

Sensitivity of microwave and infrared spectra of molecules to variation of fundamental constants

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JENAM, 7 September 2010

Fundamental constants in atomic physics

There are three fundamental constants, which influence atomic and molecular spectra:

- Fine structure constant $\alpha = e^2/(\hbar c)$ is a coupling constant in QED.
- Electron to proton mass ratio $\mu = m_e/m_p$. Because m_p is proportional to Λ_{QCD} , $\mu \sim m_e/\Lambda_{QCD}$.
- Nuclear gyromagnetic ratio g_n can be expressed in terms of Λ_{QCD} and quark masses, but for atomic physics g_n is independent constant (always enters in combination $g_n\mu$).

Dimensionless sensitivity coefficients

If fundamental constants change, the frequency of any atomic transition also change:

$$\omega = \omega_0 \left[1 + Q_\alpha \frac{\delta\alpha}{\alpha} + Q_\mu \frac{\delta\mu}{\mu} + Q_g \frac{\delta g_n}{g_n} \right],$$
$$\frac{\delta\omega}{\omega} = \frac{\delta F}{F}, \quad F = \alpha^{Q_\alpha} \mu^{Q_\mu} g_n^{Q_g}.$$

In order to detect this change we need to compare at least two transition frequencies:

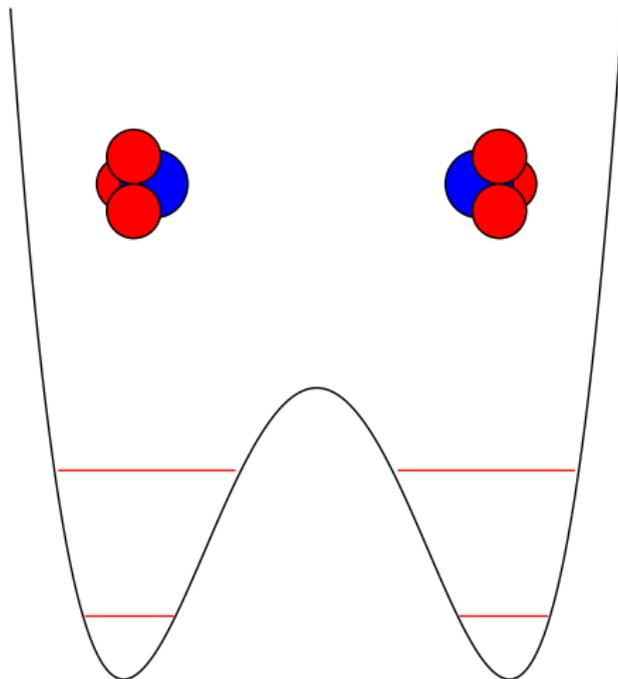
$$\frac{\omega_j}{\omega_k} = \left(\frac{\omega_j}{\omega_k} \right)_0 \left[1 + \frac{\delta\Phi}{\Phi} \right], \quad \Phi = \alpha^{\Delta Q_\alpha} \mu^{\Delta Q_\mu} g_n^{\Delta Q_g}.$$

Clearly, the effect is proportional to the differences of sensitivity coefficients ΔQ .

Sensitivity coefficients for different wavebands (in a.u.)

- For optical transitions in *light* atoms and molecules $Q_\alpha, Q_\mu, Q_g \ll 1$.
- Fine structure $\sim \alpha^2 \Rightarrow Q_\alpha = 2$.
- Vibrational structure $Q_\mu = \frac{1}{2}$.
- Rotational structure $Q_\mu = 1$.
- Magnetic hyperfine structure $Q_\alpha = 2; Q_\mu = 1; Q_g = 1$.
- Inversion line in NH_3 (1.2 cm) $Q_\mu = 4.46$.
- Mixed inversion-rotational lines in H_3O^+ $|Q_\mu| \sim 10$.
- Λ -doublet lines in $\text{OH}, \text{CH}, \text{NH}^+, \dots$ $|Q_\alpha|, |Q_\mu| \gg 1$.

Inversion line in NH_3



Analytical solution for tunneling transition [Landau & Lifshitz]

WKB approximation for tunneling frequency reads:

$$\begin{aligned}\omega_{\text{inv}} &= \frac{\omega_V}{\pi} \exp(-S) \\ &= \frac{\omega_V}{\pi} \exp\left(-\frac{1}{\hbar} \int_{-a}^a \sqrt{2M_1(U(x) - E)} dx\right), \\ \frac{\delta\omega_{\text{inv}}}{\omega_{\text{inv}}} &\approx \frac{\delta\mu}{\mu} \left(\frac{1}{2} + \frac{S}{2} + \frac{S}{4} \frac{\omega_V}{U_{\text{max}} - E}\right).\end{aligned}$$

Sensitivity coefficients Q_μ for inversion transition in different isotopologues of ammonia.

Molecule	Action S	Q_μ
$^{14}\text{NH}_3$	5.9	4.4
$^{15}\text{NH}_3$	6.0	4.4
$^{14}\text{NH}_2\text{D}$	6.5	4.7
$^{14}\text{ND}_2\text{H}$	7.3	5.1
$^{14}\text{ND}_3$	8.4	5.7
$^{15}\text{ND}_3$	8.5	5.7
$^{15}\text{ND}_3^*$		5.6

*) van Veldhoven *et al.* [Eur. Phys. J. D,**31**, 337 (2005)].

Gravitational lens PKS 1830-211 ($z = 0.89$)

The most recent extragalactic ammonia results reported by [C Henkel *et al.* *A&A*, **500**, 725 (2009)]. They observed 10 optically thin inversion lines of NH_3 and 5 rotational lines of HC_3N from molecular cloud PKS 1830-211 at $z = 0.89$ (lookback time 7 Gyr). The following three-sigma limit on μ -variation was obtained:

$$|\delta\mu/\mu| < 1.4 \times 10^{-6}.$$

Molecular clouds in the Milky Way

Emission lines of ammonia are often seen from the cold molecular clouds in the Galaxy. These lines are typically two orders of magnitude narrower than for extragalactic sources. This allows to study spatial variation of μ at the 10^{-8} level [Levshakov *et al.* *A&A*, **512**, A44 (2010)]:

$$\Delta\mu/\mu = (2.2 \pm 0.4_{\text{stat}} \pm 0.3_{\text{sys}}) \times 10^{-8}.$$

Most recent result [Levshakov *et al.* *arXiv:1008.1160*]:

$$\Delta\mu/\mu = (2.6 \pm 0.1_{\text{stat}} \pm 0.3_{\text{sys}}) \times 10^{-8}.$$

More about this in the **next talk by Levshakov**.

How we can independently test ammonia results?

To test non-zero ammonia results we need to find other transitions with high sensitivity to μ -variation, which are observed in the interstellar medium.

Other microwave and infrared transitions with high sensitivity to μ -variation:

- Mixed inversion-rotation transitions in partly deuterated ammonia NH_2D and in hydronium ion H_3O^+ ;
- Λ -doublet transitions in CH , OH , and in NH^+ .

Mixed transitions in NH_2D and ND_2H

In partly deuterated ammonia inversion lines have different ortho-para symmetry. Because of that inversion transition goes only in combination with rotational transitions. For such mixed transitions

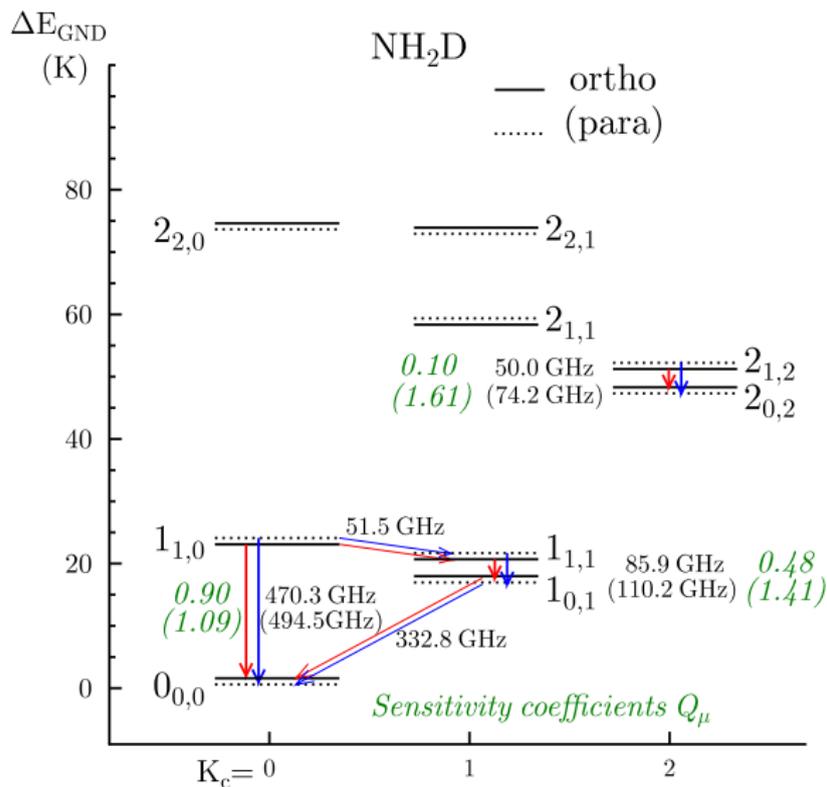
$$\omega = \omega_r \pm \omega_{\text{inv}},$$

and sensitivity coefficients are equal to

$$Q_\mu = \frac{\omega_r}{\omega} Q_{r,\mu} \pm \frac{\omega_{\text{inv}}}{\omega} Q_{\text{inv},\mu},$$

where $Q_{r,\mu} = 1$ and $Q_{\text{inv},\mu} = 4.7$ (NH_2D), or $Q_{\text{inv},\mu} = 5.1$ (ND_2H).

Spectrum of NH₂D

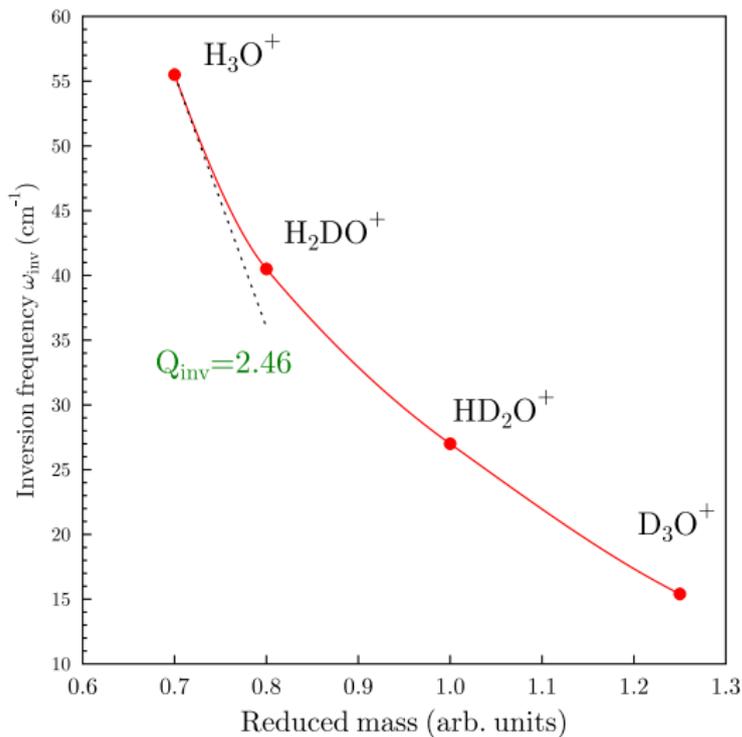


Mixed transitions in H_3O^+

In hydronium ion H_3O^+ the inversion frequency (55 cm^{-1}) is much higher, than in ammonia and is comparable to rotational frequencies. Because of that, there are several “low frequency” mixed transitions with very high sensitivities of different signs. Some of these transitions were observed from the interstellar medium.

This is extremely favorable situation for the μ -variation search!

Inversion frequencies of isotopologues of hydronium ion and sensitivity to μ -variation



Sensitivities of mixed transitions of hydronium ion

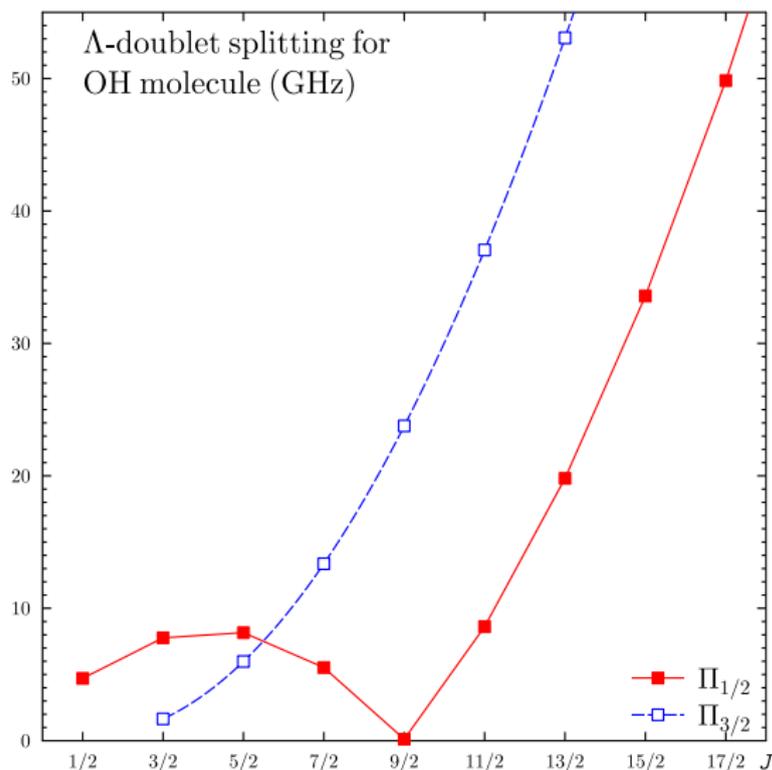
J	K	Transition				Frequency (MHz)	Q_{μ}
		s	J'	K'	s'		
1	1	-1	2	1	+1	307192.410	+9.0
3	2	+1	2	2	-1	364797.427	-5.7
3	1	+1	2	1	-1	388458.641	-5.2
3	0	+1	2	0	-1	396272.412	-5.1
0	0	-1	1	0	+1	984711.907	+3.5
4	3	-1	3	3	+1	1031293.738	-1.4
4	2	-1	3	2	+1	1069826.632	-1.2
3	2	-1	3	2	+1	1621738.993	+2.5
2	1	-1	2	1	+1	1632090.98	+2.5
1	1	-1	1	1	+1	1655833.910	+2.5

Λ -doublet transitions in OH and CH

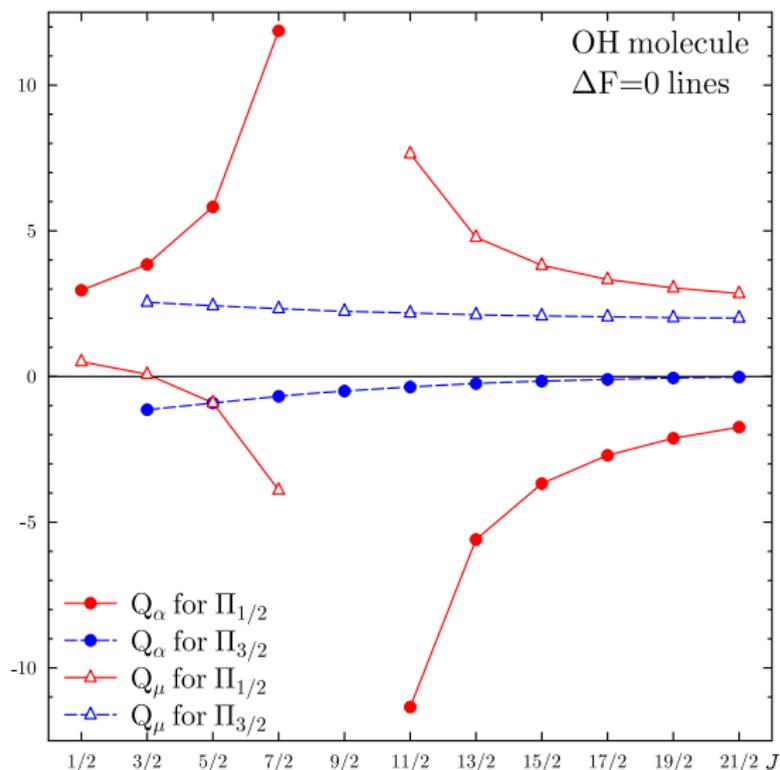
In molecules OH and CH electronic spin \mathbf{S} is weakly coupled to the molecular axis for low J and decoupled from the axis for higher J . This leads to gradual transformation of Ω -doubling into Λ -doubling.

For electronic state $\Pi_{1/2}$ of OH molecule and $\Pi_{3/2}$ state of CH molecule transformation of the coupling scheme causes line crossing and huge enhancement of the sensitivity coefficients Q_α and Q_μ . Sensitivity coefficients for two other fine structure levels smoothly depend on the quantum number J .

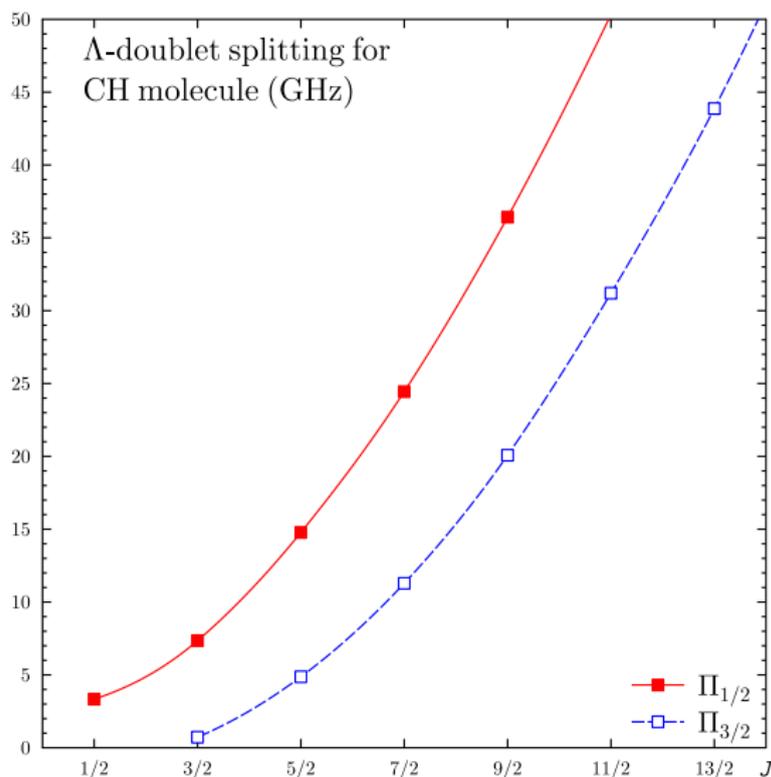
Frequencies of Λ -transitions in OH



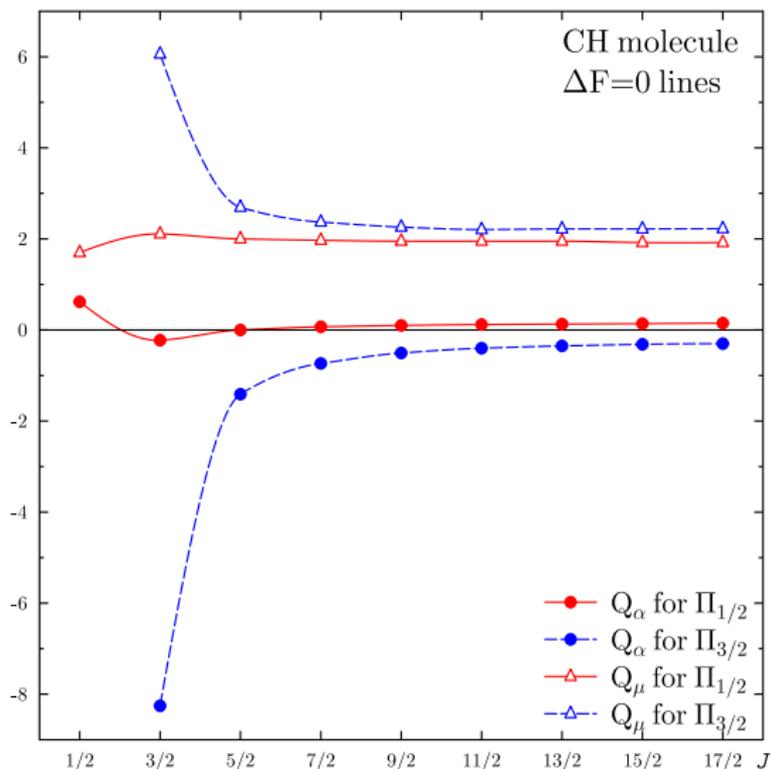
Sensitivities for Λ -transitions in OH



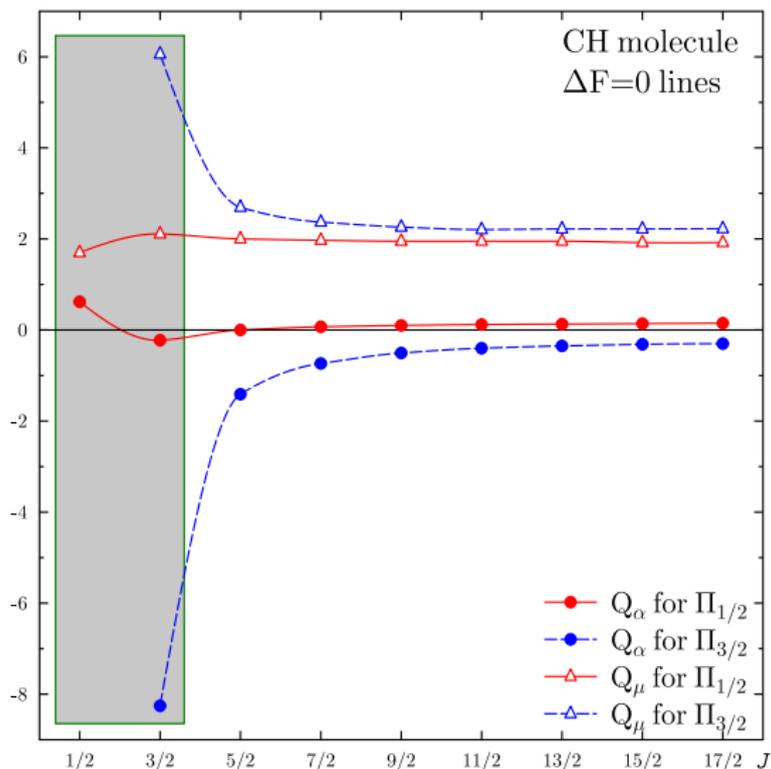
Frequencies of Λ -transitions in CH



Sensitivities for Λ -transitions in CH

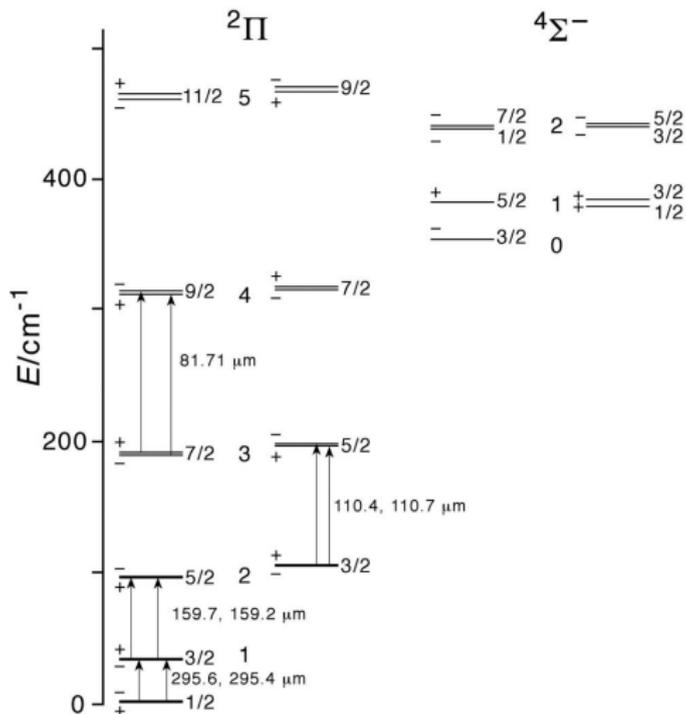


Sensitivities for Λ -transitions in CH



Level structure of NH^+ ion

[Hûbers *et al.*, Chem. Phys. Lett. **131**, 034311 (2009)]



To check ammonia results
we need laboratory frequency measurements
with relative accuracy 10^{-8} !

Publications

- V F Flambaum & M G Kozlov, Phys.Rev.Lett. **98**, 240801 (2007); arXiv: [0704.2301](#).
- S A Levshakov, P Molaro, and M G Kozlov, arXiv: [0808.0583](#).
- M G Kozlov, Phys.Rev.A, **80**, 022118 (2009); arXiv: [0905.1714](#).
- P Molaro, S A Levshakov, and M G Kozlov, Nuc. Phys. B Proceedings Supplements, **194**, 287 (2009); arXiv: [0907.1192](#).
- M G Kozlov, A V Lapinov, and S A Levshakov, J. Phys. B, **43**, 074003 (2010); arXiv: [0908.2983](#).
- S A Levshakov *et al.* arXiv: [1008.1160](#).