate the eﬀect of the deuteron binding energy variation, although one needs a systematic error which is very much greater than has been claimed in the most recent observational work.

We note that Izotov and Thuan [25], the most recent estimate for Yp in our sample, argue that systematics are at most 0.6% for that survey. On the other hand, the possibility has also been explored that the creation of 4He in population III stars might mean that the true primordial 4He abundance is lower even than that seen in the most metal-poor objects [49]. If so, the significance of the deviation of δQ/Q from zero we report in this paper would be even larger.

These results hopefully provide an extremely strong motivation to obtain substantially better measurements of all the light elements, and to explore even more intensively, the possible sources of systematic errors.

Code:

FUNCTION PLJ(IA,IB)   
INCLUDE "cin.h"   
implicit real \*8 (a-h,o-z)   
common/nnn/ee(NVM),nnn(NVM), kk(NVM),ll(NVM),jj(NVM),nlist   
COMMON /JZ/JZ(NJZMAX) /NH/NH(NJZMAX)   
T=0.d0   
NA=NH(IA)   
NB=NH(IB)   
IF (NA.NE.NB) GOTO 1000   
MA=JZ(IA)   
MB=JZ(IB)   
IF (MA.NE.MB+2) GOTO 1000   
JA=JJ(NA)   
T=JA\*(JA+2)-MA\*MB   
T=dSQRT(T)   
1000 PLJ=T   
RETUN   
END   
c   
SUBROUTINE DETS(IC,N1,N2)   
INCLUDE "cin.h"   
COMMON /NDC/NDC(NCMAX)   
IF(IC.EQ.1)THEN   
N1=1   
N2=NDC(1)   
ELSE   
II=0   
DO I=1,IC-1   
II=II+NDC(I)   
END DO   
N1=II+1   
N2=II+NDC(IC)   
END IF   
RETURN   
END   
c   
SUBROUTINE FORMH   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
COMMON /NC/NC /NE/NE /NV/NV   
COMMON /NCJ/NCJ(NCMAX) /COEF/COEF(NCOEF)   
c COMMON/AAA/MAA,III(NSTJ),JJJ(NSTJ)/AAAA/AA(NSTJ)   
common /aline/al(NXX) /nline/nind(NXX) /diag/diag(NXX)   
REAL COEF   
logical iwl   
real \*8, allocatable :: a(:)   
integer, allocatable :: iii(:),jjj(:)   
INTEGER \*2 nind   
IF(NV.GT.NXX)THEN   
PRINT 1,NV,NXX   
--   
1 FORMAT('' Too big matrix: NV='', i5,'' NXX='',i5)   
STOP   
END IF   
NDCMAX=0   
DO IC=1,NC   
NDCMAX=MAX0(NDCMAX,NDC(IC))   
END DO   
c IF(NDCMAX.GT.NSTJ)THEN   
c PRINT 23,NCMAX,NSTJ   
c 23 FORMAT('' NDCMAX='',I5,'' greater then (than?) NSTJ='',I5)   
c STOP   
c END IF   
ndcm2=NDCMAX\*\*2   
allocate (aa(ndcm2),iii(ndcm2),jjj(ndcm2))   
if(allocated(aa).and.allocated(iii).and.allocated(jjj))then   
print \*,''OK''   
else   
stop ''allocation failed in FORMH''   
end if   
print \*, '' Calculation of H:''   
c open (11,file=''/erased\_at\_5am\_monday/dzuba/cin.buf'',   
c , status=''unknown'',form=''UNFORMATTED'')   
  
IND=0   
IVV=0   
c print \*,'' nv='',nv   
DO 10 IV=1,NV   
ICI=NCJ(IV)   
CALL DETS(ICI,NI1,NI2)   
call coretest(ni1,idc1)   
NDI=NI2-NI2+1   
JVV=0   
ICJ0=0   
ii=0   
DO 20 JV=1,IV   
c iwl=iv.eq.1.and.jv.eq.1   
ICJ=NCJ(JV)   
CALL DETS(ICJ,NJ1,NJ2)   
call coretest(nj1,idc2)   
c if(idc1.eq.1.and.idc2.eq.1.and.iv.ne.jv) go to 21   
c if(iv.gt.1.and.jv.gt.1.and.iv.ne.jv) go to 21   
IF(ICJ0.NE.ICJ)THEN   
CALL MATRCO(ICI,ICJ,NI1,NI2,NJ1,NJ2,   
, MAA,III(1),JJJ(1)AA(1))   
ICJ0=ICJ   
END IF   
NDJ=NJ2-NJ1+1   
T=0.   
IF(MAA.GT.0)THEN   
DO M=1,MAA   
T=T+COEF(IVV+III(M))\*COEF(JVV+JJJ(M))\*AA(M)   
END DO   
IND=IND+1   
ii=ii+1   
if(JV.EQ.IV)then   
AL(1)=T   
nind(1)=ii   
else   
AL(ii+1)=T   
nind(ii+1)=JV   
----   
end if   
c if(t.ne.0.d0)print 6,iv,jv,ici,icj,t   
c 6 format(''H:'',2i5,'' :'',2i5,f12.6)   
end if   
21 JVV=JVV+NDJ   
20 CONTINUE   
diag(iv)=T   
IF((IV/50)\*50+1.EQ.IV)PRINT 5,IV,NT,T   
5 FORMAT(''H:'',2I6,F12.6)   
call dumpline(IV,ii)   
11 IVV=IVV+NDI   
10 CONTINUE   
call flush(ind)   
IF(NV.LT.6)PRINT 22, (AL(I),I=1,NV\*(NV+1)/2)   
22 FORMAT(5E12.4)   
deallocate(aa,iii,jjj)   
RETURN   
END   
c   
subroutine coretest(id,ind)   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
dimension idet(128)   
common/nh/nh(njzmax) /ne/ne   
common/nnn/ee(NVM), nnn(NVM), kk(NVM), ll(NVM),jj(NVM),nlist   
call gdet(id,idet)   
ind=0   
do i=1,ne   
na=nh(idet(i))   
if(nnn(na).eq.3.and.ll(na).eq.1)ind=ind+1   
end do   
if(ind.ne.6)then   
ind=1   
else   
ind=0   
end if   
return   
end   
c   
subroutine flush(ind)   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
common/matrix/a(NBLOCK) /matind/indx(NBLOCK)   
common/block/last,nb /NV/NV /MJ/MJ /NE/NE /diag/diag(NXX)   
INTEGER \*2 indx   
if(last.gt.0)then   
write(11)(a(l),l=1,last)   
write(11)(indx(l),l=1,last)   
if(last.le.6)then   
print \*,''Matrix:''   
print 1, (indx(l),l=1,last)   
1 format(6i13)   
print 2, (a(l),l=1,last)   
2 format(6e13.5)   
end if   
nb=nb+1   
else   
last=NBLOCK   
end if   
close(11)   
open(12,file=''mat.par'',status=''UNKNOWN'' ,   
! form=''UNFORMATTED'')   
--   
pro=200.\*ind/(nv\*(nv+1))   
c print \*,'' nv='' ,nv   
c print \*,'' ind='' , ind   
c print \*,'' pro='' ,pro   
c print \*,'' nb='' ,nb   
c print \*,'' nblock='' , nblock   
c print \*,'' last='' , last   
print 11,nv,nv\*(nv+1)/2,ind,pro,nb,NBLOCK,last   
11 format(''Number of states '',i10/   
/ '' Total matrix size '', i10/   
/ '' Number of non-zeros '',i10/   
/ '' Non-zero fraction '',f10.2,''%''/   
/ '' Number of blocks '', i10/   
/ '' Block size: NBLOCK= '',i10, ''last='',i10)   
write(12)mj,ne,NBLOCK,nv,ind,nb,last   
write(12)(diag(l),l=1,NV)   
close(12)   
return   
end   
с   
subroutine dumpline(iv,ii)   
INCLUDE "cin.h"   
implicit real\*8 (a-h,o-z)   
common/aline/a1(NXX) /nline/nind(NXX) /block/last,nb   
common/matrix/a(NBLOCK) /matind/indx(NBLOCK)   
INTEGER \*2 nind,indx   
if(iv.eq.1)then   
last=0   
nb=0   
end if   
nind(1)=ii   
do i=1,ii   
last=last+1   
if(last.gt.NBLOCK)then   
nb=nb+1   
print 1,nb   
1 format(''Writing block #'',i3,''...'')   
write(11)(a(l),l=1,NBLOCK)   
write(11)(indx(l),l=1,NBLOCK)   
last=1   
end if   
a(last)=al(i)   
indx(last)=nind(i)   
end do   
return   
end

More of the computer code is here:

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/cin1.docx

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/code2.rar

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/code3.rar

**References and bibliography:**

1. J. C. Berengut, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A 68, 022502 (2003).
2. J. C. Berengut, V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A 69, 044102 (2004).
3. M. G. Kozlov, V. A. Korol, J. C. Berengut, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A 70, 062108 (2004).
4. J. C. Berengut, V. A. Dzuba, V. V. Flambaum, and M. V. Marchenko, Phys. Rev. A 70, 064101 (2004).
5. J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A 72, 044501 (2005).
6. J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A 73, 012504 (2006).
7. J. C. Berengut, V. A. Dzuba, V. V. Flambaum, M. G. Kozlov, M. V. Marchenko, M. T. Murphy, and J. K. Webb (2004), physics/0408017.
8. M. T. Murphy, Probing Variations in the Fundamental Constants with Quasar Absorption Lines, Ph.D. thesis, School of Physics, UNSW (2002).
9. J.-P. Uzan, Rev. Mod. Phys. 75, 403 (2003).
10. V. V. Flambaum and E. V. Shuryak, Phys. Rev. D 65, 103503 (2002).
11. V. F. Dmitriev and V. V. Flambaum, Phys. Rev. D 67, 063513 (2003).
12. V. V. Flambaum and E. V. Shuryak, Phys. Rev. D . 67, 083507 (2003).
13. V. F. Dmitriev, V. V. Flambaum, and J. K. Webb, Phys. Rev. D 69, 063506 (2004).
14. S. K. Lamoreaux and J. R. Torgerson, Phys. Rev. D 69, 121701 (2004).
15. M. T. Murphy, J. K. Webb, V. V. Flambaum, J. X. Prochaska, and A. M. Wolfe, Mon. Not. R. Astron. Soc. 327, 1237 (2001).
16. H. Chand, P. Petitjean, R. Srianand, and B. Aracil, Astron. Astrophys. 430, 47 (2005).
17. M. P. Savedo , Nature **178**, 689 (1956).
18. J. N. Bahcall, W. L. W. Sargent, and M. Schmidt, Astrophys. J. **149**, L11 (1967).
19. V. A. Dzuba, V. V. Flambaum, and J. K. Webb, Phys. Rev. Lett. **82**, 888 (1999).
20. V. A. Dzuba, V. V. Flambaum, and J. K. Webb, Phys. Rev. A **59**, 230 (1999).
21. J. K. Webb, V. V. Flambaum, C. W. Churchill, M. J. Drinkwater, and J. D. Barrow, Phys. Rev. Lett. **82**, 884 (1999).
22. M. T. Murphy, J. K. Webb, and V. V. Flambaum, Mon. Not. R. Astron. Soc. **345**, 609 (2003).
23. R. Quast, D. Reimers, and S. A. Levshakov, Astron. Astrophys. **415**, L7 (2004).
24. R. Srianand, H. Chand, P. Petitjean, and B. Aracil, Phys. Rev. Lett. **92**, 121302 (2004).
25. H. Chand, R. Srianand, P. Petitjean, and B. Aracil, Astron. Astrophys. **417**, 853 (2004).
26. S. A. Levshakov, M. Centurion, P. Molaro, and S. D'Odorico, Astron. Astrophys. **434**, 827 (2005).
27. C. L. Steinhardt, Phys. Rev. D **71**, 043509 (2005).
28. J. K. Webb, M. T. Murphy, V. V. Flambaum, and S. J. Curran, Astrophys. Space Sci. **283**, 565 (2003).
29. M. T. Murphy, J. K. Webb, V. V. Flambaum, C. W. Churchill, and J. X. Prochaska, Mon. Not. R. Astron. Soc. **327**, 1223 (2001).
30. M. T. Murphy, J. K. Webb, V. V. Flambaum, and S. J. Curran, Astrophys. Space Sci. **283**, 577 (2003).
31. R. L. Kurucz, Phys. Scr. **T47**, 110 (2004).
32. K. Heilig and A. Steudel, At. Data Nucl. Data Tables **14**, 613 (1974).
33. P. Aufmuth, K. Heilig, and A. Steudel, At. Data Nucl. Data Tables **37**, 455 (1987).
34. T. P. Ashenfelter, G. J. Mathews, and K. A. Olive, Phys. Rev. Lett. **92**, 041102 (2004).
35. T. P. Ashenfelter, G. J. Mathews, and K. A. Olive, Astrophys. J. **615**, 82 (2004).
36. Y. Fenner, M. T. Murphy, and B. K. Gibson, Mon. Not. R. Astron. Soc. **358**, 468 (2005).
37. Y. B. Zeldovich and I. D. Novikov, Sov. Astron. **10**, 602 (1966).

1. J. D. Bekenstein and V. F. Mukhanov, Phys. Lett. B **360**, 7 (1995).
2. J. D. Bekenstein, Nuovo Cimento Lettere **11**, 467 (1974).
3. I. B. Kriplovich, Phys. Lett. B **431**, 19 (1998).
4. S. W. Hawking, Nature **248**, 30 (1974).
5. E. M. Drobyshevski, Astron. Astrophys. Trans. **21**, 65 (2002).
6. E. M. Drobyshevski, M. E. Drobyshevski, T. Y. Izmodenova, and D. S. Telnov, Astron. Astrophys. Trans. **22**, 263 (2003).
7. E. M. Drobyshevski (2004), astro-ph/0402367.
8. S. Hawking, Mon. Not. R. Astron. Soc. **152**, 75 (1971).
9. V. V. Flambaum and J. C. Berengut, Phys. Rev. D **63**, 084010 (2001).
10. P. Mueller, L.-B.Wang, R. J. Holt, Z.-T. Lu, T. P. O'Connor, and J. P. Schi er, Phys. Rev. Lett. **92**, 022501 (2004).
11. Z.-T. Lu, R. J. Holt, P. Mueller, T. P. O'Connor, J. P. Schi er, and L.-B. Wang, Nucl. Phys. A **754**, 361 (2005).
12. H. A. Bethe and E. E. Salpeter, **Quantum Mechanics of One- and Two-Electron** **Atoms** (Academic Press, New York, 1957).
13. I. I. Sobel'man, **Introduction to the Theory of Atomic Spectra** (Pergamon, New York, 1972).
14. I. Lindgren and J. Morrison, **Atomic Many-Body Theory** (Springer-Verlag, New York, 1986).
15. V. A. Dzuba, V. V. Flambaum, M. G. Kozlov, and M. Marchenko, Phys. Rev. A **66**, 022501 (2002).
16. V. A. Dzuba, V. V. Flambaum, M. T. Murphy, and J. K. Webb, Phys. Rev. A **63**, 042509 (2001).
17. W. H. King, **Isotope Shifts in Atomic Spectra** (Plenum Press, New York, 1984).
18. L. D. Landau and E. M. Lifshitz, **Quantum Mechanics Non-Relativistic Theory**, volume 3 of **Course of Theoretical Physics** (Pergamon, New York, 1977), third edition.
19. V. M. Shabaev, Phys. Rev. A **57**, 59 (1998).
20. W. H. King, J. Opt. Soc. Am. **53**, 638 (1963).
21. D. S. Hughes and C. Eckart, Phys. Rev. **36**, 694 (1930).
22. J. P. Vinti, Phys. Rev. **56**, 1120 (1939).

1. J. Bauche and R.-J. Champeau, Adv. Atom. Mol. Phys. **12**, 39 (1976).
2. A.-M. Martensson and S. Salomonson, J. Phys. B **15**, 2115 (1982).
3. E. Lindroth and A.-M. Martensson-Pendrill, Z. Phys. A **309**, 277 (1983).

•

[63] S. H•orb•ack, A.-M. Martensson-Pendrill, S. Salomonson, and U. Osterberg, Phys. Scr. **28**, 469 (1983).

[64] S. H•orb•ack, A.-M. Pendrill, L. Pendrill, and M. Pettersson, Z. Phys. A **318**, 285 (1984).

[65] E. Lindroth, A.-M. Martensson-Pendrill, and S. Salomonson, Phys. Rev. A **31**, 58 (1985).

[66] A. C. Hartley and A.-M. Martensson-Pendrill, J. Phys. B **24**, 1193 (1991).

[67] A.-M. Martensson-Pendrill, A. Ynnerman, and H. Warston, Phys. Rev. A **45**, 4675 (1992).

[68] A.-M. Martensson-Pendrill and A. Ynnerman, J. Phys. B **25**, L551 (1992).

[69] A.-M. Martensson-Pendrill, D. S. Gough, and P. Hannaford, Phys. Rev. A **49**, 3351 (1994).

[70] L. Veseth, J. Phys. B **18**, 3463 (1985).

[71] L. Veseth, J. Phys. B **20**, 235 (1987).

[72] M. S. Safronova and W. R. Johnson, Phys. Rev. A **64**, 052501 (2001). [73] C. W. Clark, Opt. Lett. **8**, 572 (1983).

[74] C. W. Clark, Astrophys. J. **285**, 322 (1984).

[75] A. Aspect, J. Bauche, M. Godefroid, P. Grangier, J. E. Hansen, and N. Vaeck, J. Phys. B **24**, 4077 (1991).

[76] P. J•onsson and C. Froese Fischer, Phys. Rev. A **50**, 3080 (1994).

[77] J. Carlsson, P. J•onsson, M. R. Godefroid, and C. Froese Fischer, J. Phys. B **28**, 3729 (1995).

[78] P. J•onsson, C. Froese Fischer, and M. R. Godefroid, J. Phys. B **29**, 2393 (1996). [79] P. J•onsson, C. Froese Fischer, and M. R. Godefroid, J. Phys. B **32**, 1233 (1999). [80] M. Godefroid, C. Froese Fischer, and P. J•onsson, J. Phys. B **34**, 1079 (2001).

[81] M. R. Godefroid, C. Froese Fischer, and P. J•onsson, Phys. Scr. **T65**, 70 (1996). [82] M. Godefroid and C. Froese Fischer, Phys. Rev. A **60**, R2637 (1999).

[83] P. J•onsson and M. Godefroid, Mol. Phys. **98**, 1141 (2000).

1. C. Froese Fischer, P. J•onsson, and M. Godefroid, Phys. Rev. A **57**, 1753 (1998).
2. F. W. King, Phys. Rev. A **40**, 1735 (1989).
3. Z.-W. Wang, X.-W. Zhu, and K. T. Chung, Phys. Scr. **47**, 65 (1993).
4. V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).
5. E. M. Lifshitz, L. P. Pitaevskii, and V. B. Berestetskii, **Quantum Electrodynamics**, volume 4 of **Course of Theoretical Physics** (Pergamon, Oxford, 1982), second edition.
6. W. R. Johnson and J. Sapirstein, Phys. Rev. Lett. **57**, 1126 (1986).
7. W. R. Johnson, M. Idrees, and J. Sapirstein, Phys. Rev. A **35**, 3218 (1987).
8. W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A . **37**, 307 (1988).
9. J. Sapirstein and W. R. Johnson, J. Phys. B **29**, 5213 (1996).
10. W. R. Johnson, **Lectures on Atomic Physics** (1994), publicly available from W. R. Johnson's website: http://www.nd.edu/~johnson/.
11. V. A. Dzuba and W. R. Johnson, Phys. Rev. A **57**, 2459 (1998).

[95] P. Bogdanovich and G. Zukauskas, Sov. Phys. Collection **23**, 18 (1983).

[96] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. Sushkov, J. Phys. B **20**, 1399 (1987).

[97] M. G. Kozlov and S. G. Porsev, Opt. Spectrosc. **87**, 352 (1999).

[98] C. E. Moore, **Atomic Energy Levels - v. I,II, NSRDS-NBS 35** (U. S. Government Printing O ce, Washington D.C., 1971).

[99] V. A. Dzuba, O. P. Sushkov, W. R. Johnson, and U. I. Safronova, Phys. Rev. A **66**, 032105 (2002).

[100] V. A. Dzuba, U. I. Safronova, and W. R. Johnson, Phys. Rev. A **68**, 032503 (2003).

[101] J. E. Hansen, A. Steudel, and H. Walther, Phys. Lett. **19**, 565 (1965).

[102] P. Villemoes, F. A. Arnesen, Heijkenskj•old, and A. W•annstr•om, J. Phys. B **26**, 4289 (1993).

[103] X. Zhao, N. Yu, H. Dehmelt, and W. Nagourney, Phys. Rev. A **51**, 4483 (1995).

[104] K. Wendt, S. A. Ahmad, F. Buchinger, A. C. Mueller, R. Neugart, and E.-W. Otten, Z. Phys. A **318**, 125 (1984).

[105] K. Wendt, S. A. Ahmad, C. Ekstrom, W. Klempt, R. Neugart, and E.-W. Otten, Z. Phys. A **329**, 407 (1988).

1. K. Pescht, H. Gerhardt, and E. Matthias, Z. Phys. A **281**, 199 (1977).
2. G. Huber, F. Touchard, S. B•uttgenbach, C. Thibault, R. Klapisch, H. T. Duong,
   1. Liberman, J. Pinard, J. L. Vialle, P. Juncar, and P. Jacquinot, Phys. Rev. C **18**, 2342 (1978).
3. Y. P. Gangrsky, D. V. Karaivanov, K. P. Marinova, B. N. Markov, L. M. Mel-nikova, G. V. Mishinsky, S. G. Zemlyanoi, and V. I. Zhemenik, Eur. Phys. J. A **3**, 313 (1998).
4. R. E. Drullinger, D. Wineland, and J. C. Bergquist, Appl. Phys. **22**, 365 (1980).
5. F. Touchard, P. Guimbal, S. B•uttgenbach, R. Klapisch, M. D. S. Simon, J. M. Serre, C. Thibault, H. T. Duong, P. Juncar, S. Liberman, J. Pinard, and J. L. Vialle, Phys. Lett. B **108**, 169 (1982).
6. F. Kurth, T. Gudjons, B. Hilbert, T. Reisinger, G. Werth, and A.-M. Martensson-Pendrill, Z. Phys. D **34**, 227 (1995).
7. S. Maleki and A. T. Goble, Phys. Rev. A **45**, 524 (1992).
8. W. N•ortersh•auser, K. Blaum, K. Icker, P. M•uller, A. Schmitt, K. Wendt, and
   1. Wiche, Eur. Phys. J. D **2**, 33 (1998).
9. H. D. Wohlfahrt, E. B. Shera, M. V. Hoehn, Y. Yamazaki, and R. M. Ste en, Phys. Rev. C **23**, 533 (1981).
10. C. W. P. Palmer, P. E. G, Baird, S. A. Blundell, and J. R. Brandenberger, J. Phys. B **17**, 2197 (1984).
11. K. Matsubara, U. Tanaka, H. Imajo, S. Urabe, and M. Watanabe, Appl. Phys. B **76**, 209 (2002).
12. U. Sterr, K. Sengstock, J. H. M•uller, and W. Ertmer, Appl. Phys. B **56**, 62 (1993).
13. L. Hallstadius, Z. Phys. A **291**, 203 (1979).
14. S. L. Boiteux, A. Klein, J. R. R. Leite, and M. Ducloy, J. Phys. (France) **49**, 885 (1988).
15. L. Hallstadius and J. E. Hansen, Z. Phys. A **285**, 365 (1978).
16. C. Novero, A. Godone, and G. M. Tino, Nuovo Cimento D **14**, 955 (1992).
17. R. A. Bernheim and C. Kittrell, Spectrochim. Acta B **35**, 51 (1980).
18. C. R. Burnett, Phys. Rev. **80**, 494 (1950).
19. J. R. Holmes, J. Opt. Soc. Am. **41**, 360 (1951).
20. J. K. Webb, M. T. Murphy, V. V. Flambaum, V. A. Dzuba, J. D. Barrow, C. W. Churchill, J. X. Prochaska, and A. M. Wolfe, Phys. Rev. Lett. **87**, 091301 (2001).

1. M. T. Murphy, J. K. Webb, V. V. Flambaum, V. A. Dzuba, C. W. Churchill, J. X. Prochaska, J. D. Barrow, and A. M. Wolfe, Mon. Not. R. Astron. Soc. **327**, 1208 (2001).
2. D. C. Morton, Astrophys. J. Suppl. Ser. **77**, 119 (1991).
3. D. C. Morton, Astrophys. J. Suppl. Ser. **149**, 205 (2003).
4. I. Labazan, E. Reinhold, W. Ubachs, and V. V. Flambaum, Phys. Rev. A **71**, 040501 (2005).
5. U. Griesmann and R. Kling, Astrophys. J. **536**, L113 (2000).
6. P. Juncar, J. Pinard, J. Hamon, and A. Chartier, Metrologia **17**, 77 (1981).
7. M. Aldenius, S. Johansson, and M. T. Murphy, submitted to Mon. Not. R. Astron. Soc. (2006).
8. J. C. Pickering, A. P. Thorne, and J. K. Webb, Mon. Not. R. Astron. Soc. **300**, 131 (1998).
9. J. C. Pickering, A. P. Thorne, J. E. Murray, U. Litzen, S. Johansson, V. Zilio, and J. K. Webb, Mon. Not. R. Astron. Soc. **319**, 163 (2000).
10. J. C. Pickering, M. P. Donnelly, H. Nilsson, A. Hibbert, and S. Johansson, Astron. Astrophys. **396**, 715 (2002).
11. G. Nave, R. C. M. Learner, A. P. Thorne, and C. J. Harris, J. Opt. Soc. Am. B **8**, 2028 (1991).
12. V. F. Bratsev, G. B. Deyneka, and I. I. Tupitsyn, Bull. Acad. Sci. USSR, Phys. Ser. (Engl. Transl.) **41**, 173 (1977).
13. S. A. Kotochigova and I. I. Tupizin, J. Phys. B **20**, 4759 (1987).
14. E. R. Davidson, J. Comput. Phys. **17**, 87 (1975).
15. A. Stathopoulos and C. F. Fischer, Comput. Phys. Commun. **79**, 268 (1994).

[5.141] PhD thesis of Julian Berengut. UNSW University Press. Sydney. Australia. 2006.

[8.142] Y.V. Stadnik and V.V. Flambaum. Searching for dark matter and variation of fundamental constants with laser and maser interferometry. March 2015.

[8.143] Dirac, P. A. M. The Cosmological Constants. Nature

(London) 139, 323-323 (1937).

[8.144] H. Terazawa, Cosmological Origin of Mass Scales.

Phys. Lett. B 101, 43 (1981).

[8.145] Uzan, J.-P. The fundamental constants and their

variation: observational and theoretical status.

Rev. Mod. Phys. 75, 403 (2003).

[8.146] Calmet, X. and Fritzsch, H. The cosmological evolution

of the nucleon mass and the electroweak coupling con-

stants. Eur. Phys. J. C 24, 639 (2002).

[8.147] Webb, J. K. et. al. Indications of a Spatial Variation

of the Fine Structure Constant. Phys. Rev. Lett. 107,

191101 (2011).

[8.148] King, J. A. et. al. Spatial variation in the \_ne-structure

constant - new results from VLT/UVES. MNRAS 422,

3370 (2012).

[8.149] Webb, J. K., Flambaum, V. V., Churchill, C. W.,

Drinkwater, M. J. & Barrow, J. D. Search for time vari-

ation of the \_ne structure constant. Phys. Rev. Lett. 82,

884-887 (1999).

[8.150] Murphy, M. T., Webb, J. K. & Flambaum, V. V. Fur-

ther evidence for a variable \_ne structure constant from

Keck/HIRES QSO absorption spectra. MNRAS 345, 609

(2003).

[8.151] Berengut, J. C. & Flambaum, V. V. Manifestations of

a spatial variation of fundamental constants in atomic

and nuclear clocks, Oklo, meteorites, and cosmological

phenomena. Europhys. Lett. 97, 20006 (2012).

[8.152] Rosenband, T. et. al. Frequency Ratio of Al+ and Hg+

Single-Ion Optical Clocks; Metrology at the 17th Decimal Place. Science 319, 1808-1812 (2008).

[8.153] Bertone, G. (Ed.) Particle Dark Matter: Observations,

Models and Searches. (Cambridge University Press, Cam-

bridge, 2010).

[8.154] Peccei, R. D. & Quinn, H. R. CP Conservation in the

Presence of Pseudoparticles. Phys. Rev. Lett. 38, 1440

(1977).

[8.155] Peccei, R. D. & Quinn, H. R. Constraints imposed

by CP conservation in the presence of pseudoparticles. Phys. Rev. D 16, 1791 (1977).

[8.156] J. E. Kim, Weak-Interaction Singlet and Strong CP In-

variance. Phys. Rev. Lett. 43, 103 (1979).

[8.157] M. A. Shifman, A. I. Vainshtein, and V. I. Zakharov,

Can con\_nement ensure natural CP invariance of strong

interactions? Nucl. Phys. B 166, 493 (1980).

[8.158] A. R. Zhitnitsky, The Weinberg Model Of The CP

Violation And T Odd Correlations In Weak Decays.

Yad. Fiz. 31, 1024 (1980) [Sov. J. Nucl. Phys. 31, 529

(1980)].

[8.159] M. Dine, W. Fischler, and M. Srednicki, A simple solu-

tion to the strong CP problem with a harmless axion.

Phys. Lett. B 104, 199 (1981).

[8.160] Sikivie, P. & Yang, Q. Bose-Einstein Condensation of

Dark Matter Axions. Phys. Rev. Lett. 103, 111301

(2009).

[8.161] P. Sikivie, Experimental Tests of the "Invisible" Axion.

Phys. Rev. Lett. 51, 1415 (1983).

[8.262] Asztalos, S. J. et. al. SQUID-Based Microwave Cavity

Search for Dark-Matter Axions. Phys. Rev. Lett. 104,

041301 (2010).

[8.163] P. W. Graham and S. Rajendran, Axion dark matter

detection with cold molecules. Phys. Rev. D 84, 055013

(2011).

[8.164] P. W. Graham and S. Rajendran, New observables for

direct detection of axion dark matter. Phys. Rev. D 88,

035023 (2013).

[8.165] Stadnik, Y. V. & Flambaum, V. V. Axion-induced ef-

fects in atoms, molecules, and nuclei: Parity noncon-

servation, anapole moments, electric dipole moments,

and spin-gravity and spin-axion momentum couplings.

Phys. Rev. D 89, 043522 (2014).

[8.166] Budker, D., Graham, P. W., Ledbetter, M., Rajen-

dran, S. & Sushkov, A. O. Proposal for a Cosmic Axion

Spin Precession Experiment (CASPEr). Phys. Rev. X 4,

021030 (2014).

[8.167] B. M. Roberts, Y. V. Stadnik, V. A. Dzuba, V. V. Flam-

baum, N. Leefer, and D. Budker. Limiting P-Odd Inter-

actions of Cosmic Fields with Electrons, Protons, and Neutrons. Phys. Rev. Lett. 113, 081601 (2014).

[8.168] B. M. Roberts, Y. V. Stadnik, V. A. Dzuba, V. V. Flam-

baum, N. Leefer, and D. Budker. Parity-violating inter-

actions of cosmic \_elds with atoms, molecules, and nu-

clei: Concepts and calculations for laboratory searches

and extracting limits. Phys. Rev. D 90, 096005 (2014).

[8.169] Derevianko, A. & Pospelov, M. Hunting for topological

dark matter with atomic clocks. Nature Physics 10, 933-

936 (2014).

[8.170] Olive, K. A. & Pospelov, M. Environmental dependence

of masses and coupling constants. Phys. Rev. D 77,

043524 (2008).

[8.171] Vilenkin, A. Cosmic strings and domain walls.

Phys. Rep. 121, 263-315 (1985).

[8.172] D. J. E. Marsh and A.-R. Pop, Axion dark matter, soli-

tons, and the cusp-core problem. arXiv:1502.03456.

[8.173] Pospelov, M. et. al. Detecting domain walls of

axionlike models using terrestrial experiments.

Phys. Rev. Lett. 110, 021803 (2013).

[8.174] Stadnik, Y. V. & Flambaum, V. V. Searching for Topo-

logical Defect Dark Matter via Nongravitational Signa-

tures. Phys. Rev. Lett. 113, 151301 (2014).

[8.175] Hinkley, N. et. al. An Atomic Clock with 1018 Instability.

Science 341, 1215-1218 (2013).

[8.176] Bloom, B. J. et. al. An optical lattice clock with accuracy

and stability at the 1018 level. Nature (London) 506, 71-

75 (2014).

[8.177] Je\_erts, S. R. Atomic Clocks: Primary Frequency Stan-

dards at NIST (8th Annual DOE Laser Safety O\_cer

Workshop, Menlo Park, 2013).

[8.178] Kosteleck\_y, V. A. & Russell, N. Data tables for Lorentz

and CPT violation. Rev. Mod. Phys. 83, 11 (2011).

[8.179] Massimo, B. (Ed.) Advanced Interferometers and the

Search for Gravitational Waves: Lectures from the First

VESF School on Advanced Detectors for Gravitational

Waves. (Springer, Cham, 2014).

[8.180] A. Arvanitaki, J. Huang, and K. Van Tilburg, Searching

for dilaton dark matter with atomic clocks. Phys. Rev. D

91, 015015 (2015).

[8.181] D. Meiser, J. Ye, D. R. Carlson, and M. J. Hol-

land, Prospects for a Millihertz-Linewidth Laser.

Phys. Rev. Lett. 102, 163601 (2009).

[8.182] J. G. Bohnet, Z. Chen, J. M. Weiner, D. Meiser,

M. J. Holland and J. K. Thompson. A steady-state su-

perradiant laser with less than one intracavity photon.

Nature (London) 484, 78 (2012).

[8.183] J. G. Bohnet, Z. Chen, J. M. Weiner, K. C. Cox,

and J. K. Thompson. Relaxation Oscillations, Stability,

and Cavity Feedback in a Superradiant Raman Laser.

Phys. Rev. Lett. 109, 253602 (2012).

[8.184] V. V. Flambaum and A. F. Tedesco, Dependence of nu-

clear magnetic moments on quark masses and limits on

temporal variation of fundamental constants from atomic

clock experiments. Phys. Rev. C 73, 055501 (2006).

[8.185] V. A. Dzuba, V. V. Flambaum, and J. K. Webb,

Calculations of the relativistic e\_ects in many-electron

atoms and space-time variation of fundamental con-

stants. Phys. Rev. A 59, 230 (1999).

[8.186] T. H. Dinh, A. Dunning, V. A. Dzuba, and V. V. Flam-

baum, The sensitivity of hyper\_ne structure to nuclear

radius and quark mass variation. Phys. Rev. A 79, 054102

(2009).

[8.187] Godun, R. M. et. al. Frequency Ratio of Two Op-

tical Clock Transitions in 171Yb+ and Constraints on the Time Variation of Fundamental Constants.

Phys. Rev. Lett. 113, 210801 (2014).

[8.188] Huntemann, N. et. al. Improved Limit on a Temporal

Variation of mp=me from Comparisons of Yb+ and Cs

Atomic Clocks. Phys. Rev. Lett. 113, 210802 (2014).

[8.189] Reinhold, E. et. al. Indication of a Cosmological Varia-

tion of the Proton-Electron Mass Ratio Based on Lab-

oratory Measurement and Reanalysis of H2 Spectra.

Phys. Rev. Lett. 96, 151101 (2006).

[8.190] Dzuba, V. A., Flambaum, V. V. & Webb, J. K. Space-

Time Variation of Physical Constants and Relativistic

Corrections in Atoms. Phys. Rev. Lett. 82, 888 (1999).

[8.191] NIST, Computational Chemistry Comparison and

Benchmark DataBase, http://cccbdb.nist.gov/

default.htm

[8.192] TAMA Collaboration, Observation results by the

TAMA300 detector on gravitational wave bursts from

stellar-core collapses. Phys. Rev. D 71, 082002 (2005).

[8.193] Ligo Scienti\_c Collaboration and Virgo Collaboration,

Sensitivity Achieved by the LIGO and Virgo Gravita-

tional Wave Detectors during LIGO's Sixth and Virgo's

Second and Third Science Runs. arXiv:1203.2674.

[8.194] K. L. Dooley, Status of GEO600. arXiv:1411.6588.

[8.195] A. Chou et. al. The Fermilab Holometer: A program to

measure Planck scale indeterminacy, Fermilab publica-

tion, 2009.

[1.111] http://fy.chalmers.se/~f3ail/Publications/BoundQED.pdf

[201] Michael Murphy. PhD Thesis. 2002.

[202] Abgrall H., Roue® E., Launay F., Roncin J. Y., Subtil J. L., 1993a, A&AS, 101, 273

[203] Abgrall H., Roue® E., Launay F., Roncin J. Y., Subtil J. L., 1993b, A&AS, 101, 323

[204] Albrecht A., Magueijo J., 1999, Phys. Rev. D, 59, 043516

[205] Andrews S. M., Meyer D. M., Lauroesch J. T., 2001, ApJ, 552, L73

[206] Antoniadis I., Arkani-Hamed N., Dimopoulos S., Dvali G., 1998, Phys. Lett. B, 436,

257

[207] Arkani-Hamed N., Dimopoulos S., Dvali G., 1998, Phys. Lett. B, 429, 263

[208] Avelino P. P. et al., 2001, Phys. Rev. D, 64, 103505

[209] Bahcall J. N., Salpeter E. E., 1965, ApJ, 142, 1677

[210] Bahcall J. N., Sargent W. L. W., Schmidt M., 1967, ApJ, 149, L11

D., 1987, Phys. Rev. D, 35, 1805

[211] Barrow J. D., 1990, in Bertotti B., Balbinot R., Bergia S., Messina A., eds, Modern

Cosmology in Retrospect. Cambridge Univ. Press, Cambridge, UK, p. 67

[212] Barrow J. D., 1996, MNRAS, 282, 1397

[213] Barrow J. D., 1999, Phys. Rev. D, 59, 043515

[214] Barrow J. D., 2002, From Alpha to Omega: The Constants of Nature. Jonathan

Cape, London, UK

[215] Barrow J. D., Magueijo J., 1998, Phys. Lett. B, 443, 104

[216] Barrow J. D., Magueijo J., 1999a, Phys. Lett. B, 447, 246

[217] Barrow J. D., Magueijo J., 1999b, Classical Quantum Gravity, 16, 1435

[218] Barrow J. D., Magueijo J., 2000, ApJ, 532, L87

182 References

[219] Barrow J. D., O'Toole C., 2001, MNRAS, 322, 585

[221] Barrow J. D., Tipler F. J., 1986, The anthropic cosmological principle. Clarendon

Press, Oxford, UK

[222] Battye R. A., Crittenden R., Weller J., 2001, Phys. Rev. D, 63, 043505

[223] Bekenstein J. D., 1979, Comments on Astrophys., 8, 89

[224] Bekenstein J. D., 1982, Phys. Rev. D, 25, 1527

[225] Bennett C. L. et al. 1996, ApJ, 464, L1

[226] BergstrÄom L., Iguri S., Rubinstein H., 1999, Phys. Rev. D, 60, 045005

[227] Bethe H. A., Salpeter E. E., 1977, Quantum mechanics of one- and two-electron

atoms. Plenum, New York, NY, USA

[228] Biggs A. D., Browne I. W. A., Wilkinson P. N., 2001, MNRAS, 323, 995

[229] Black J. H., Cha®ee F. H., Foltz C. B., 1987, ApJ, 317, 442

[230] Brans C., Dicke R. H., 1961, Phys. Rev., 124, 924

[231] Briggs F. H., Wolfe A. M., Turnshek D. A., Schae®er J., 1985, ApJ, 293, 387

[232] Browne I. W. A., Patnaik A. R., Walsh D., Wilkinson P. N., 1993, MNRAS, 263,

L32

[233] Burbidge E. M., Lynds C. R., Burbidge G. R., 1966, ApJ, 144, 447

Cahn R. N., 1996, Rev. Mod. Phys., 68, 951

Calmet X., Fritzsch H., 2002, Euro. Phys. J. C, 24, 639

Campbell B. A., Olive K. A., 1995, Phys. Lett. B, 345, 429

Carilli C. L., Menten K. M., Reid M. J., Rupen M. P., 1997, ApJ, 474, L89

Carilli C. L., Menten K. M., Reid M. J., Rupen M. P., Yun M. S., 1998, ApJ, 494,

175

Carilli C. L. et al., 2000, Phys. Rev. Lett., 85, 5511 (C00)

Carilli C. L., Perlman E. S., Stocke J. T., 1992, ApJ, 400, L13

Carilli C. L., Rupen M. P., Yanny B., 1993, ApJ, 412, L59

Chamoun N., Landau S. J., Vucetich H., 2001, Phys. Lett. B, 504, 1

References 183

Chandrasekhar S., 1939, Nat, 139, 757

Chen H., Lanzetta K. M., Webb J. K., Barcons X., 1998, ApJ, 498, 77

Chodos A., Detweiler S., 1980, Phys. Rev. D, 21, 2167

Churchill C. W., Le Brun V., 1998, ApJ, 499, 677

Churchill C. W., Mellon R. R., Charlton J. C., Jannuzi B. T., Kirhakos S., Steidel

C. C., Schneider D. P., 2000a, ApJS, 130, 91

Churchill C. W., Mellon R. R., Charlton J. C., Jannuzi B. T., Kirhakos S., Steidel

C. C., Schneider D. P., 2000b, ApJ, 543, 577

Churchill C. W. et al., 2003a, in preparation

Churchill C. W., Mellon R. R., Charlton J. C., Vogt S. S., 2003b, ApJ, submitted,

preprint (astro-ph/0212120)

Churchill C. W., Vogt S. S., 2001, AJ, 122, 679

Clayton M. A., Mo®at J. W., 1999, Phys. Lett. B, 460, 263

Clayton M. A., Mo®at J. W., 2000, Phys. Lett. B, 477, 269

Clayton M. A., Mo®at J. W., 2001, Phys. Lett. B, 506, 177

Combes F., Wiklind T., 1995, A&A, 303, L61

Cowie L. L., Songaila A., 1995, ApJ, 453, 596

Cowie L. L., Songaila A., Kim T., Hu E. M., 1995, AJ, 109, 1522

Crawford I. A., Howarth I. D., Ryder S. D., Stathakis R. A., 2000, MNRAS, 319,

L1

Curran S. J., Murphy M. T., Webb J. K., PihlstrÄom Y. M., 2003, MNRAS, 340, 139

Curran S. J., Murphy M. T., Webb J. K., RantakyrÄo F., Johansson L. E. B., Nikoli¶c

S., 2002a, A&A, 394, 763

Curran S. J., Webb J. K., Murphy M. T., Bandiera R., Corbelli E., Flambaum

V. V., 2002b, Publ. Astron. Soc. Austral., 19, 455

Curran S. J., Webb J. K., Murphy M. T., Carswell R. F., 2003b, in preparation

Damour T., Dyson F., 1996, Nucl. Phys. B, 480, 37

Damour T., Polyakov A. M., 1994, Nucl. Phys. B, 423, 532

184 References

Dav¶e R., Hernquist L., Katz N., Weinberg D. H., 1999, ApJ, 511, 521

Dent T., Fairbairn M., 2003, Nucl. Phys. B, 653, 256

Dicke R. H., 1957, Rev. Mod. Phys., 29, 355

Dicke R. H., 1961, Nat, 192, 440

Dicke R. H., 1962, Phys. Rev., 125, 2163

Dirac P. A. M., 1937, Nat, 139, 323

Drinkwater M. J., Webb J. K., Barrow J. D., Flambaum V. V., 1998, MNRAS, 295,

457 (D98)

Drullinger R. E., Wineland D. J., Bergquist J. C., 1980, Appl. Phys., 22, 365

Du® M. J., Okun L. B., Veneziano G., 2002, J. High Energy Phys., 2002, 023

Dyson F. J., 1967, Phys. Rev. Lett., 19, 1291

Dyson F. J., 1972, in Salam A., Wigner E. P., eds, Aspects of Quantum Theory.

Cambridge Univ. Press, Cambridge, UK, p. 213

Dzuba V. A., Flambaum V. V., Kozlov M. G., Marchenko M., 2002, Phys. Rev. A,

66, 022501

Dzuba V. A., Flambaum V. V., Murphy M. T., Webb J. K., 2001a, in Karshenboim

S. G., Pavone F. S., Bassani G. F., Inguscio M., HÄansch T. W., eds, Lecture

Notes in Physics Vol. 570, The Hydrogen Atom: Precision Physics of Simple

Atomic Systems. Springer-Verlag, Berlin, Germany, p. 564

Dzuba V. A., Flambaum V. V., Murphy M. T., Webb J. K., 2001b, Phys. Rev. A,

63, 42509

Dzuba V. A., Flambaum V. V., Webb J. K., 1999a, Phys. Rev. A, 59, 230

Dzuba V. A., Flambaum V. V., Webb J. K., 1999b, Phys. Rev. Lett., 82, 888

Edlen B., 1953, J. Opt. Soc. Am., 43, 339

Edlen B., 1966, Metrologia, 2, 71

Essen L., Donaldson R. W., Bangham M. J., Hope E. G., 1971, Nat, 229, 110

Feretti L., Dallacasa D., Govoni F., Giovannini G., Taylor G. B., Klein U., 1999,

A&A, 344, 472

References 185

Fernandez-Soto A., Lanzetta K. M., Barcons X., Carswell R. F., Webb J. K., Yahil

A., 1996, ApJ, 460, L85

Filippenko A. V., 1982, PASP, 94, 715

Finn G. D., Mugglestone D., 1965, MNRAS, 129, 221

Fisher R. A., 1958, Statistical Methods for Research Workers. Harper, New York,

NY, USA

Flambaum V. V., Shuryak E. V., 2002, Phys. Rev. D, 65, 103503

Flowers J. L., Petley B. W., 2001, Rep. Prog. Phys., 64, 1191

Foltz C. B., Cha®ee F. H., Black J. H., 1988, ApJ, 324, 267

Forg¶acs P., Horv¶ath Z., 1979, Gen. Relativ. Gravitation, 11, 205

Freund P. G. O., 1982, Nucl. Phys. B, 209, 146

Fujii Y., Iwamoto A., Fukahori T., Ohnuki T., Nakagawa M., Hidaka H., Oura Y.,

MÄoller P., 2000, Nucl. Phys. B, 573, 377

Gaillard M. K., Grannis P. D., Sciulli F. J., 1999, Rev. Mod. Phys., 71, 96

Gamow G., 1967, Phys. Rev. Lett., 19, 913

Gay P. L., Lambert D. L., 2000, ApJ, 533, 260

Ge J., Bechtold J., 1997, ApJ, 477, L73

Ge J., Bechtold J., 1999, in Carilli C. L., Radford S. J. E., Menten K. M., Langstom

G. I., eds, ASP Conf. Ser. Vol. 156, Highly Redshifted Radio Lines. Astron. Soc.

Pac., San Francisco, CA, U.S.A, p. 121

Ge J., Bechtold J., Kulkarni V. P., 2001, ApJ, 547, L1

Gill P. E., Murray W., Wright M. H., 1981, Practical optimization. Academic Press,

London, UK

Griesmann U., Kling R., 2000, ApJ, 536, L113

Gunn J. E., Peterson B. A., 1965, ApJ, 142, 1633

Haehnelt M. G., Steinmetz M., Rauch M., 1998, ApJ, 495, 647

Haldane J. B. S., 1937a, Nat, 139, 1002

Haldane J. B. S., 1937b, Nat, 158, 555

186 References

Hallstadius L., 1979, Z. Phys. A, 291, 203

Hannestad S., 1999, Phys. Rev. D, 60, 023515

Harris D. L., 1948, ApJ, 108, 112

Hazard C., 1963, MNRAS, 126, 489

Herbig G. H., 1975, ApJ, 196, 129

Hogan C. J., 2000, Rev. Mod. Phys., 72, 1149

Ho·rava P., 1996, Phys. Rev. D, 54, 7561

Ho·rava P., Witten E., 1996, Nucl. Phys. B, 475, 94

Huml¶³·cek J., 1979, J. Quant. Spectrosc. Radiat. Transfer, 21, 309

Huml¶³·cek J., 1982, J. Quant. Spectrosc. Radiat. Transfer, 27, 437

Hummer D. G., 1965, MNRAS, 70, 1

Ivanchik A. V., Potekhin A. Y., Varshalovich D. A., 1999, A&A, 343, 439

Ivanchik A. V., Rodriguez E., Petitjean P., Varshalovich D. A., 2002, Astron. Lett.,

28, 423

Ivanchik A. V., Rodriguez E., Petitjean P., Varshalovich D. A., 2003, in Martins

C. J. A. P., ed., The cosmology of extra dimensions and varying fundamental

constants. Kluwer, Netherlands

Jenkins E. B., Peimbert A., 1997, ApJ, 477, 265

Jenkins E. B., Wo¶zniak P. R., So¯a U. J., Sonneborn G., Tripp T. M., 2000, ApJ,

538, 275

Jenniskens P., Desert F.-X., 1994, A&AS, 106, 39

Jordan P., 1937, Naturwiss., 25, 513

Jordan P., 1939, Z. Phys., 113, 660

Kaluza T., 1921, Preuss. Akad. Wiss. K, 1, 966

Kaplinghat M., Scherrer R. J., Turner M. S., 1999, Phys. Rev. D, 60, 023516

Kelly R. L., 1987, J. Phys. Chem. Ref. Data Suppl., 16, 1

Klein O., 1926, Z. Phys., 37, 895

References 187

Kolb E. W., Perry M. J., Walker T. P., 1986, Phys. Rev. D, 33, 869

Kothari D. S., 1938, Nat, 142, 354

Kujat J., Scherrer R. J., 2000, Phys. Rev. D, 62, 023510

Kupka F., Piskunov N., Ryabchikova T. A., Stempels H. C., Weiss W. W., 1999,

A&AS, 138, 119

Landau L. D., 1955, in Pauli W., ed., Neils Bohr and the Development of Physics.

McGraw-Hill, New York, NY, USA, p. 52

Landau S. J., Harari D. D., Zaldarriaga M., 2001, Phys. Rev. D, 63, 083505

Landau S. J., Vucetich H., 2002, ApJ, 570, 463

Langacker P., Segrµe G., Strassler M. J., 2002, Phys. Lett. B, 528, 121

Lanzetta K. M., Bowen D. V., 1992, ApJ, 391, 48

Lanzetta K. M., Bowen D. V., Tytler D., Webb J. K., 1995, ApJ, 442, 538

Lauroesch J. T., Meyer D. M., Blades J. C., 2000, ApJ, 543, L43

Le Brun V., Bergeron J., 1998, A&A, 332, 814

Le Brun V., Bergeron J., Boisse P., 1996, A&A, 306, 691

Ledoux C., Srianand R., Petitjean P., 2002, A&A, 392, 781

Levshakov S. A., Dessauges-Zavadsky M., D'Odorico S., Molaro P., 2002a, MNRAS,

333, 373

Levshakov S. A., Dessauges-Zavadsky M., D'Odorico S., Molaro P., 2002b, ApJ,

565, 696

Levshakov S. A., Molaro P., Centuri¶on M., D'Odorico S., Bonifacio P., Vladilo G.,

2000, A&A, 361, 803

Levy-Leblond J. M., 1979, in Toraldo di Francini G., ed., Proc. Enrco Fermi Int.

School Phys. Vol. 52, Problems in the foundations of physics. Elsevier, Netherlands,

p. 237

Li L., Gott J. R. III, 1998, Phys. Rev. D, 58, 103513

Lineweaver C. H., Tenorio L., Smoot G. F., Keegstra P., Banday A. J., Lubin P.,

1996, ApJ, 470, 38

188 References

Liske J., 2003, A&A, 398, 429

Litzen U., Brault J. W., Thorne A. P., 1993, Phys. Scr., 47, 628

Livio M., Stiavelli M., 1998, ApJ, 507, L13

Lopez S., Reimers D., Rauch M., Sargent W. L. W., Smette A., 1999, ApJ, 513, 598

Lu L., Sargent W. L. W., Barlow T. A., Churchill C. W., Vogt S. S., 1996, ApJS,

107, 475

Lu L., Sargent W. L. W., Womble D. S., Takada-Hidai M., 1996, ApJ, 472, 509

Lynds R., 1971, ApJ, 164, L73

Maeda K. I., 1988, Mod. Phys. Lett. A, 3, 242

Magueijo J., 2000, Phys. Rev. D, 62, 103521

Magueijo J., Barrow J. D., Sandvik H. B., 2002, Phys. Lett. B, 549, 284

Maller A., Somerville R. S., Prochaska J. X., Primack J. R., 1999, in Bunker A. J.,

van Breugel W. J. M., eds, ASP Conf. Ser. Vol. 193, The Hy-Redshift Universe:

Galaxy Formation and Evolution at High Redshift. Astron. Soc. Pac., San Francisco,

CA, U.S.A, p. 608

Marciano W. J., 1984, Phys. Rev. Lett., 52, 489

Marcy G. W., Butler R. P., 1992, PASP, 104, 270

Martin W. C., Zalubas R., 1983, J. Phys. Chem. Ref. Data, 12, 323

Martins C. J. A. P., ed., 2003, Proceedings of JENAM2002, The cosmology of extra

dimensions and varying fundamental constants. Kluwer, Netherlands

Martins C. J. A. P., Melchiorri A., Trotta R., Bean R., Rocha G., Avelino P. P.,

Viana P. T. P., 2002, Phys. Rev. D, 66, 023505

Maurette M., 1976, Annu. Rev. Nuc. Sci., 26, 319

McDonald P., Miralda-Escud¶e J., 1999, ApJ, 519, 486

Menten K. M., Reid M. J., 1996, ApJ, 465, L99

Mills I., Cvitas T., Homann K., Kallay N., Kuchitsu K., 1988, in Quantities, Units

and Symbols in Physical Chemistry. Blackwell Scienti¯c Publications, Oxford, UK

Milne E. A., 1935, Relativity, Gravitation and World Structure. Clarendon Press,

References 189

Oxford, UK

Milne E. A., 1937, Proc. R. Soc. A, 158, 324

Miralda-Escude J., Cen R., Ostriker J. P., Rauch M., 1996, ApJ, 471, 582

Mo®at J., 1993, Int. J. Mod. Phys. D, 2, 351

Mohr P. J., Taylor B. N., 2000, Rev. Mod. Phys., 72, 351

Molaro P., Bonifacio P., Centuri¶on M., D'Odorico S., Vladilo G., Santin P., Di

Marcantonio P., 2000, ApJ, 541, 54

Molaro P., Levshakov S. A., D'Odorico S., Bonifacio P., Centuri¶on M., 2001, ApJ,

549, 90

Monaghan J. J., 1971, MNRAS, 152, 509

Moore C. E., 1971, Atomic Energy Levels as Derived from Analyses of Optical

Spectra. Natl. Stand. Rel. Data Ser. Vol. 1{3, Natl. Bur. Stand. (USA), US Govt.

Printing O±ce, Washington DC, USA

Morton D. C., 1991, ApJS, 77, 119

Morton D. C., 1992, ApJS, 81, 883

Morton D. C., Dinerstein H. L., 1976, ApJ, 204, 1

Murphy M. T., Curran S. J., Webb J. K., 2003b, MNRAS, 342, 830

Murphy M. T., Webb J. K., Flambaum V. V., 2003c, MNRAS, accepted, preprint

(astro-ph/0306483)

Murphy M. T., Webb J. K., Flambaum V. V., Churchill C. W., Prochaska J. X.,

2001b, MNRAS, 327, 1223

Murphy M. T., Webb J. K., Flambaum V. V., Curran S. J., 2002, in Dong S., Burchat

P., eds, Proceedings of the XXII Physics in Collision Conference. Stanford,

CA, U.S.A, p. 116

Murphy M. T., Webb J. K., Flambaum V. V., Curran S. J., 2003a, Ap&SS, 283,

577

Murphy M. T.,Webb J. K., Flambaum V. V., Drinkwater M. J., Combes F., Wiklind

T., 2001d, MNRAS, 327, 1244

190 References

Murphy M. T., Webb J. K., Flambaum V. V., Dzuba V. A., Churchill C. W.,

Prochaska J. X., Barrow J. D., Wolfe A. M., 2001a, MNRAS, 327, 1208

Murphy M. T., Webb J. K., Flambaum V. V., Prochaska J. X., Wolfe A. M., 2001c,

MNRAS, 327, 1237

Nagourney W., Dehmelt H. G., 1981, Bull. Am. Phys. Soc., 26, 805

Naudet R., 1974, Bull. Inf. Sci. Tech., 193, 1

Nave G., Learner R. C. M., Thorne A. P., Harris C. J., 1991, J. Opt. Soc. Am. B,

8, 2028

Nollett K. M., Lopez R. E., 2002, Phys. Rev. D, 66, 063507

Norl¶en G., 1973, Phys. Scr., 8, 249

Nulsen P. E. J., Barcons X., Fabian A. C., 1998, MNRAS, 301, 168

O'Dea C. P., Baum S. A., Stanghellini C., Dey A., van Breugel W., Deustua S.,

Smith E. P., 1992, AJ, 104, 1320

Olive K. A., Pospelov M., Qian Y.-Z., Coc A., Cass¶e M., Vangiona-Flam E., 2002,

Phys. Rev. D, 66, 045022

Outram P. J., Carswell R. F., Theuns T., 2000, ApJ, 529, L73

Outram P. J., Cha®ee F. H., Carswell R. F., 1999, MNRAS, 310, 289

Pagel B. E. J., 1977, MNRAS, 179, 81P

Palmer B. A., Engleman R., 1983, Technical report, Atlas of the Thorium spectrum.

Los Alamos National Laboratory, NM, USA

Patnaik A. R., Browne I. W. A., King L. J., Muxlow T. W. B., Walsh D., Wilkinson

P. N., 1993, MNRAS, 261, 435

Peacock J. A., 1999, Cosmological physics. Cambridge Univ. Press, Cambridge, UK

Peck E. R., Reeder K., 1972, J. Opt. Soc. Am., 62, 958

Peebles P. J., Dicke R. H., 1962, Phys. Rev., 128, 2006

Peebles P. J. E., 1993, Principles of physical cosmology. Princeton Univ. Press,

Princeton, NJ, USA

Perlman E. S., Carilli C. L., Stocke J. T., Conway J., 1996, AJ, 111, 1839

References 191

Petitjean P., Rauch M., Carswell R. F., 1994, A&A, 291, 29

Petitjean P., Srianand R., Ledoux C., 2000, A&A, 364, L26

Petitjean P., Srianand R., Ledoux C., 2002, MNRAS, 332, 383

Petrov Y. V., 1977, Sov. Phys. Uspekhi, 20, 937

Pettini M., King D. L., Smith L. J., Hunstead R. W., 1997, ApJ, 478, 536

Pickering J. C., Donnelly M. P., Nilsson H., Hibbert A., Johansson S., 2002, A&A,

396, 715

Pickering J. C., Thorne A. P., Murray J. E., Litz¶en U., Johansson S., Zilio V., Webb

J. K., 2000, MNRAS, 319, 163

Pickering J. C., Thorne A. P., Webb J. K., 1998, MNRAS, 300, 131

Pickett H. M., Poynter R. L., Cohen E. A., Delitsky M. L., Pearson J. C., Muller

H. S. P., 1998, J. Quant. Spectrosc. Radiat. Transfer, 60, 883

Piskunov N. E., Kupka F., Ryabchikova T. A., Weiss W. W., Je®ery C. S., 1995,

A&AS, 112, 525

Poppe G. P. M., Wijers C. M. J., 1990, Trans. Math. Software, 16, 38

Potekhin A. Y., Ivanchik A. V., Varshalovich D. A., Lanzetta K. M., Baldwin J. A.,

Williger G. M., Carswell R. F., 1998, ApJ, 505, 523

Prestage J. D., Tjoelker R. L., Maleki L., 1995, Phys. Rev. Lett., 74, 3511

Price R. J., Crawford I. A., Barlow M. J., 2000, MNRAS, 312, L43

Prochaska J. X., 2003, ApJ, 582, 49

Prochaska J. X., Wolfe A. M., 1996, ApJ, 470, 403

Prochaska J. X., Wolfe A. M., 1997, ApJ, 474, 140

Prochaska J. X., Wolfe A. M., 1999, ApJS, 121, 369

Prochaska J. X., Wolfe A. M., 2000, ApJ, 533, L5

Prochaska J. X. et al., 2001, ApJS, 137, 21

Randall L., Sundrum R., 1999a, Phys. Rev. Lett., 83, 3370

Randall L., Sundrum R., 1999b, Phys. Rev. Lett., 83, 4690

192 References

Rao S. M., Turnshek D. A., 2000, ApJS, 130, 1

Rauch M., 1998, ARA&A, 36, 267

Riazuelo A., Uzan J., 2002, Phys. Rev. D, 66, 023525

Rosman K. J. R., Taylor P. D. P., 1998, J. Phys. Chem. Ref. Data, 27, 1275

Safronova M. S., Johnson W. R., 2001, Phys. Rev. A, 64, 52501

Sandvik H. B., Barrow J. D., Magueijo J., 2002, Phys. Rev. Lett., 88, 31302

Savedo® M. P., 1956, Nat, 178, 689

Schaye J., 2001, ApJ, 559, L1

Schmidt M., 1963, Nat, 197, 1040

Shlyakhter A. I., 1976, Nat, 264, 340

Sievers J. L. et al., 2002, ApJ, submitted, preprint (astro-ph/0205387)

Smoot G. F. et al., 1992, ApJ, 396, L1

Sommerfeld A., 1911, Z. Phys., 12, 1057

Songaila A., Cowie L. L., 1996, AJ, 112, 335

Songaila A. et al., 1994, Nat, 371, 43

Sortais Y. et al., 2001, Phys. Scr., T95, 50

Srianand R., Petitjean P., 1998, A&A, 335, 33

Srianand R., Petitjean P., Ledoux C., 2000, Nat, 408, 931

Stockton A. N., Lynds C. R., 1966, ApJ, 144, 451

Struve O., Elvey C. T., 1934, ApJ, 79, 409

Teller E., 1948, Phys. Rev., 73, 801

Theuns T., Leonard A., Efstathiou G., 1998a, MNRAS, 297, L49

Theuns T., Leonard A., Efstathiou G., Pearce F. R., Thomas P. A., 1998b, MNRAS,

301, 478

Thompson R. I., 1975, Astron. Lett., 16, 3

Timmes F. X., Clayton D. D., 1996, ApJ, 472, 723

Tripp T. M., Lu L., Savage B. D., 1998, ApJ, 508, 200

References 193

Tubbs A. D., Wolfe A. M., 1980, ApJ, 236, L105

Uzan J., 2003, Rev. Mod. Phys., 75, 403

Valenti J. A., Butler R. P., Marcy G. W., 1995, PASP, 107, 966

Varshalovich D. A., Levshakov S. A., 1993, J. Exp. Theor. Phys. Lett., 58, 237

Varshalovich D. A., Panchuk V. E., Ivanchik A. V., 1996, Astron. Lett., 22, 6

Varshalovich D. A., Potekhin A. Y., 1995, Space Sci. Rev., 74, 259

Varshalovich D. A., Potekhin A. Y., 1996, Astron. Lett., 22, 1 (VP96)

Varshalovich D. A., Potekhin A. Y., Ivanchik A. V., 2000, in Dunford R. W., Gemmel

D. S., Kanter E. P., Kraessig B., Southworth S. H., Young L., eds, AIP Conf.

Proc. Vol. 506, X-Ray and Inner-Shell Processes. Argonne National Laboratory,

Argonne, IL, USA, p. 503 (VPI00)

Vogt S. S. et al., 1994, in Crawford D. L., Craine E. R., eds, Proc. SPIE Vol. 2198,

Instrumentation in Astronomy VIII. p. 362

Walker M., Wardle M., 1998, ApJ, 498, L125

Weast R. C., 1979, Handbook of Chemistry and Physics, 60th edn. CRC Press, Boca

Raton, FL, USA

Webb J. K., 1987, PhD thesis, Univ. Cambridge

Webb J. K., Flambaum V. V., Churchill C. W., Drinkwater M. J., Barrow J. D.,

1999, Phys. Rev. Lett., 82, 884 (W99)

Webb J. K., Murphy M. T., Flambaum V. V., 2003, in preparation

Webb J. K., Murphy M. T., Flambaum V. V., Curran S. J., 2003, Ap&SS, 283, 565

Webb J. K., Murphy M. T., Flambaum V. V., Dzuba V. A., Barrow J. D., Churchill

C. W., Prochaska J. X., Wolfe A. M., 2001, Phys. Rev. Lett., 87, 091301

Weinberg S., 1983, Phil. Trans. R. Soc. London, 310, 249

Wells R. J., 1999, J. Quant. Spectrosc. Radiat. Transfer, 62, 29

Whaling W., Anderson W. H. C., Carle M. T., Brault J. W., Zarem H. A., 1995, J.

Quant. Spectrosc. Radiat. Transfer, 53, 1

Wheeler J. A., 1980, in Woolf H., ed., Some strangeness in the proportion. Addison194

References

Wesley, London, UK, p. 341

Wiklind T., Combes F., 1994, A&A, 286, L9

Wiklind T., Combes F., 1995, A&A, 299, 382

Wiklind T., Combes F., 1996, A&A, 315, 86

Wiklind T., Combes F., 1997, A&A, 328, 48

Wiklind T., Combes F., 1998, ApJ, 500, 129

Wolfe A. M., Brown R. L., Roberts M. S., 1976, Phys. Rev. Lett., 37, 179

Wolfe A. M., Davis M. M., 1979, AJ, 84, 699

Wolfe A. M., Prochaska J. X., 2000, ApJ, 545, 603

Wu Y., Wang Z., 1986, Phys. Rev. Lett., 57, 1978

Tables list:

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/tables4phd4physics.rtf

Formulas list:

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/formulas\_17jan07.rtf

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/formulas\_18jan07.rtf

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/formulas\_19jan07.rtf

http://michaelmarchenko.weebly.com/uploads/3/0/2/7/30272185/formulas25mar07\_\_.rtf