Modelling of precision laser spectroscopy experiments

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Methodology

1. High accuracy theoretical calculations of spectra
2. High precision laser spectroscopy measurement
3. Juxtaposition of theory with experiment

→ **(improved) values of fundamental particle characteristics:**

- particle masses (m_p/m_e, $m_{\bar{p}}/m_e$, $m_{\pi\pm}/m_e$)
- magnetic moments ($\mu_{\bar{p}}$)
- charge distribution (proton r.m.s. and Zemach radii)
- Ry, α, $d\alpha/dt$, etc.

Simple atomic systems

- Strong requirements to the accuracy of theory (10^{-10}, 10^{-11},?)

  achievable in simple 2 or 3 body systems only!

  → **Restricted choice of atomic systems:**

- Hydrogen atom
- Positronium e^+e^- and Muonium μ^+e^-
- Hydrogen molecular ions H_2^+, HD^+, D_2^+
- Exotic hydrogen $p^+\mu^-$, $p^+\pi^-$,…
- Exotic helium $He^{++}e^-p^-$, $He^{++}e^-\pi^-$, etc.

The 3 experimental projects of interest

- **ASACUSA (CERN)**

  laser spectroscopy of antiprotonic and pionic helium

  → antiproton magnetic moment, m_{p-}/m_e, $m_{\pi-}/m_e$ → CPT
- **FAMU (INFN+RIKEN-RAL)**

  laser spectroscopy of muonic hydrogen

  → muonic Zemach radius → proton size puzzle
- **PREMOL (University of Dusseldorf)**

  laser spectroscopy of trapped H2+, HD+ and D2+

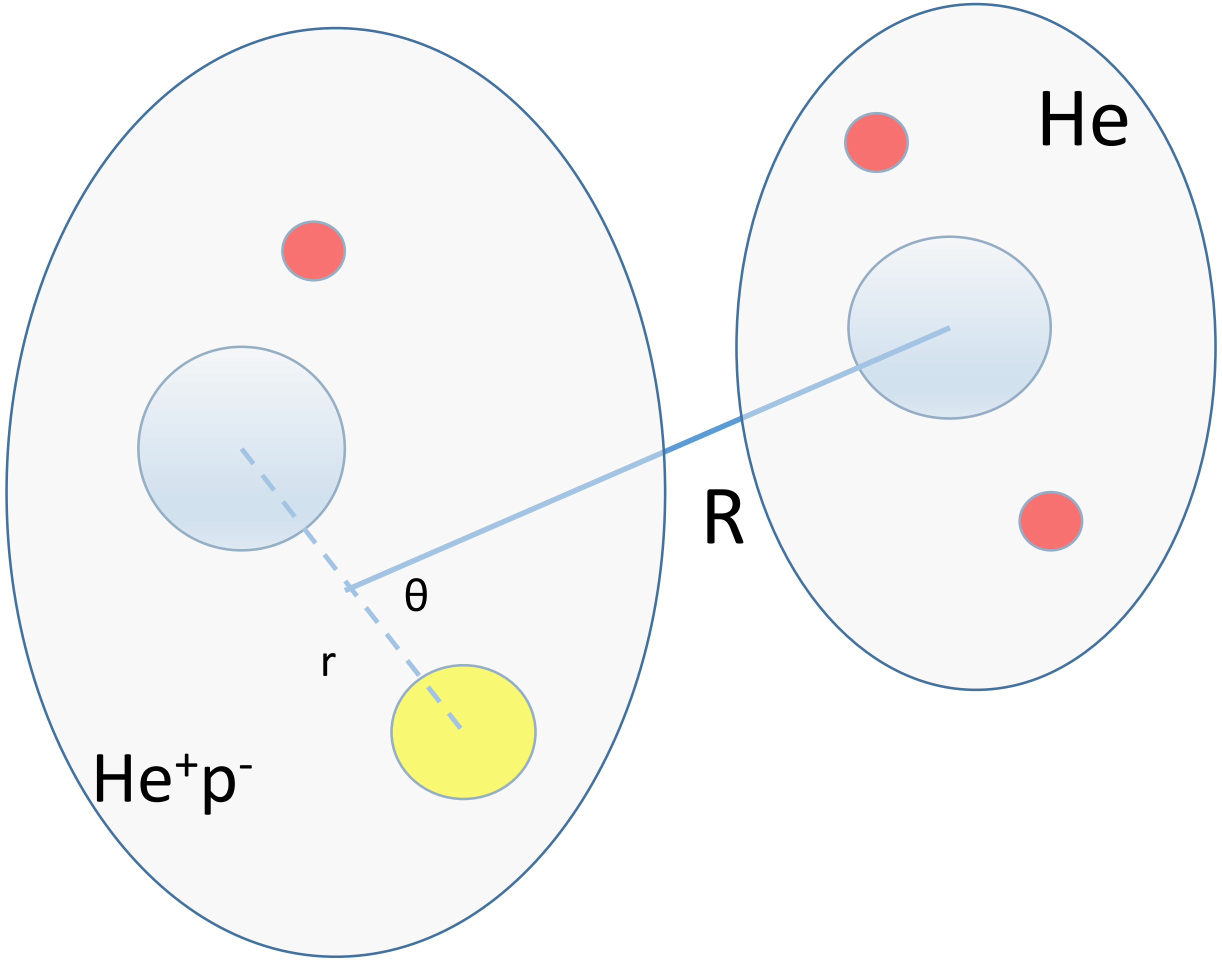
  → m_p/m_e, m_d/m_e,… → molecular clocks, $d\alpha/dt$

Modelling tasks

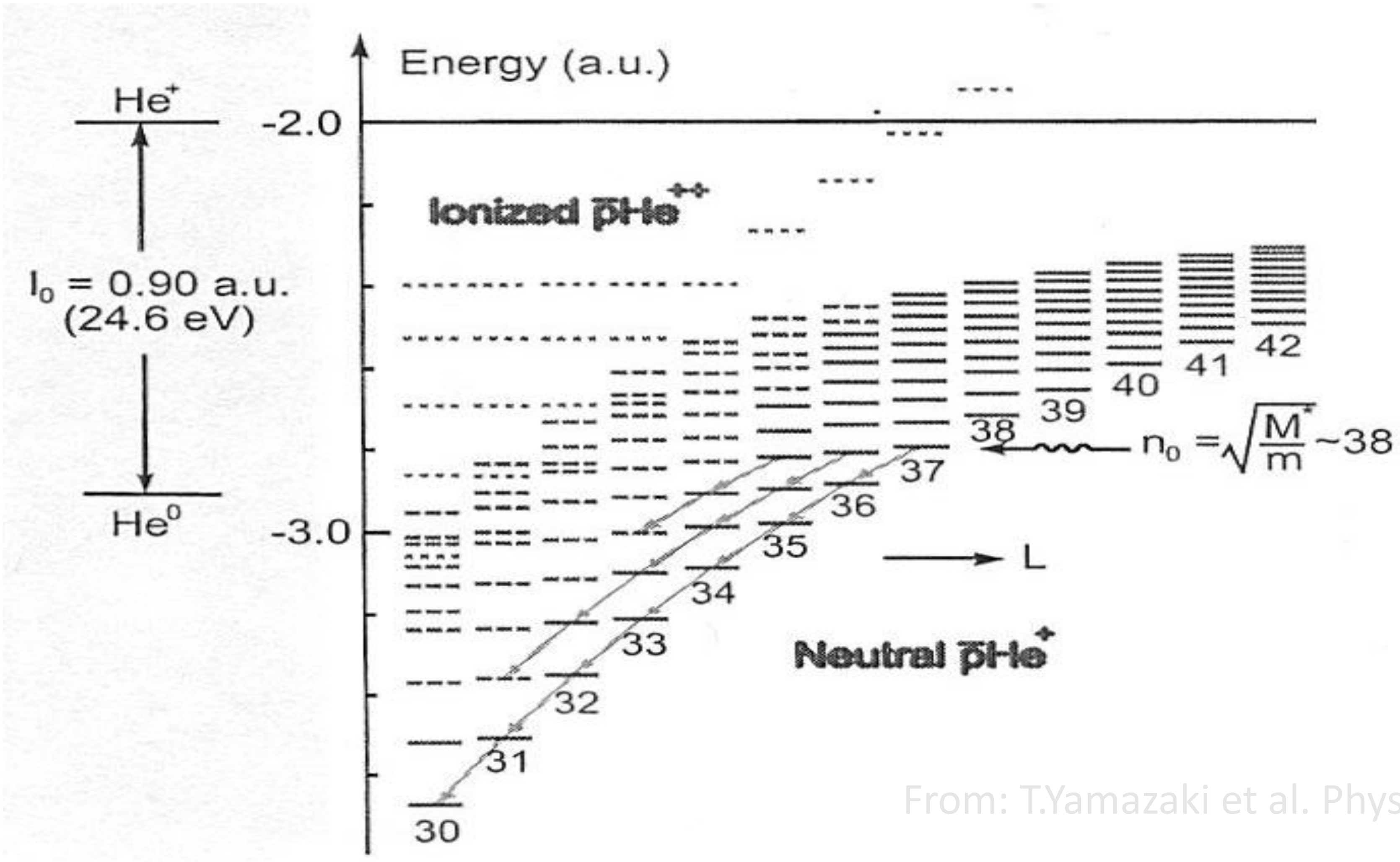
1. Evaluation of the systematic effects
   - External field effects (Zeeman, a.c. and d.c.Stark)
   - Density shift and broadening
2. Minimization of the systematic effects
   - Optimal selection of appropriate spectral lines
3. Optimization of the experimental conditions
   - Search for maximal efficiency of the set-up

ASACUSA (1): exotic helium atom

- Exotic helium: one electron (red dot) in He is replaced by p^- or π^- (yellow dot)
- Formed when antiproton (or pion) beam is stopped in He gas.
- Very accurate theory for <u>isolated</u> He^+p^- (Korobov,…)
- Main systematic effect: interaction with neighbor He atoms (density shift & broad.)



ASACUSA (2): isolated atom energy spectrum



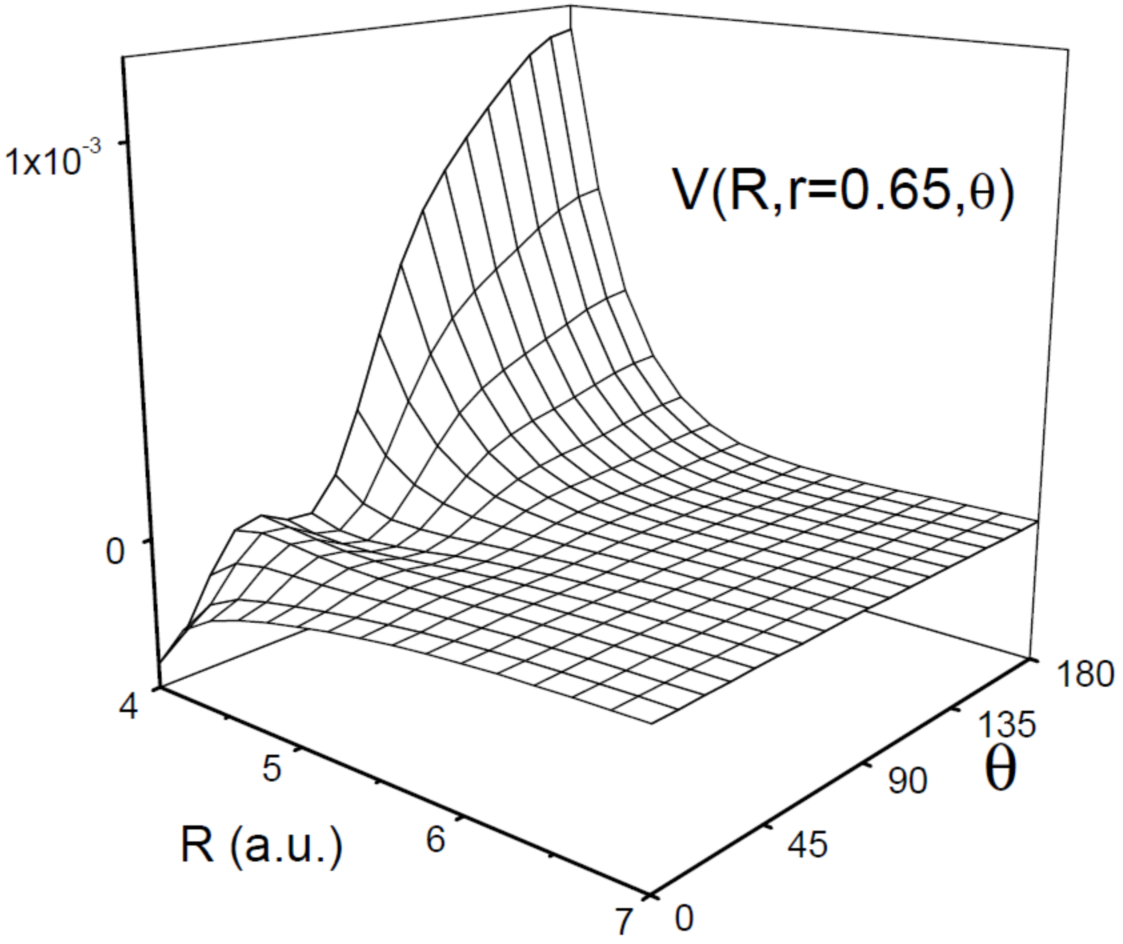
From: T.Yamazaki et al. Phys.Rep.366

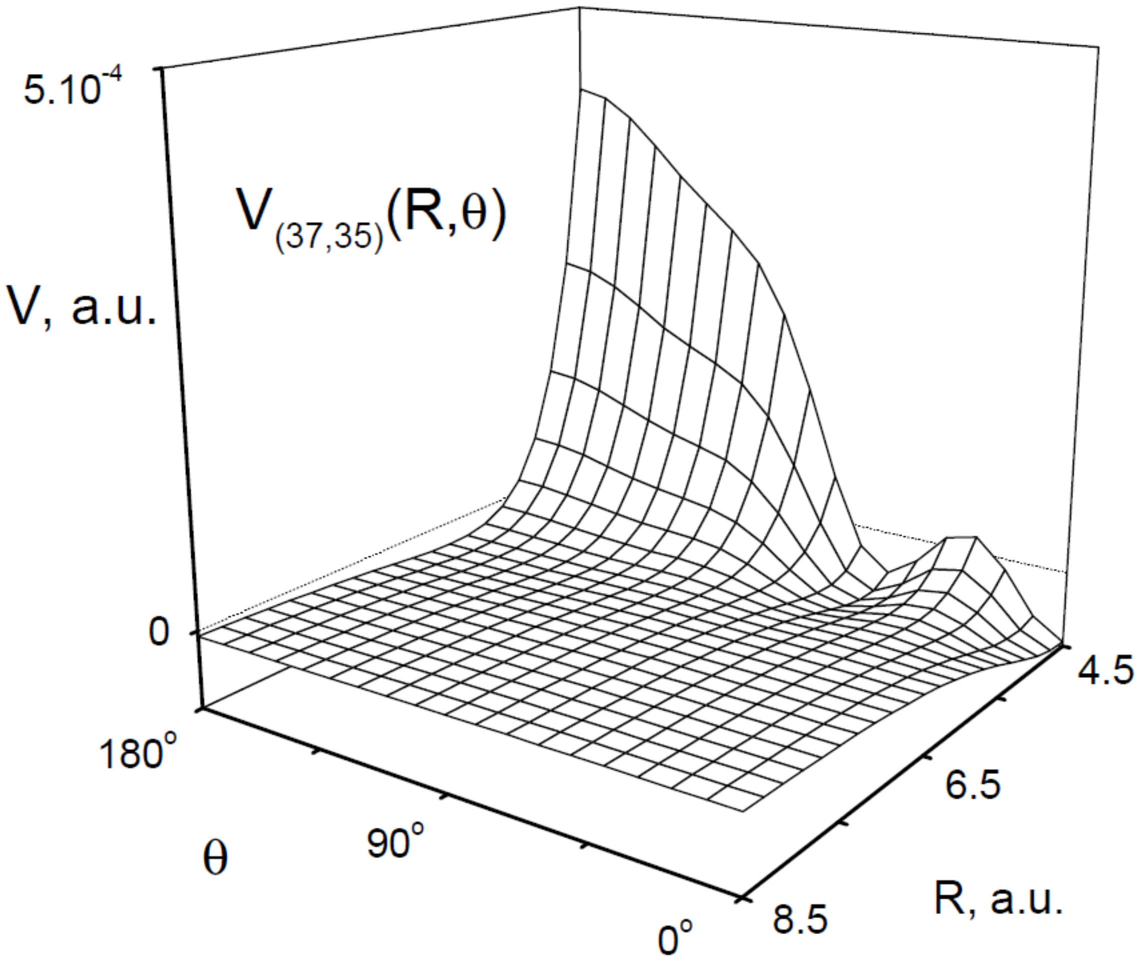
ASACUSA (3): Density shift & broadening

- Depends on the interaction of He^+p^- with He
- In the lowest order approximation: binary potential $V(R,r,\theta)$

  $V(R,r,\theta)$ = E(6-body system) – $E(He^+p-)$ – E(He)
- E(6-body system): calculated using Quantum chemistry methods
- 1999 calculation: $V(R,r,\theta)$ evaluated on a grid of 395 points
  accuracy $\sim 10^{-3}$, 8 hours CPU/point (SAPT, Szalewicz, Jeziorski)
- 2019 calculation: 25000 pts grid, 1 hour/point (Przybytek, Jeziorski)
- Density effect evaluation: Semiclassical; fully QM
- Precise PES needed for E1 and 2-photon laser spectroscopy.

ASACUSA (4): The PES





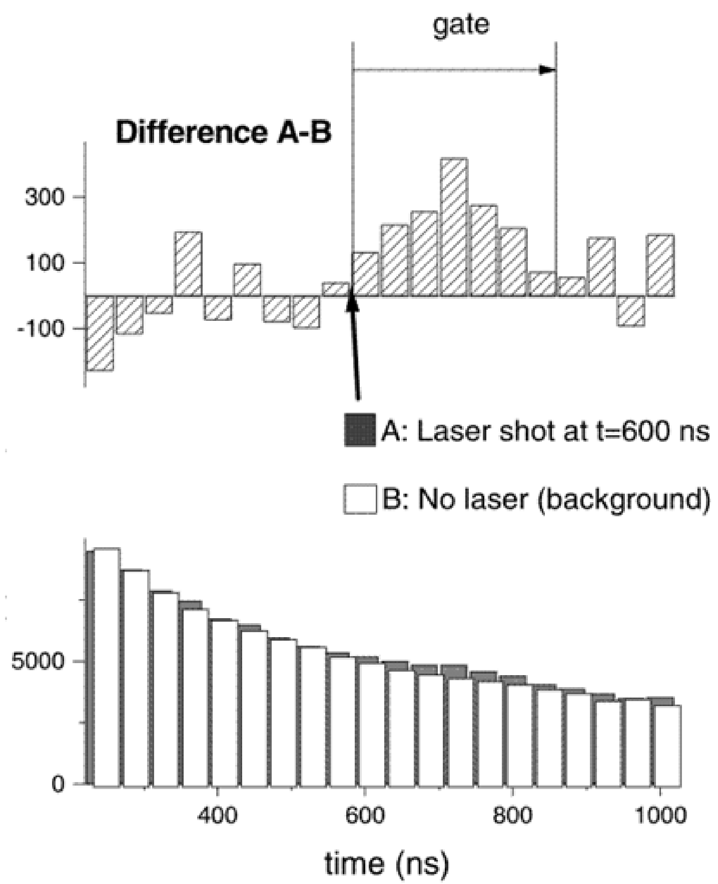
FAMU (1): IR laser spectroscopy of $\mu^{-}p$

- The goal: determine the proton Zemach radius R_Z
- Motivation: the Proton size puzzle (Pohl, 2010):

  the r.m.s. proton charge radii measured in ordinary and muonic hydrogen differ by 7σ; necessary to compare the Zemach radii
- Method: to extract R_Z measure the hyperfine splitting Δe^{hfs} in $(\mu p)_{1s}$

$$\Delta e^{hfs}[\text{meV}] = 182.819[\text{meV}] - 1.301[\text{meV/fm}]R_Z + 0.064[\text{meV}]$$

FAMU (2): The experimental method



- Muons are stopped in H_2/O_2 gas
- $(p\mu)_{1s}$ are formed
- IR laser pulses excite $(p\mu)_{1s}$
- The time distribution of the events of muon transfer as signature of resonant excitation of F=1 spin state.
- Signal Δ: count difference in gate
- Noise σ: sq.root of counts in gate

FAMU (3): The experiment

FAMU is a "frontier" spectroscopy experiment, because

- Muonic hydrogen atoms are very rare: only 10^3/second at RIKEN-RAL (standard optical spectroscopy techniques non applicable)
- Laser-induced spin-flip is a very weak M1 transition (standart detection methods not applicable)
- Pulsed IR laser at λ=6.7 nm did not exist; now have only ~2 mJ/pulse
- IR multi-pass cavity of ultra high reflectivity R>0.9995 needed

Detailed modelling of every step required to grant sufficient efficiency

FAMU: Beam and target optimization

- Slowing down and stopping of muons: multiple scattering
- Position of muon stops – many parameters to optimize:

    - initial muon beam characteristics,

    - composition, density, temperature of the target and gas

- Optimization by Monte Carlo simulations – very time consuming

→ Smooth fit to MC results, analytical optimization

→ Reliable extrapolation to unexplored materials [JINST(2016)]

Example: breakdown momentum $p_B(d,\rho)=26.6\ d^{0.2969}\ \rho^{0.2342}$ MeV/c

FAMU: Multi-pass cavity optimization

- Need to maximize the signal-to-noise ratio Δ/σ

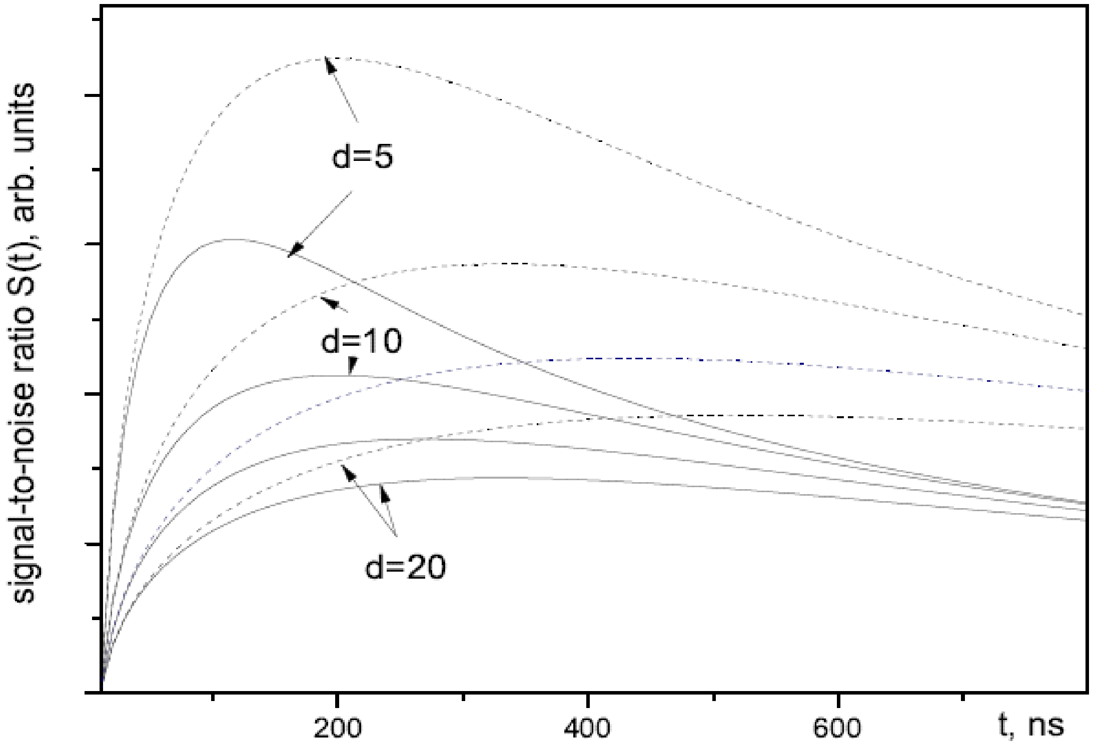


Figure 4. Dependence of the signal-to-noise ratio $S(t) = \Delta/\sigma$ (in arbitrary units) on the measurement time gate t, for a set of inter-mirror distances $d = 5(5)20$ cm, mirror reflectivity $R = 0.998$ (solid lines) or $R - 0.999$ (dashed lines), and laser pulse length τ_L=20 ns.

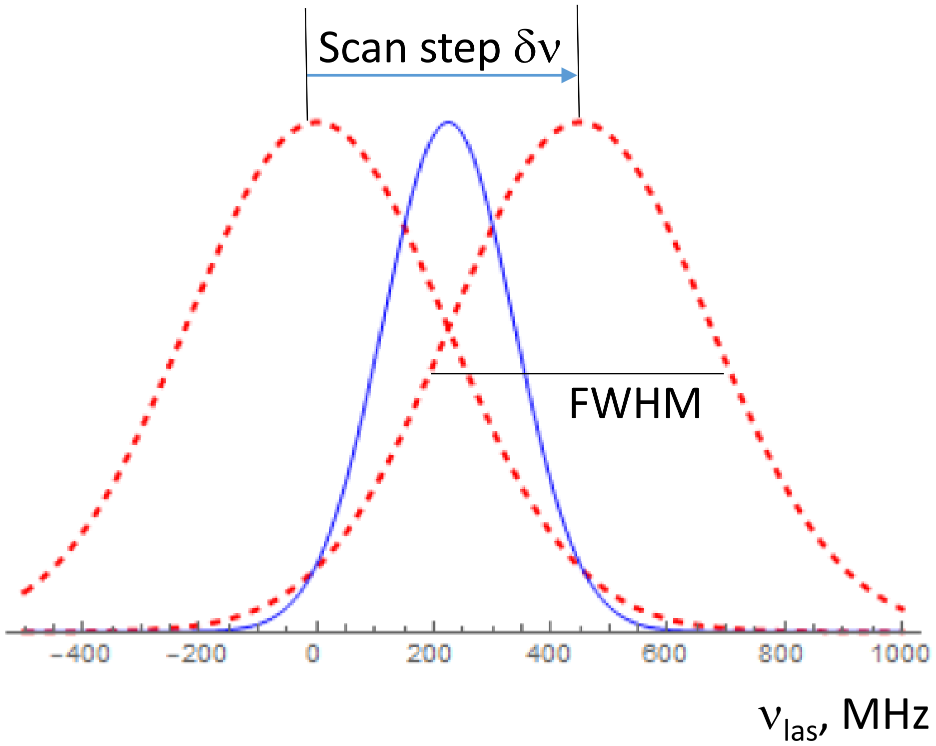
FAMU: Measurement strategy optimization

- Muons are "expensive"

  → Minimize the beam time

- Optimal frequency step for scanning the investigate range with the tunable IR laser:

$$\delta\nu = FWHM \, . \, (8Log(2))^{-1/2}$$



PREMOL

- High precision laser spectroscopy of trapped ions H_2^+,HD^+,D_2^+
- Comparison with theory (Korobov, …) →

  improved values of fundamental constants

To evaluate (prior to comparison): all systematic effects:

- external magnetic fields (Zeeman)
- external electric fields (a.c. & d.c. Stark)
- laser polarization effects, …

PREMOL: Zeeman splitting

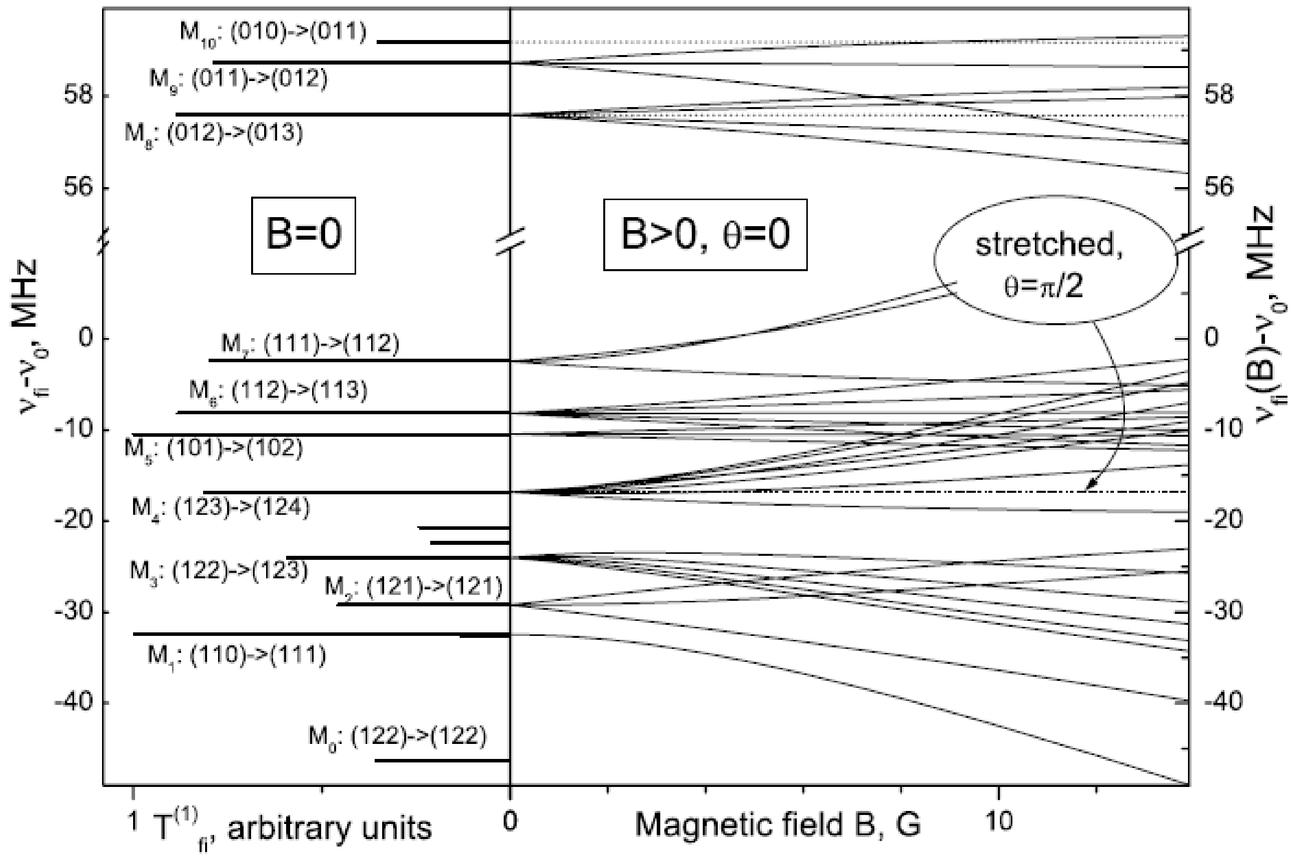
Zeeman shift (up to O(B2))

$\Delta E_Z = t\ M\ B + (q + r\ M^2)\ B^2$

Selected E1 spectral lines with minimal sensitivity to external magnetic field

Similar for M1, E2 and 2-photon

Similar for Stark shifts



PREMOL: Homonuclear molecular ions H_2^+,D_2^+

Possible transitions:

- ~~E1 (electric dipole)~~
- Forbidden E1
- 2-photon electric
- E2 electric quadrupole
- …
- …

PREMOL: Polarization effects in E2-lines

$T^{(2)}_M$ – amplitudes of E2-transitions with ΔM=q=-2,-1,…,2

Linear polarization

$$|\widehat{T}^{(2)0}|^2 = \tfrac{1}{4}\sin^2 2\beta\cos^2(\alpha-\theta),$$
$$|\widehat{T}^{(2)\pm1}|^2 = \tfrac{1}{12}(1+\sin^2(\alpha-\theta)\cos 2\beta+\cos^2(\alpha-\theta)\cos 4\beta),$$
$$|\widehat{T}^{(2)\pm2}|^2 = \tfrac{1}{24}\sin^2\beta\,(3+\cos 2\beta-2\sin^2\beta\cos 2(\alpha-\theta)),$$

circular polarization

$$|\widehat{T}^{(2)\,0}|^2 = \tfrac{1}{8}\sin^2 2\beta,$$
$$|\widehat{T}^{(2)\,\pm1}|^2 = \frac{1}{3}\begin{pmatrix}\sin^4\beta/2\\ \cos^4\beta/2\end{pmatrix}(1\pm2\cos\beta)^2,$$
$$|\widehat{T}^{(2)\,\pm2}|^2 = \frac{1}{3}\begin{pmatrix}\sin^4\beta/2\\ \cos^4\beta/2\end{pmatrix}\sin^2\beta.$$

Still more complicated expressions for elliptical polarization

PREMOL: Molecular clocks

- Appropriateness for molecular clocks: spectral lines with
  - as small as possible natural width
  - lowest overall sensitivity to systematic effects.
- Successful selection of several such lines: [PRL113(2014)]

  systematic uncertainty 5×10^{-17}
- Composite frequencies $\nu_c=\beta_1\nu_1+\beta_2\nu_2+\ldots\beta_k\nu_k$

  systematic uncertainty 10^{-18}
- Currently: completion and refinement of the selection in progress