The α-dependence of transition frequencies for multi-electron ions

M. G. Kozlov[1], V. V. Dzuba[2], V. V. Flambaum[2] and M. Marchenko[2]

[1] *Petersburg Nuclear Physics Institute, Gatchina, Russia*
[2] *University of the New South Wales, Sydney, Australia*

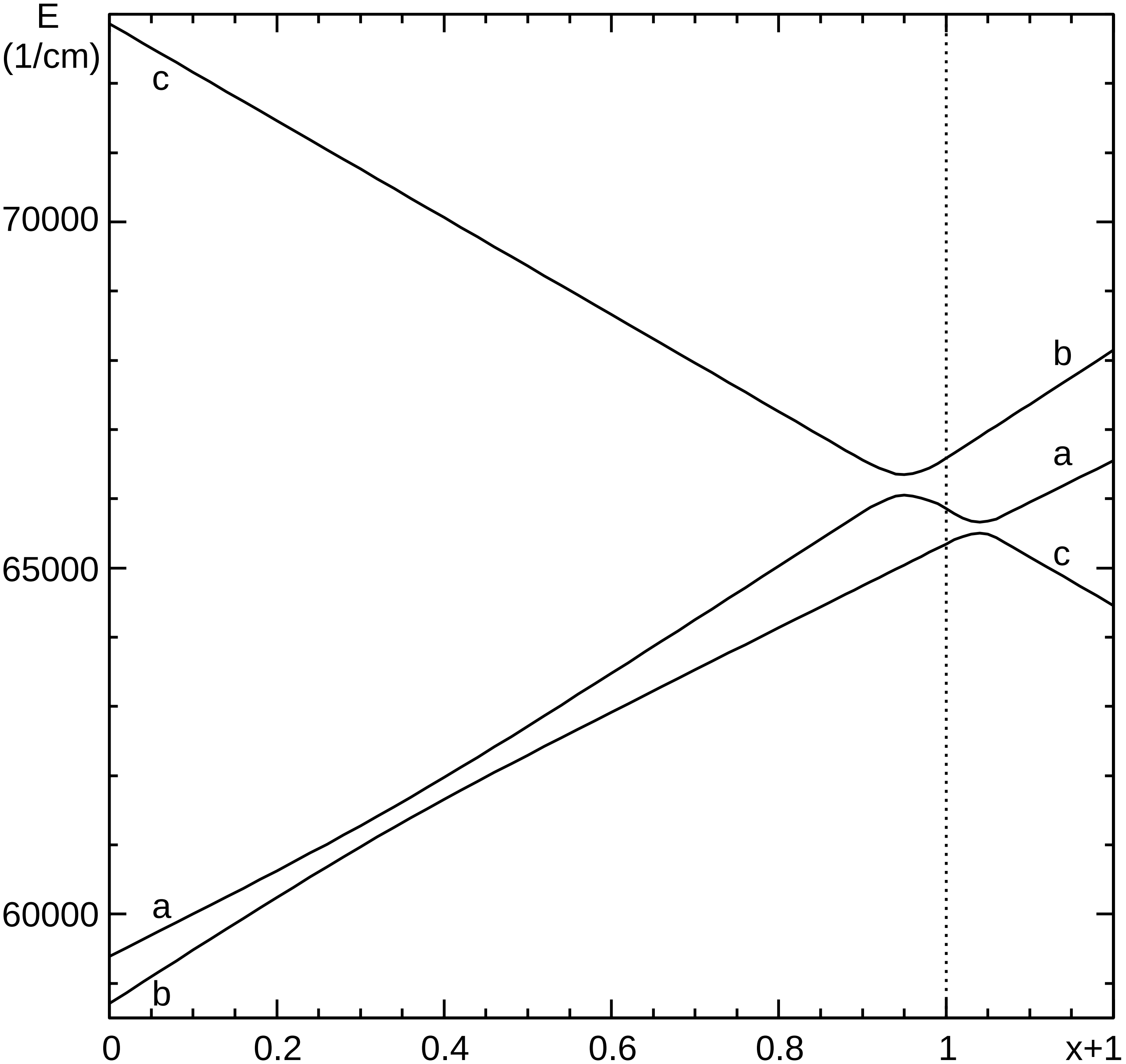
An exceptional precision of experimental methods in atomic physics allows to use atoms as test systems to study fundamental laws of nature. Recently there was an intensive discussion of the possible space-time variation of the fine structure constant $\alpha = e^2/hc$ at the cosmological scale. The first evidence for such variation has been reported from the analysis of the astrophysical data [J. K. Webb *et al*, Phys. Rev. Lett. **87**, 091301 (2001)]. Here we discuss the reliability of the underlying atomic theory.

- $\diamond$ How to search for the possible variation of $\alpha = \frac{e^2}{hc}$.
- $\diamond$ Brief discussion of the experimental situation.
- $\diamond$ Method of calculation of the α-dependence of the frequencies of the atomic transitions.
- $\diamond$ Level-crossings. Spectra of Ni II and Fe II.
- $\diamond$ Conclusions.

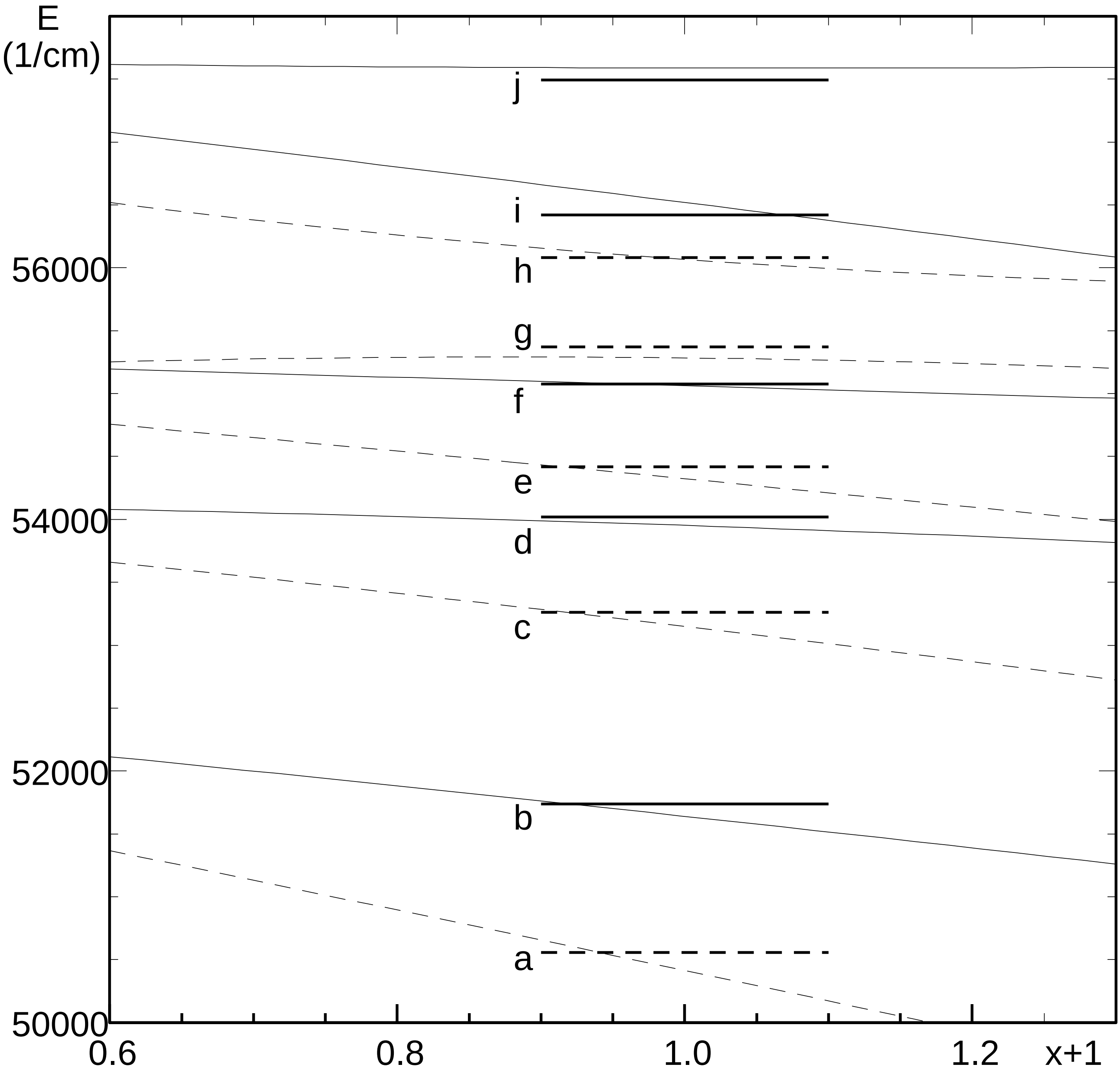
Parameters q for Si II, Cr II, Fe II, Ni II, and Zn II. Estimated errors are in brackets.

Ion	Transition			ω_0 (cm^{-1})	q (cm^{-1})		
					this work		[1]
Si II	$^2P^o_{1/2}$	$\rightarrow$	$^2D_{3/2}$	55309.337	520	(30)	530
		$\rightarrow$	$^2S_{1/2}$	65500.449	50	(30)	70
Cr II	$^6S_{5/2}$	$\rightarrow$	$^6P^o_{3/2}$	48398.868	−1360	(150)	−1290
		$\rightarrow$	$^6P^o_{5/2}$	48491.053	−1280	(150)	−1200
		$\rightarrow$	$^6P^o_{7/2}$	48632.055	−1110	(150)	−1060
Fe II	$^6D_{9/2}$	$\rightarrow$	$^6D^o_{9/2}$	38458.987	1330	(150)	1450
		$\rightarrow$	$^6D^o_{7/2}$	38660.049	1490	(150)	1620
		$\rightarrow$	$^6F^o_{11/2}$	41968.064	1460	(150)	1640
		$\rightarrow$	$^6F^o_{9/2}$	42114.833	1590	(150)	1780
		$\rightarrow$	$^6P^o_{7/2}$	42658.240	1210	(150)	1420
		$\rightarrow$	$^4F^o_{7/2}$	62065.528	1100	(300)	1210
		$\rightarrow$	$^6P^o_{7/2}$	62171.625	−1300	(300)	1280
Ni II	$^2D_{5/2}$	$\rightarrow$	$^2F^o_{7/2}$	57080.373	−700	(250)	−300
		$\rightarrow$	$^2D^o_{5/2}$	57420.013	−1400	(250)	−700
		$\rightarrow$	$^2F^o_{5/2}$	58493.071	−20	(250)	800
Zn II	$^2S_{1/2}$	$\rightarrow$	$^2P^o_{1/2}$	48481.077	1584	(25)	1577
		$\rightarrow$	$^2P^o_{3/2}$	49355.002	2490	(25)	2479

[1] Murphy *et al.*, Mon. Not. R. Astron. Soc. **327**, 1208 (2001).



Example of the typical level-crossings in the upper band of Fe II
($x = (\alpha/\alpha_0)^2 - 1$).
$a = {}^4F^o_{7/2}(3d^64p)$, $b = {}^4D^o_{7/2}(3d^64p)$, and $c = {}^6P^o_{7/2}(3d^54s4p)$.



Dependence of the odd levels of Ni II on $(\alpha/\alpha_0)^2 = x + 1$. Solid lines correspond to $J = 5/2$ and dashed lines to $J = 7/2$. The experimental positions of the lines are all shifted down by 1000 cm^{-1}. The assignment of the levels from bottom up: $^4D^o_{7/2,5/2}$ (a, b), $^4G^o_{7/2,5/2}$ (c, d), $^4F^o_{7/2,5/2}$ (e, f), $^2G^o_{7/2}$ (g), $^2F^o_{7/2}$ (h), $^2D^o_{5/2}$ (i), and $^2F^o_{5/2}$ (j).

Transition frequencies ω from the ground state $^6D_{9/2}$, g-factors, and parameters $q_\pm$ for Fe II (in cm^{-1}).

	Experiment		Theory				
	ω	g	ω	g	$g(LS)$	q_-	q_+
$^6D^o_{9/2}$	38459	1.542	38352		1.556	1359	1363
$^6D^o_{7/2}$	38660	1.584	38554	1.586	1.587	1522	1510
$^6F^o_{11/2}$	41968		41864		1.455	1496	1508
$^6F^o_{9/2}$	42115	1.43	42012		1.434	1615	1631
$^6F^o_{7/2}$	42237	1.399	42141	1.396	1.397	1738	1737
$^6P^o_{7/2}$	42658	1.702	42715	1.709	1.714	1241	1261
$^4D^o_{7/2}$	44447	1.40	44600	1.345	1.429	1791	1837
$^4F^o_{7/2}$	44754	1.29	44386	1.327	1.238	1608	1601
$^8P^o_{7/2}$	54490		54914	1.936	1.937	-2084	-2086
$^4G^o_{7/2}$	60957	0.969	63624	0.978	0.984	1640	1640
$^4H^o_{7/2}$	61157	0.720	63498	0.703	0.667	1296	1247
$^4D^o_{7/2}$	61726	1.411	66145	1.398	1.429	1194	1240
$^4F^o_{7/2}$	62066	1.198	65528	1.252	1.238	1071	1052
$^6P^o_{7/2}$	62172	1.68	65750	1.713	1.714	-1524	-1514
$^2G^o_{7/2}$	62323		64798	0.882	0.889	1622	1605

Zn II

- The ground state configuration is $[1s^2 \ldots 3d^{10}]4s$.
- Transition of interest is $4s \to 4p_j$.
- The theory here is simple, so we can use Zn II to study the importance of different corrections:

  Core-valence correlations can be included in the Brueckner approximation:

  $$(H_{\mathrm{DHF}} + \Sigma(E))\,\Psi = E\Psi,$$

  with the self-energy operator $\Sigma(E)$ calculated in the second order of many-body perturbation theory.

  Breit correction was estimated by calculating the operator H_{DHF} with the magnetic part of the Breit operator included self-consistently.

Transition frequencies and parameters q for Zn II (in cm^{-1}).

Transition			Exper.	DHFC	DHFCB	BC	BCB
			transition frequencies				
$4s_{1/2}$	$\to$	$4p_{1/2}$	48481.077	44610.1	44608.1	48391.2	48389.4
	$\to$	$4p_{3/2}$	49355.002	45346.9	45330.0	49263.8	49244.6
			parameters $q = (q_+ + q_-)/2$				
$4s_{1/2}$	$\to$	$4p_{1/2}$		1362	1359	1594	1590
	$\to$	$4p_{3/2}$		2129	2109	2500	2479

DHFC(B) = Dirac-Hartree-Fock-Coulomb(-Breit),
BC(B) = Brueckner-Coulomb(-Breit).

Interaction of the level ${}^6P^o_{7/2}$ with levels of the configuration $3d^64p$.

The level ${}^6P^o_{7/2}$ interacts with the levels ${}^2G^o_{7/2}$, ${}^4F^o_{7/2}$, and ${}^4D^o_{7/2}$. The slopes and g-factors of the latter are relatively close to each other, so we can simply take the average for all three:

$$\bar{g} = 1.185; \quad \bar{q} = 1297.$$

Now we can use experimental g-factor of the state ${}^6P^o_{7/2}$ to determine the mixing:

$$C^2 = \frac{1.68 - \bar{g}}{1.713 - \bar{g}} = 0.937,$$

$$q({}^6P^o_{7/2}) = C^2 q_0({}^6P^o_{7/2}) + (1 - C^2)\bar{q} = -1342,$$

i.e. the correction for the mixing $\delta q({}^6P^o_{7/2}) = +177$ is not very large. That corresponds to the fact that experimental g-factor of the level ${}^6P^o_{7/2}$ is significantly larger than any g-factors of the levels of the configuration $3d^64p$.