HIGH ACCURACY METHANOL LINES FOR SEARCH OF SPATIAL-TEMPORAL VARIATIONS OF THE FUNDAMENTAL CONSTANTS

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Objective: High accuracy measurements of frequencies of some methanol lines

- Extensive search of spatial-temporal variations of the fundamental constants
- Method: observations of atomic and molecular spectral lines in the interstellar medium
- Some transition frequencies of molecules with intramolecular motions have extremely high sensitivity to variations of $\mu=m_p/m_e$

$$\frac{\Delta \nu}{\nu}=K_\mu \frac{\Delta \mu}{\mu}$$

- The most promising probe: methanol CH_3OH – sensitivity up to

$$K_\mu=-32.8$$

- Relative accuracy of laboratory measurements: 10^{-8}-10^{-9}.
- Absolute uncertainty of laboratory measurements: sub kilohertz.
- Main purpose of this work: to improve accuracy of line frequency measurements up to sub kilohertz level for some methanol lines

Methanol lines as a probe for search for spatial-temporal variations of the fundamental constants

At present abilities of the search of possible spatial-temporal variations of fundamental constants are limited by

- Accuracy of astrophysical data
- Accuracy of laboratory measurements

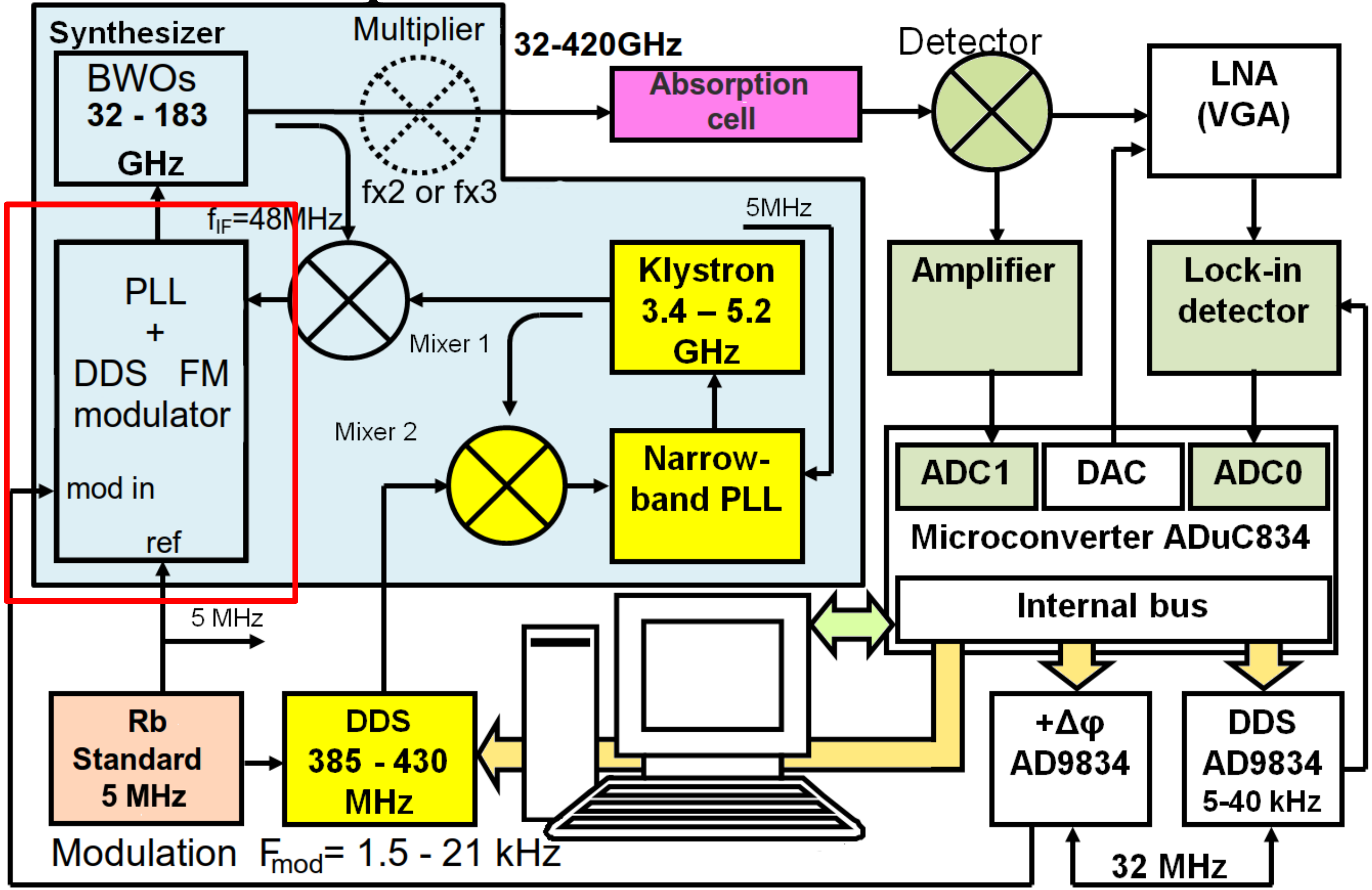
Transition	ν_{Lab1} [1]	ν_{Lab2} [2]	ν_{Lab1} - ν_{Lab1}	ν_z=0.88582	K_μ
$3_{-1} - 2_0$ E	12178.597(4)	12178.587	0.0**100**	6457.985	-32.8
$0_0 - 1_0$ A^+	48372.4558(7)	48372.460	-0.0**012**	25650.6219	-1.0
$0_0 - 1_0$ E	48376.892(10)	48376.887	0.0**050**	25652.974	-1.0
$2_{-1} - 1_0$ E	60531.489(10)	60531.477	0.0**120**	32098.233	-7.4

[1] A&A 428, p.1019 [2] Mol Phys 111, p.1923

Principal laboratory accuracy limitation:

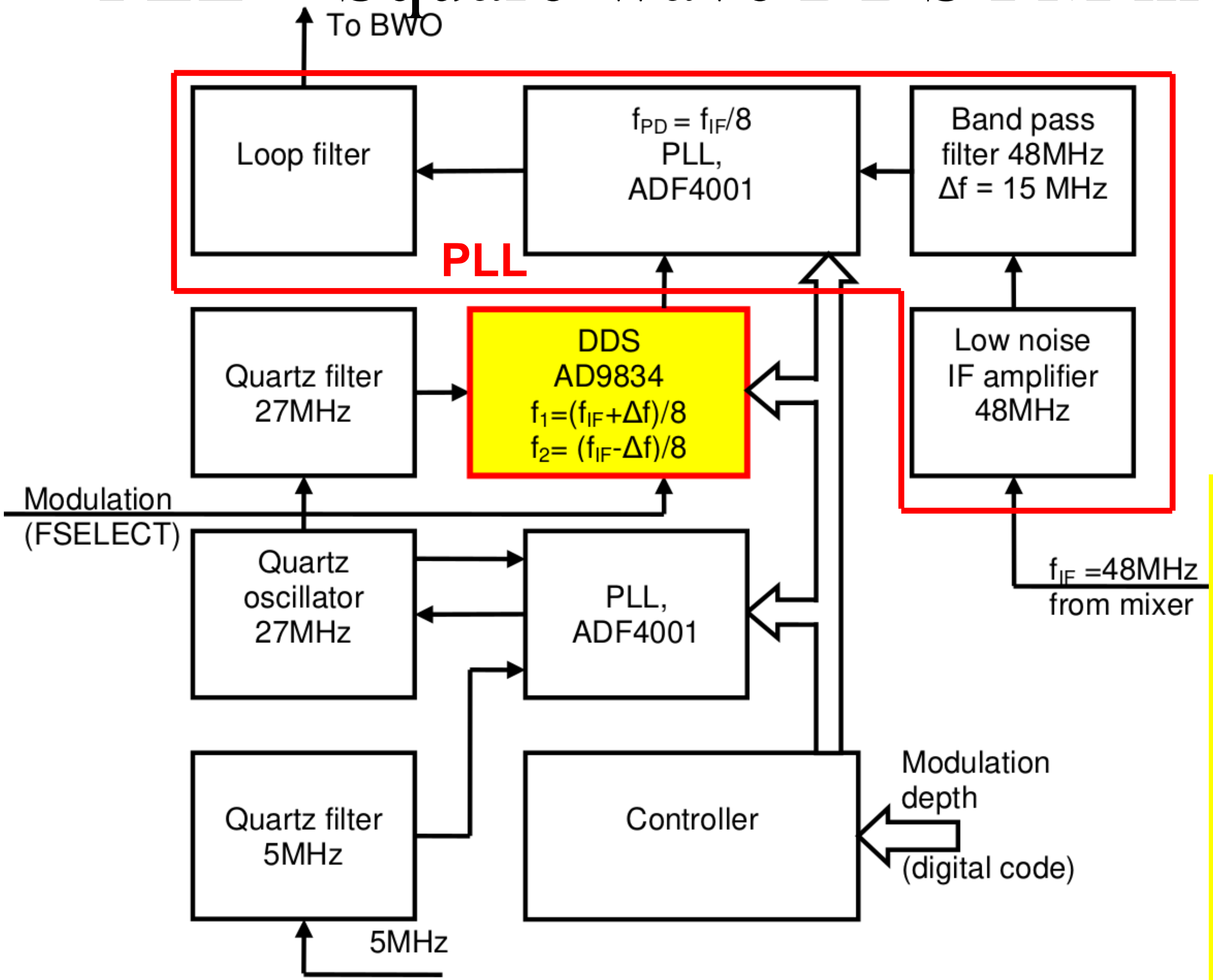
- Majority of modern microwave spectrometers operate with Frequency Modulated (FM) source and lock-in detection in the receiving system
- Recorded lineshapes are effected by:
  - Modulation distortions
  - Distortions caused by reflections in absorbing cell (standing wave)
- To reach the highest accuracy of line frequency measurements it is necessary to take into account both kinds of distortions

Block-Diagram of the Microwave Spectrometer IRA NASU



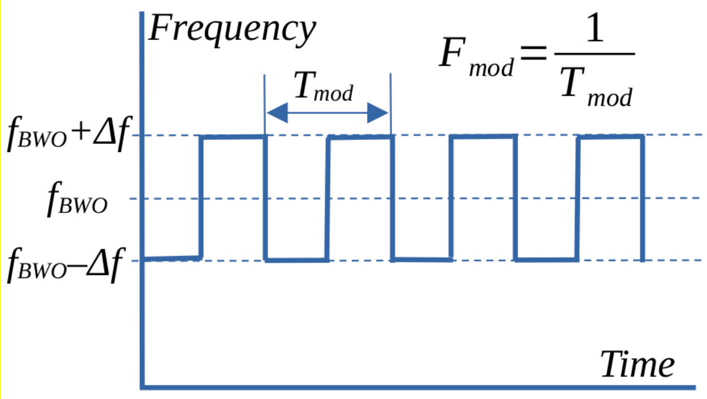
- Absorption Spectrometer
- Range 32-420GHz
- Frequency-modulated source
- The first harmonic 1*f* lock-in detection

PLL + Square-wave DDS FM modulator



DDS provides fast frequency switching with continuous phase. PPL reference signal (f_{IF}) will be FM-modulated => output signal of BWO will be FM-modulated

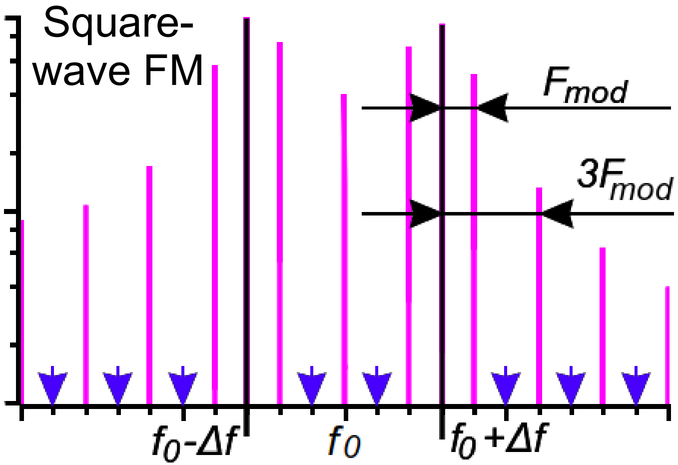
Frequency of output signal of BWO (square-wave FM-modulated)

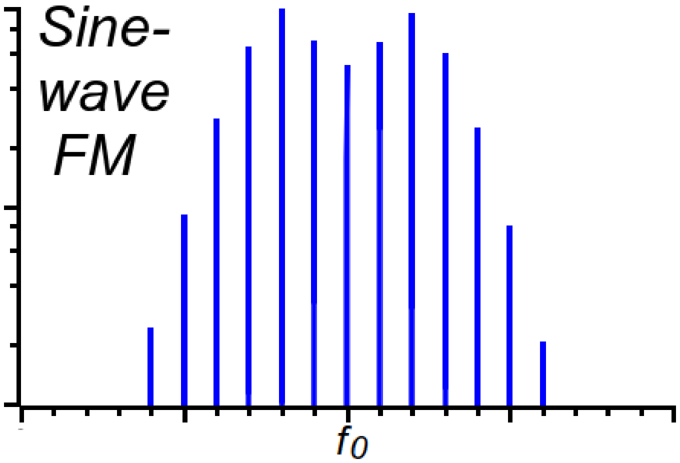


Modulation distortions of lineshape

- In order to take into account lineshape distortions parameters of FM should be known with high accuracy
- Modern Direct Digital Synthesizers (DDS) are capable to provide frequency-shift keying (**square-wave FM**) between two frequencies known with very high accuracy – Parameters of FM are known with high accuracy
- Problem: all previously elaborated approaches were intended for analysis of lineshapes obtained with sine-wave FM
- To use square-wave FM (by means of DDS) we need to develop corresponding lineshape analysis

Some peculiarities of square-wave FM

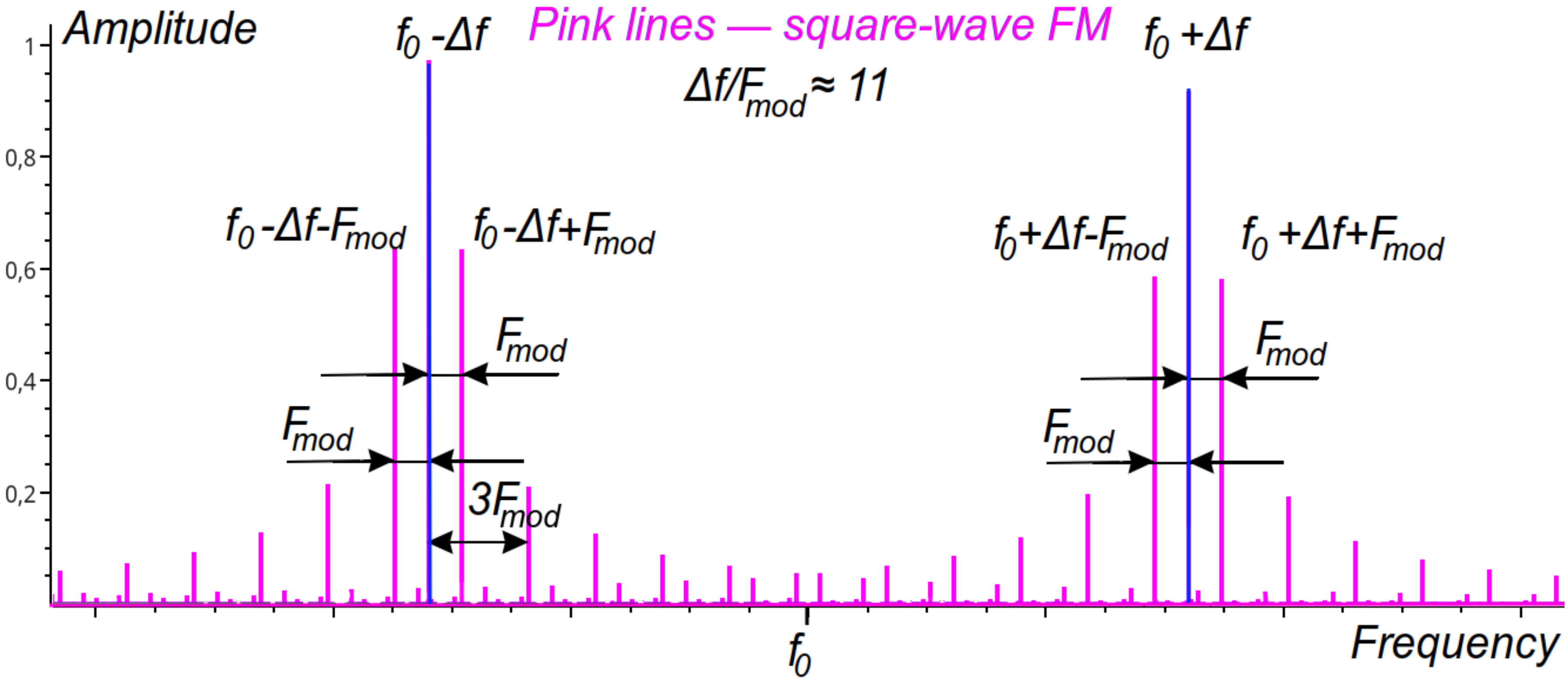




- Square-wave FM signal is dominated by **odd harmonics** of modulation frequency F_{mod}
- In square-wave FM signal **even harmonics** of modulation frequency are suppressed
- Square-wave FM is suitable for 1*f* lock-in detection only (not suitable for 2*f* lock-in detection!)
- Square-wave FM signal is rather different from usual sine-wave FM signal
- Analysis of spectra records should take into account peculiarities of the square-wave FM (which differs significantly from usual sine-wave modulation)

“Frequency domain” approach: Spectrum of FM signal ($\Delta f/F_{mod} \approx 11$)

Δf – modulation depth F_{mod} – frequency of modulation

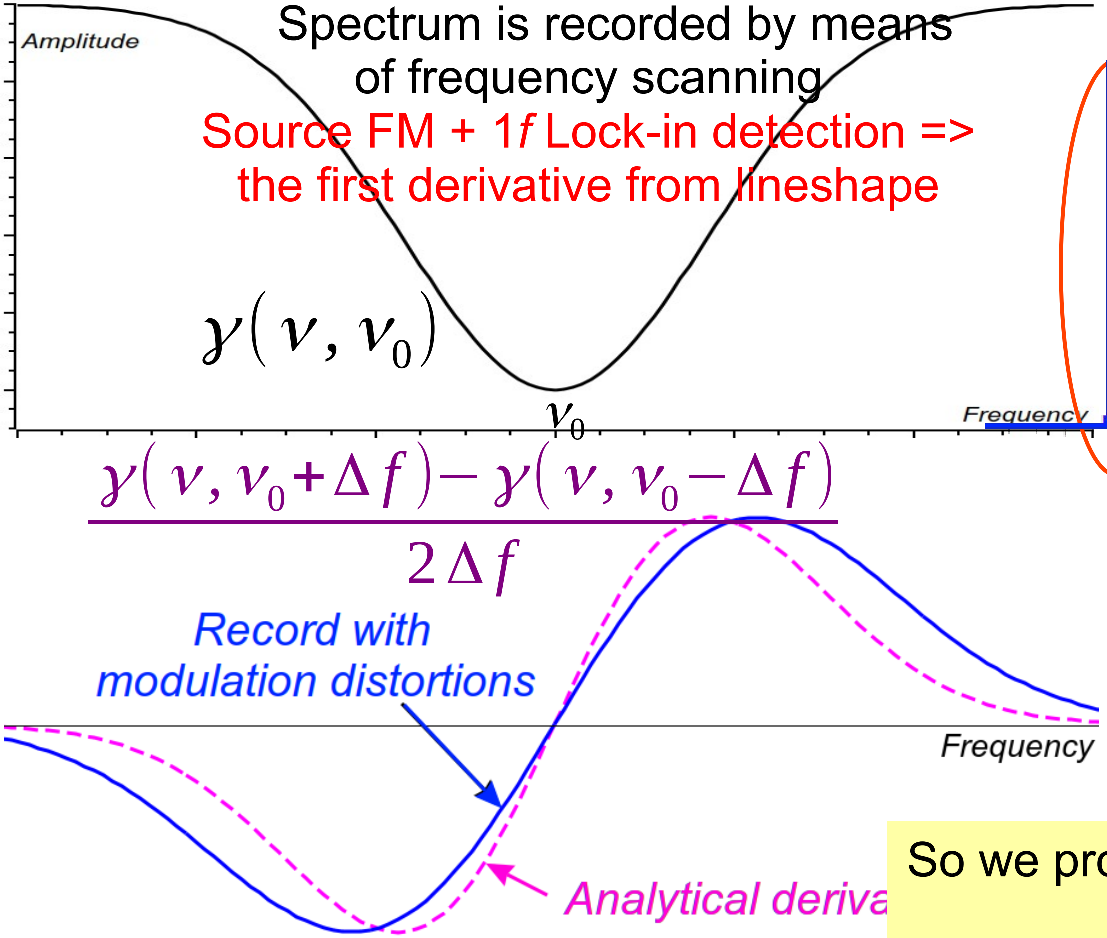


“Numerical derivative” approach

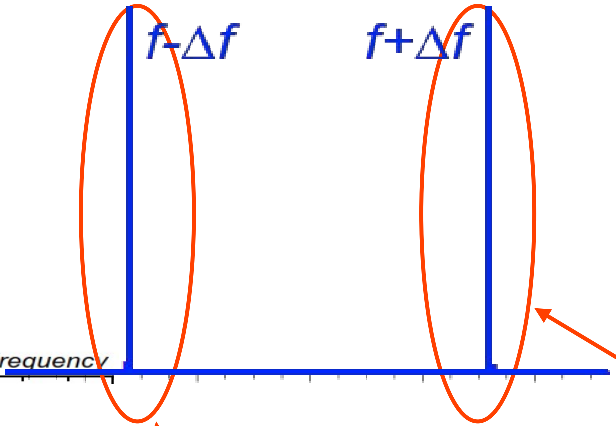
Spectrum is recorded by means of frequency scanning

Source FM + 1*f* Lock-in detection => the first derivative from lineshape

$$\gamma(\nu, \nu_0)$$



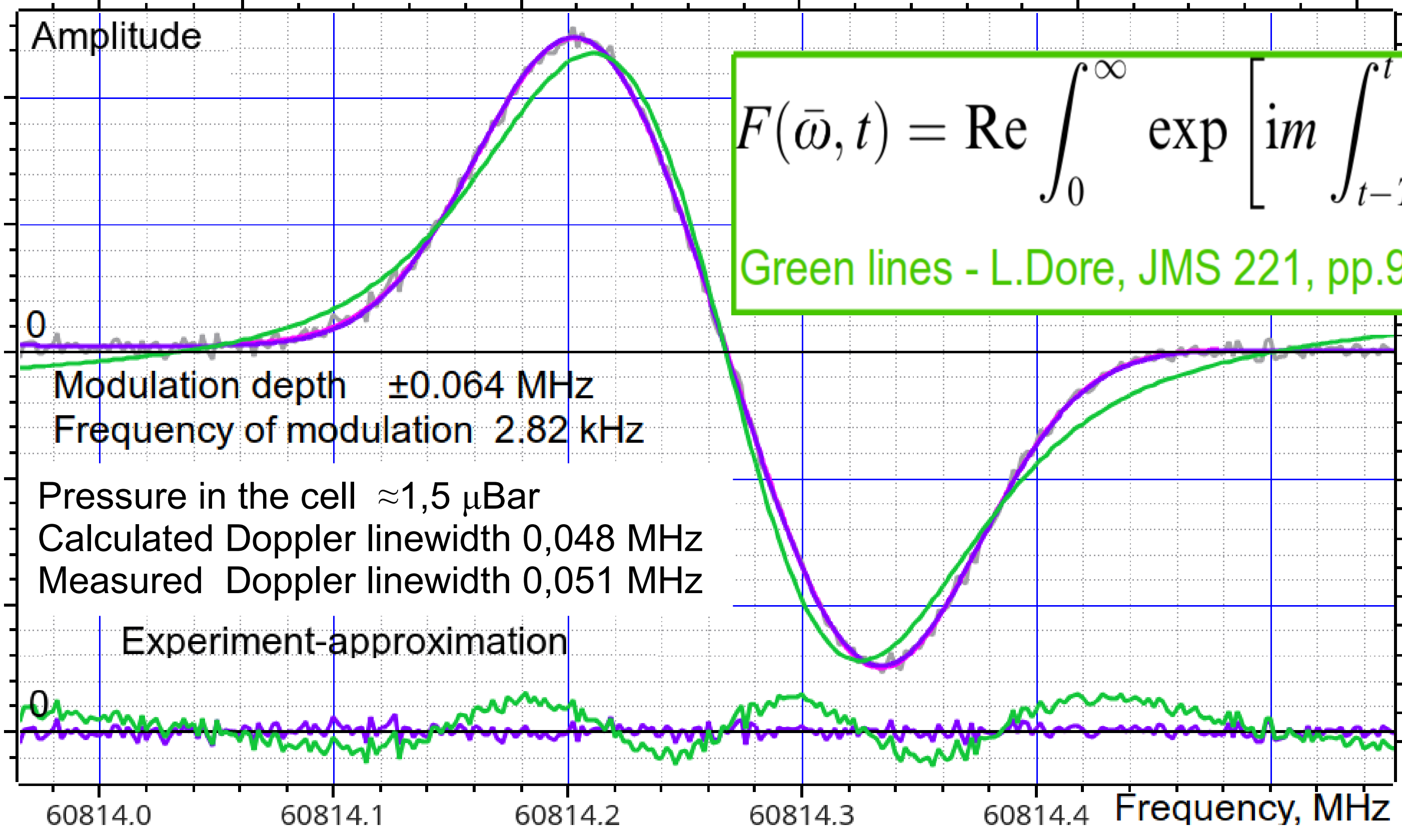
$$\frac{\gamma(\nu, \nu_0 + \Delta f) - \gamma(\nu, \nu_0 - \Delta f)}{2\Delta f}$$



Real record may be expressed as a numerical derivative obtained as difference of lineshapes at upper and lower frequency

So we propose to apply the numerical derivative as approximation function

Approximation of record obtained at middle modulation depth



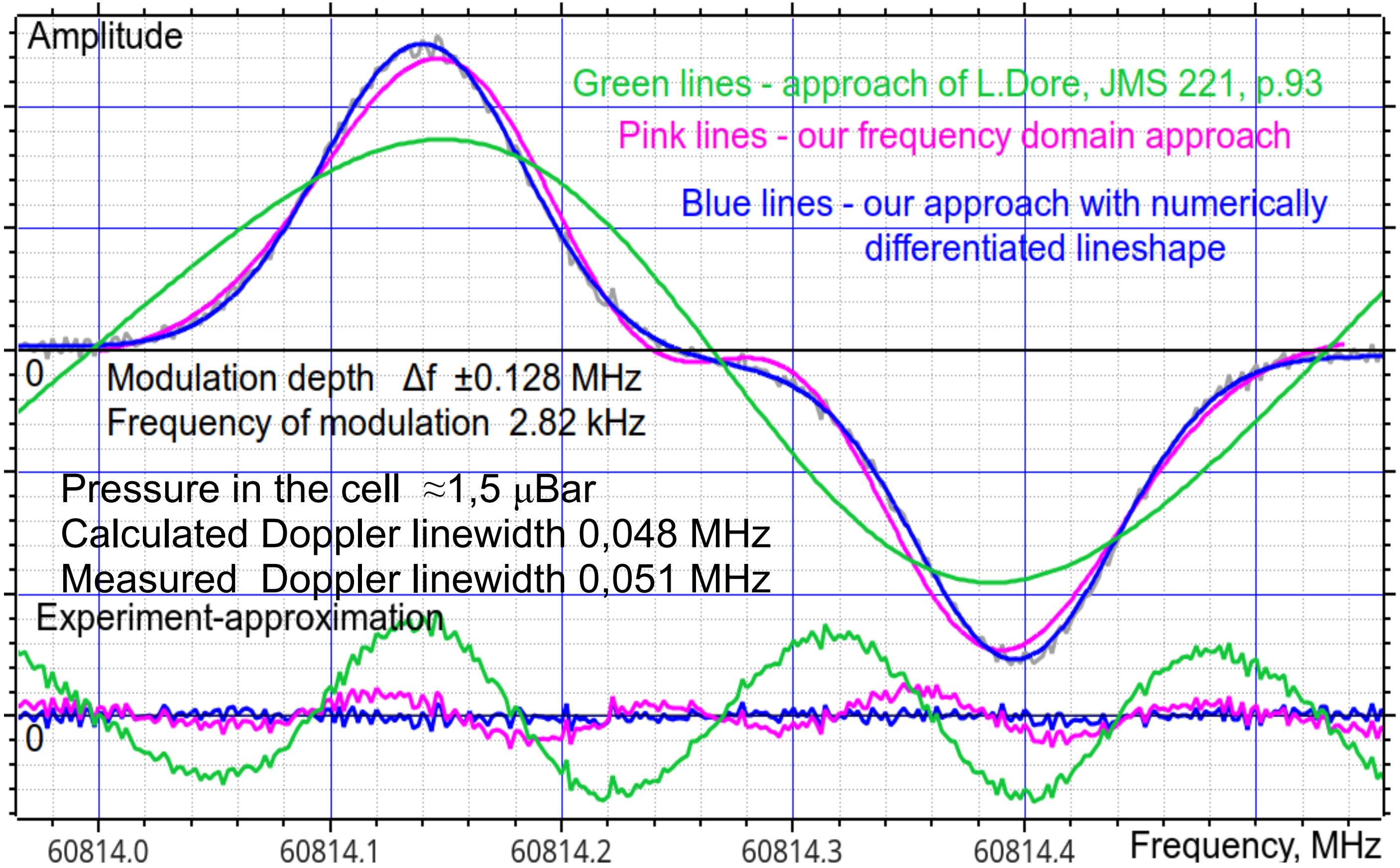
$$F(\bar{\omega}, t) = \mathrm{Re} \int_0^{\infty} \exp\left[\mathrm{i}m \int_{t-T}^{t} \cos \omega_m t' \, \mathrm{d}t' \right] \mathrm{e}^{-\mathrm{i}\bar{\omega} T} \Phi(T) \, \mathrm{d}T$$

Green lines - L.Dore, JMS 221, pp.93-98 $\omega(t) = \bar{\omega} - m \cos \omega_m t$

Approximation using sine-wave FM spectrum deviates from observed lineshape

Both proposed approaches show good quality of approximation

Approximation of record obtained at large modulation depth



Approximation using sine-wave FM is not able to reproduce experiment

"Numerical derivative" approach shows very good quality of approximation

Lineshape distortions caused by reflections in the cell (standing wave)*

Beer–Lambert–Bouguer law $i(\nu) = i_0(\nu)e^{-\gamma(\nu)l}$

With low absorption may be expanded in Taylor series $i(\nu) \approx i_0(\nu)(1-\gamma(\nu)l)$

where $\gamma(\nu)$ is true lineshape and l is length of the cell

* Source FM + 1*f* Lock-in detection => Spectra are recorded as the first derivative from true lineshape

$$i'(\nu) = i'_0 - l\, i'_0\, \gamma(\nu) - l\, i_0\, \gamma'(\nu)$$

* Usual approach: $i_0 = const$ (since i_0 varies very slowly)

The second term with $\gamma(\nu)$ vary rather quickly.
It introduces appreciable distortions of recorded line.
Since i_0 *a priori* is unknown we don't know ratio between the second and the third terms

* An idea of such approach was induced by paper of H.M.Pickett Appl.Optics. 19(16), pp.2745-2749

How to take into account distortions of observed lineshape?

Principal idea: consider ratio k between lineshape and distortions as fitted parameter. Observed lineshape will be fitted with following equation:

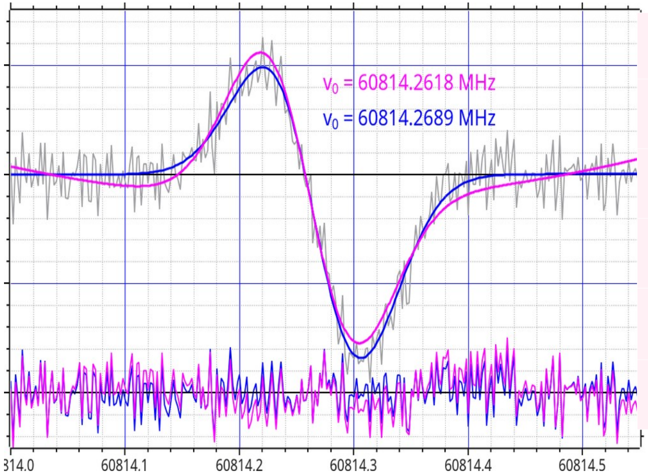
$$s(\nu) = (a\,\nu + b) + k\,\gamma(\nu, \nu_0) + \frac{\gamma(\nu, \nu_0 + \Delta f) - \gamma(\nu, \nu_0 - \Delta f)}{2\Delta f}$$

Observed lineshape — Baseline variations — Distortions due to reflections — Numerical derivative of Lineshape

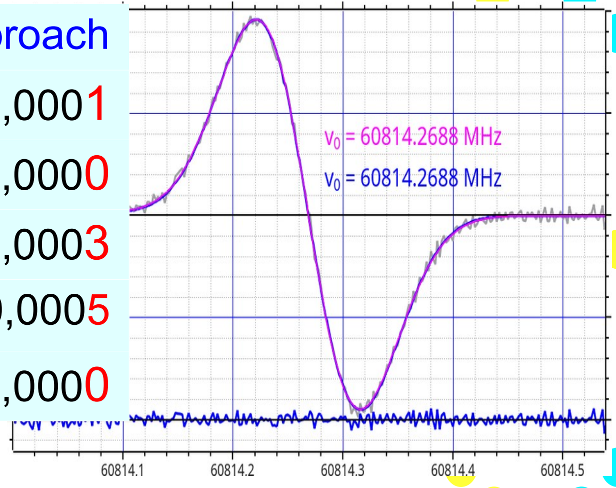
Usually such distortions lead to frequency determination error up to **±5** kHz and sometimes even **±10** kHz

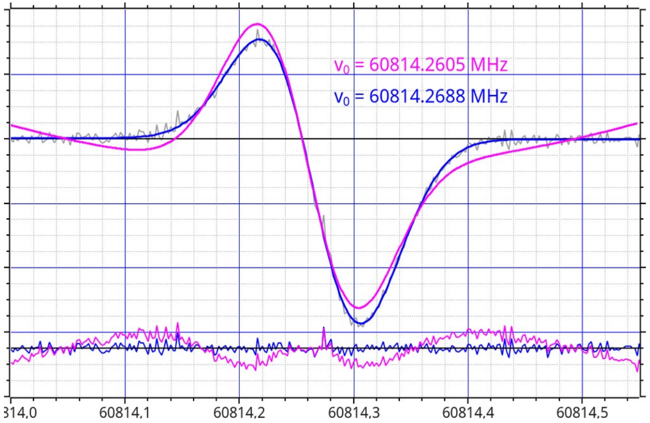
Taking into account distortions caused by reflections in the absorbing cell we obtained the reproducibility of about **±0.1 kHz** for OCS *J*=5-4 transition frequency

Approximation of OCS line obtained under different standing-wave conditions



Usual approach		Proposed approach	
60814,2618	0,0070	60814,2689	-0,0001
60814,2706	-0,0018	60814,2688	0,0000
60814,2651	0,0037	60814,2691	-0,0003
60814,2583	0,0105	60814,2683	0,0005
60814,2605	0,0083	60814,2688	0,0000





- Reflections in an absorbing cell lead to distortions (asymmetry) of lineshape
- Undistorted lines are measured with high accuracy
- Any distortions give errors during frequency measurements up to tens of kHz
- Proposed approach allows to reduce frequency determination error down to unities of kHz

Measured frequency of methanol lines

Transition	ν_{Lab} [1]	$\nu_{z=0.88582}$	K_μ	Our measurements	Correction
$3_{-1} - 2_0$ E	12178.597(4)	6457.985	-32.8	Out of range	Correction
$0_0 - 1_0$ A^+	48372.4558(7)	25650.6219	-1.0	48372.4644±0.0005	-0.0086
$0_0 - 1_0$ E	48376.892(10)	25652.974	-1.0	48376.8906±0.0005	0.0014
$2_{-1} - 1_0$ E	60531.489(10)	32098.233	-7.4	60531.4905±0.0005	-0.0015

Values of all frequencies were considerably corrected !

Conclusions

- Measured frequencies of three methanol lines were considerably improved
- Improvement was achieved by application of
    - DDS that allows to use square-wave FM with modulation parameters known with high-accuracy
    - “Numerical derivative” which gives very high quality of approximation at all values of modulation depth including also sub-Doppler resolution measurements using Lamb-dip technique

Thank you for your attention!