Hyperfine spectroscopy of muonic hydrogen and the PSI Lamb shift experiment

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1. Introduction

The recent measurement at PSI of the Lamb shift in the muonic hydrogen atom [1–3] has had an important impact for the following reasons:

1. A new value of the r.m.s. charge radius of the proton, $r_p = 0.84184(67)$ fm has been obtained with experimental uncertainty $8 \times 10^{-4}$, more than one order of magnitude below the uncertainty of earlier results. This new value is to be used as input in the analysis of high accuracy atomic spectroscopy data, and also opens room for much more stringent tests of the existence of new physics have been put forward; none of them, however, has been acknowledged to be satisfactory so far;

2. The new value of $r_p$ is incompatible with the CODATA value [4], as well as with the latest update of the r.m.s. charge radius value obtained from $e-p$ scattering data [5]. This puzzle has been widely discussed since the publication of Ref. [1], and explanations varying from possible inaccuracies in the experimental methods or the underlying theoretical calculations to new physics have been put forward; none of them, however, has been acknowledged to be satisfactory so far;

3. This pioneering laser spectroscopy experiment in the FIR frequency range paves the way for more applications of laser spectroscopy to exotic atoms.

In what follows we analyze the new horizons for the measurement of the hyperfine splitting of the ground state of the muonic hydrogen atom, opened by the successful PSI Lamb shift experiment. We also give quantitative estimates of the efficiency of the experimental methods under consideration as function of the IR laser source power, and of the statistical uncertainty of the experimental data – the two known “bottle-necks” of the proposal.

2. Hyperfine splitting of the s-states of muonic hydrogen atoms

The theoretical expression for the hyperfine splitting, $\Delta E_n^{\text{HFS}}$, of the muonic hydrogen atom ($\mu^+p$) in the s-state ($ns$) with principal quantum number $n = 1, 2, \ldots$, is traditionally put in the form [6,7]

$$\Delta E_n^{\text{HFS}} = \Delta E_n(1 + \delta^{\text{QED}} + \delta^{\text{str}}),$$

where $\Delta E_n$ is the leading order Fermi term, expressed in terms of particle masses $m_p, m_\mu$, and the dipole magnetic moment of the proton $\mu_p$ (in units $\hbar = c = 1$):

$$\Delta E_n = \frac{8\pi^2}{3\hbar^2} \frac{m_p^2 m_\mu^2}{(m_p + m_\mu)^2} \mu_p$$

while $\delta^{\text{QED}}$ and $\delta^{\text{str}}$ are the pure QED correction and a term that describes the effects of proton structure. (Note that these two effects cannot be separated in higher orders.) The explicit expressions of the few first terms in the power series expansion of $\delta^{\text{QED}}$ in terms of the fine structure $\alpha$ can be found in, e.g. [6,7]. The proton-structure-depending correction $\delta^{\text{str}}$ is further put in the form

$\Delta E_n^{\text{HFS}} = \Delta E_n(1 + \delta^{\text{QED}} + \delta^{\text{str}})$
\[ \delta_{\text{str}} = \delta_{\text{rec}} + \delta^2 + \delta_{\text{pol}} + \delta_{\text{hvp}} \]  

(3)

in order to distinguish the contributions \( \delta_{\text{rec}}, \delta^2, \delta_{\text{pol}} \) and \( \delta_{\text{hvp}} \) of recoil, of the static charge and magnetic distribution within the proton, of the dynamical polarizability effects and of hadronic vacuum polarization respectively (though, strictly speaking, this representation holds only in the lowest order). The recoil term, of order \( O(2m_p|\vec{m}_s|) \), is independent of proton finite size effects; its explicit expression can be found in [6]. The dominating contribution to \( \delta_{\text{str}} \) comes from \( \delta^2 \) which, in the leading order approximation, has the form

\[ \delta^2 = -2.\pi \frac{m_p m_e}{m_e + m_p} \rho_p \]  

(4)

where \( \rho_p \) denotes the Zemach radius of the proton, defined as the first moment of the convolution of the proton charge and magnetic dipole momentum spatial distributions \( \rho_e \) and \( \rho_m \):

\[ \rho_p = \int \vec{d} \rho_p(\vec{r}) = \int \vec{d} \rho_p(\vec{r}) \rho_p(\vec{r} - \vec{r}). \]  

(5)

The radiative corrections to \( \delta^2 \) of order \( O(\alpha^2) \), analogous to what was calculated for normal hydrogen in Ref. [8], are yet to be computed. The corrections \( \delta_{\text{pol}} \) and \( \delta_{\text{hvp}} \) have been calculated in [9] with the use of phenomenological input data.

The latest theoretical values, calculated with account of all known corrections are \( \Delta E_{\text{exp}}^{\text{HFS}} = 182.725 \pm 0.062 \) meV [10], \( \Delta E_{\text{the}}^{\text{HFS}} = 22.8148 \pm 0.0078 \) meV [11]. While \( \Delta E_{\text{str}} \) scales as \( 1/\alpha \) (see Eq. 2), the dimensionless corrections \( \delta_{\alpha}, X = \text{QED, Z, pol, hvp} \), \( \delta_{\text{pol}} \) and \( \delta_{\text{hvp}} \) may vary slower with \( \alpha \). In what follows we use the estimates of their magnitude and uncertainty of Table 1 of Ref. [12].

3. The Zemach radius of the proton from measurements of the hyperfine splitting of muonic hydrogen

Measuring the hyperfine splitting in muonic hydrogen (and, in principle, in any hydrogen-like atom) and juxtaposing the experimentally observed value \( \Delta E_{\text{exp}}^{\text{HFS}} \) with \( \Delta E_{\text{the}}^{\text{HFS}} \) will provide – through Eqs. (1)–(5) – information on the electromagnetic structure of the proton. The overall uncertainty of \( \Delta E_{\text{the}}^{\text{HFS}} \) – of the order of \( 10^{-3} \) – is predominantly due to the uncertainty of the theoretical estimates of \( \delta_{\alpha} = \delta^2 + \delta_{\text{pol}} \), the not-yet-calculated higher order terms in \( \delta_{\text{pol}} \) and the uncertainty in \( \delta_{\text{hvp}} \), being of order \( 10^{-6} \) [12]. The accuracy of the current value of \( \delta_{\alpha} \) may be improved by a measurement of the hyperfine splitting in muonic hydrogen if the experimental uncertainty of \( \Delta E_{\text{exp}}^{\text{HFS}} \) is below \( 10^{-4} \). Unlike \( \delta^2 \), the proton polarizability correction \( \delta_{\text{pol}} \) is not directly related to a single parameter of the proton but is expressed instead in terms of its structure functions [9]. We therefore confirm the conclusion of Ref. [12] that measurements of \( \Delta E_{\text{exp}}^{\text{HFS}} \) should be regarded as measurements of \( \rho_p \), the Zemach radius of the proton.

Several authors have already extracted the value of \( \rho_p \) from the hyperfine splitting in the ground state of normal hydrogen [12–15]; however, the extracted values differ substantially [16]. The value of \( \rho_p \) has also been evaluated in [17] using the convolved distribution of Eq. (5) obtained from the assembly of the fits of the proton form factors of Refs. [5,18]; their value is only compatible with the results of Refs. [12] and [14]. It has already been pointed out that this puzzle might be solved by an independent measurement of \( \Delta E_{\text{exp}}^{\text{HFS}} \) in muonic hydrogen. The recent measurement of the Lamb shift in muonic hydrogen [1] has provided as a by-product the value of the hyperfine splitting in the 2s state \( \Delta E_{\text{exp}}^{\text{HFS}} \approx 23 \) meV, evaluated through the difference of the 2s(1s(F = 1) → 2p2p(F = 2) and 2S1/2(F = 0) → 2P3/2(F = 1) transition energies [19]. The experimental uncertainty of \( \Delta E_{\text{exp}}^{\text{HFS}} \) is estimated to \( \approx 6 \) meV, that leads to a relative uncertainty for the value of \( \rho_p \) of the order of 4% – too high to select the correct one among the competing theoretical predictions for the proton Zemach radius mentioned above. Recently, the experimental value of the hyperfine splitting in the ground state of muonic hydrogen \( \Delta E_{\text{exp}}^{\text{HFS}} = 211 \pm 19 \) meV has been obtained in [20] directly from spectroscopy data about the (3p–1s) transitions. The uncertainty of 9%, however, is too large to enable the determination of \( \rho_p \).

As already pointed out, the accurate knowledge of the Zemach radius of the proton offers an efficient tool for testing quantitatively the models of proton structure. In comparison to the r.m.s. proton charge radius, \( \rho_p \) has the important feature to be sensitive to the magnetic dipole moment distribution as well. In particular, the measurement of \( \rho_p \) with an uncertainty below 0.5% would impose independent experimental bounds on the low transfer momentum limit of the proton charge to magnetic form factors ratio [12]. Further on, comparing the values of \( \rho_p \) obtained in normal and muonic hydrogen might also help resolve the puzzle with the discrepancy between the values of the r.m.s. charge radius of the proton [1]. While the different moments of the convolved charge and magnetic distributions in the proton are independent and \( \rho_p \) cannot be used as an estimate of the third Zemach moment appearing in calculations of the Lamb shift [1], the measurement of \( \rho_p \) may provide firm ground for the exclusion of exotic proton structure models such as [21], which have been shown to produce first moments quite far from the expected range (see the third column of Table 1 of Ref. [17]). An important independent test of QED would be the evaluation of the Sternheim interval \( D_Z = \Delta E_{\text{exp}}^{\text{HFS}} - \Delta E_{\text{the}}^{\text{HFS}} \), in which the leading \( O(\alpha^2) \) order proton structure corrections are cancelled. All this, together with the recent progress in the development of fine tunable lasers in the FIR range, provides sufficient arguments to revive the projects for measuring the hyperfine splitting in the ground state of muonic hydrogen [22–24] that were abandoned for more than a decade.

4. Experimental methods for the measurement of the hyperfine splitting of the ground state of muonic hydrogen

The experimental method for the measurement of the hyperfine splitting in the ground state of the muonic hydrogen atom, initially proposed in [22], combines elementary particle with laser spectroscopy techniques. The muonic hydrogen atoms are formed when muons are slowed down and stopped in a pure hydrogen target between two parallel gold or aluminium plates. At sufficient hydrogen target densities the atoms are quickly de-excited, de-polarized and thermalized. The life of a muonic hydrogen atom ends up either with the decay of the muon, or in a collision with the walls of the target volume that leads to the transfer of the muon to the heavier gold or aluminium nucleus, followed by the prompt Coulomb de-excitation of the muonic (gold or aluminium) atom that is easily recognized by the accompanying emission of characteristic X-rays. The experimental method consists in studying the time distribution of the events of muon transfer from the proton to the heavier nucleus. When the target is irradiated with a laser tuned at the resonance wave length \( 2\nu_ch/\Delta E_{\text{exp}}^{\text{HFS}} \approx 6.76 \) μm and a muonic hydrogen atom in the ground singlet \( 1s(F = 0) \) state absorbs a photon of the resonance energy, it is excited to the triplet state \( 1s(F = 1) \) and later collisionally de-excited back to the singlet state. The de-excited atom is accelerated (about 2/3 of the de-excitation energy is transformed into kinetic energy), its free path grows up, and so does the probability for it to hit the target volume walls. The increase of the number of muon transfer events \( R = R(v) \) in an appropriate time gate and its variation in response to the variations of the laser wavelength \( v \) may therefore be used as a signature of the tuning of the laser source at the
resonance wavelength \( \nu_0 \) and provides a way to measure it. The efficiency of the method has been studied with Monte-Carlo simulations of the processes [22,23] based on the use of the differential cross sections of \( \mu^- \)–atoms by \( \text{H}_2 \) molecules, calculated \textit{ab initio} in [25]. The feasibility of the proposed measurement depends crucially on several factors that have been discussed only qualitatively; we present here their first quantitative estimates.

4.1. Tunable IR laser power

To estimate the required power of fine tunable sources of monochromatic radiation in the 6.7 \( \mu \)m wavelength range, we evaluate the probability for a spin–flip transition in the ground state of \( \mu^- \) stimulated by external oscillating magnetic field of frequency \( \nu \), \( \mathbf{B}(t) = \mathbf{B}_0 \cos 2 \pi \nu t \). The transition matrix element is (if choosing the quantization axis parallel to \( \mathbf{B}_0 \))

\[
\langle (1s)F = 1 | - \epsilon \hbar \cos 2 \pi \nu t (\hat{m}_y \mathbf{B}_0 \cdot \mathbf{s}_p - \hat{m}_y \mathbf{B}_0 \cdot \mathbf{s}_n) \rangle \langle (1s)F = 0 \rangle = \frac{-\epsilon \hbar}{2} \cos 2 \pi \nu t \left( \frac{m_e \mathbf{m}_p}{\mathbf{p}_p} \mathbf{s}_n - \frac{m_e \mathbf{m}_p}{\mathbf{p}_p} \mathbf{s}_n \right) ,
\]

where \( m_p, m_n, \mathbf{s}_p \), and \( \mathbf{s}_n \) denote the mass and the spin operator of the proton and the muon, and the proton and muon quantum moments \( \mu_p \) and \( \mu_n \) are in units \( \epsilon \hbar(2m_p) \) and \( \hbar(2m_p) \), respectively. The probability per unit \( dP/dt \) time for the spin–flip transition then is

\[
dP(v, \nu_0)/dt = \frac{1}{\hbar^2} \langle \mu_r | B_0 \rangle \, (m_e \mathbf{m}_p)^2 \left( \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} + \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} \right)^2 \delta(v - \nu_0),
\]

where \( \mu_r \) denotes the Bohr magneton and \( \nu_0 \) is the resonance frequency. The probability distribution of \( v_0 \) around the resonance frequency at rest \( \nu_0 = |H_{\text{RPS}}|/\hbar \) is \( \rho(v_0) = \left( \sigma_0/2 \pi \right)^{-1} \exp \left( -|v_0 - \nu_0|^2/2 \sigma_0^2 \right) \), with \( \sigma_0 = \nu_0 \times \sqrt{1/(m_p + m_n) c^2} \). Denote the laser line profile by \( \rho_l(v) \), and its width by \( \sigma_l \). The observable spin–flip probability \( dP/dt \) then becomes:

\[
dP(v, \nu_0)/dt = \int d\nu_0 \rho_l(\nu_0) \int d\nu_0 \rho_l(\nu_0) \, dP(v, \nu_0)/dt
\]

In the cases of interest \( \sigma_l \ll \sigma_0 \) that leads (if the laser is tuned at resonance) to

\[
dP/dt \approx \left( \frac{m_p + m_n}{\hbar^2 k T} \right)^2 \frac{\hbar^2 (m_p + m_n)^2}{\left( \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} + \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} \right)^2} \mathbf{B}_0^2 .
\]

The amplitude of the oscillating magnetic field \( \mathbf{B}_0 \) is related to the average density \( |F| \) of the energy flux carried by the electromagnetic wave through \( \mathbf{B}_0 = (2\mu_0/c) |F| \), where \( \mu_0 \) is the permeability of vacuum. The integration over the duration \( \tau \) of the laser pulse gives for the spin–flip probability \( P \)

\[
P = \frac{2\mu_0 \mu_0^2}{\hbar^2 c^2 v_0} \left( \frac{m_p + m_n}{\hbar^2 k T} \right)^2 \frac{\hbar^2 (m_p + m_n)^2}{\left( \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} + \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} \right)^2} \tau |F| .
\]

We now express the energy flux density \( |F| \) in terms of the energy output \( E \), the duration of the laser pulse \( \tau \) and the cross section of the laser beam \( S : |F| = E/(S \tau) \). After substituting the numerical values of the constants involved we finally get:

\[
P \approx 8 \times 10^{-5} \frac{E}{S \tau} \frac{\hbar^2 c^2 v_0}{\left( \frac{m_p + m_n}{\hbar^2 k T} \right)^2 \left( \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} + \frac{m_e}{\mathbf{p}_p} \frac{m_e}{\mathbf{p}_p} \right)^2} \, \tau |F| .
\]

where we assume that the value of \( E \) is given in J, of \( S \) in m², and of \( T \), the target temperature in K.

Using Eq. 9 we see, for instance, that the IR laser pulses of 0.25 mJ, produced by the laser system developed for the measurement of the Lamb shift in muonic hydrogen [1], if focused on a surface of 1 cm², would invert the spin of an atom within the irradiated volume at \( T = 300 \) K with the probability of only \( 1.2 \times 10^{-5} \) – too low for the proposed experiment to be feasible. The spin–flip probability could be increased by lowering the target temperature \( T \). To avoid the formation of molecular \( \mu^- \mu^+ \) ions [26], the temperature should not go below \(-10 \) K that limits the gain to a factor \(-6 \).

The efficiency may be increased much more substantially if the laser beam is squeezed by reducing its cross section with a factor \( k \) (thus increasing the energy flux density and the spin–flip probability \( P \) with the same factor), and the target is placed within a multipass cavity that provides \( k \) reflections (thus preserving the irradiated target volume unchanged). The PSI Lamb shift experimental team used a multipass cavity with \( k \approx 2 \times 10^3 \) [1]; using a similar one would bring the value of \( P \) to the reasonable 12%. There are, however, severe technical difficulties to have the target volume divided into thin slices with gold walls placed in a multipass cavity of high reflectivity.

The latter initiated the development of a modification of the experimental method of Ref. [22] in which the time distribution of the events of muon transfer to the nuclei of an appropriate gaseous admixture to the hydrogen target – rather than to the nuclei of the target walls – is used as signature of the laser-stimulated spin–flip in a muonic hydrogen atom [24]. While quantum mechanics predicts that, in the general case, the rate of muon transfer should be independent of the collision energy in the low energy limit, there are experimental evidences that the muon transfer rate to oxygen has a resonance-like behavior around 0.1 eV [27] and theoretical results [28,29] indicating that other gases may also exhibit a strong energy dependence in the same range of interest. The Monte-Carlo simulations of [24] have shown that the modified method has an efficiency that competes with the original one while imposing no restrictions on the use of a multipass cavity.

4.2. Muon sources

Both the experimental method proposed in [22,23] and the alternative version considered in [24,28] have the disadvantage that the “signal” (the increase of the number of muon transfer events in an appropriate time gate following the laser pulse) is accompanied by a significant “noise” (the background consisting of the muon transfer events from atoms that have not absorbed any photon of resonance frequency). If denoting the signal-to-noise ratio by \( \rho \), the relative statistical uncertainty \( \Delta v_0/v_0 \) of the experimental value of the resonance frequency \( v_0 \) may be approximately estimated as:

\[
\Delta v_0 \approx \frac{0.866}{\sqrt{m}} \left( \frac{t}{\rho} \right) \frac{1 + 3.35 \times 10^{-5}}{\sqrt{1 + 15 \times 10^{-6}}} \left( \frac{v_0}{\Gamma} - 1 \right)^2 - 11.25 \frac{\Gamma^2}{\sqrt{m}} \rho^2 .
\]

where \( \Gamma \) is the width of the interval of scanned frequencies, \( m \) is the number of measurements in this interval, and \( t \) is related to the confidence level \( 1 - \alpha = \epsilon t (t/2) \). The details of the derivation of Eq. (10) are given in the Appendix A.

The model-based Monte Carlo simulations in Ref. [24] showed that a signal-to-noise ratio of the order of \( \rho \approx 10 \) can be achieved in a wide variety of experimental conditions using bunches of 500,000 muons at each sampling frequency. According to Eq. (10), however, this wouldn’t guarantee a relative accuracy beyond \( 10^{-2} \). Further improvement could only be achieved with much higher values of \( \rho \) that requires in turn orders of magnitude higher statistics, that could possibly be reached using the recently developed muon sources at RAL [31]. The value of \( \rho \) could be further increased by carefully selecting the length and delay of the measurement time gate; as long as the purpose of the earlier
Monte Carlo simulations of Ref. [24] was only to demonstrate that the response of the time distribution was really observable, the values of the signal-to-noise ratio discussed there are far from the optimal ones. Since the magnitude of $\mu$ is sensitive to the details of the dependence of the muon transfer rate at epithe ral energies [28], it is worth studying quantitatively the behavior of the muon transfer rate to gases other than oxygen, carbon or neon and their applicability in the alternative experimental method of [24].

4.3. Doppler and density broadening

At room temperature, $T \approx 300$ K, the relative Doppler-broadening at FWHM of the para-to-ortho hyperfine transition line in the ground state of the muonic hydrogen atom is $1.17 \times 10^{-5}$ and practically sets no restrictions on the experimental accuracy. The density broadening and shift are yet to be evaluated, but the first estimates show that they would be negligible in the envisaged experimental conditions.

5. Conclusions

We demonstrate that the measurement of the hyperfine splitting of the ground state in muonic hydrogen has become particularly important after the recent successful Lamb shift experiment at PSI, in the frame of the open discussions about the incompatibility of the proton radii extracted using different methods. At the same time, we show that this measurements is technically closer to its realization than ever. We have revisited the existing experimental ideas for this measurement and analyzed the main methodological difficulties related to (1) the power of the available IR laser sources and (2) the relativistic low signal-to-noise ratio requiring an extended duration of the measurements. Each of these aspects is currently the subject to dedicated efforts; possible solutions for new laser sources are being envisaged [30], the existing high intensity pulsed muon sources are considered [31], and in-depth theoretical studies of the muon transfer with account to spin and molecular effects are in progress [32]. All these activities have good chances to converge into the realization of an experimental project almost as old as the measurement of the hyperfine splitting of hydrogen back in 1971 [33].

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Appendix A

To estimate the statistical uncertainty of the resonance frequency of IR laser $v_0$ (or, equivalently, the hyperfine splitting $\Delta_{\text{HI}}^{\text{para/ortho}} = h v_0$) we adopt the following simple model for the experiment described above: the “number of events of muon transfer $R(v)$” is repeatedly measured at $m$ different frequencies $v = v_i, i = 1, \ldots, m$ in the vicinity of the (unknown) resonance frequency $v_0$, and the frequency for which $R(v_0)$ is maximal is taken to be the experimental value of $v_0$. Denote by $y_i$ the number of counts at $v_i$, $y_i$ are values of the random variables $Y_i$ that are supposed to be independent and normally distributed: $Y_i \sim N(y_i, \sigma_i^2)$.

The resonance frequency $v_0$ is determined as follows: (1) the values $y_i$ are approximated with an appropriate smooth function $y = f(v; p_1, p_2, \ldots)$; (2) the values of the parameters $p_k$ are determined by the least square method from the equations

$$\frac{\partial}{\partial p_k} \sum_{i=1}^{m} [f(v_i; \{p_k\}) - y_i] = 0, \quad j = 1, 2, \ldots;$$

(3) the resonance frequency is then determined from $f(v; \{p_k\})|_{v=v_0} = 0$. To estimate the uncertainty of the values $v_0$ obtained this way, we use a simplified model in which (1) the experimental spectrum is fitted with the quadratic polynomial $f(v) = -a v^2/2 + b v + c$, and (2) the sampling frequencies are equidistant: $v_i = h(i - 1), i = 1, 2, \ldots, m$. The least square method then gives:

$$a = 2 \left(\frac{S_1 - S_3}{2} T_0 + (S_1 - S_3) T_1 + (S_0 - S_2) T_2\right)$$

$$b = \left(\frac{S_1 - S_3}{2} T_0 + (S_1 - S_3) T_1 + (S_0 - S_2) T_2\right)$$

where

$$S_k = \sum_{i=1}^{m} \frac{y_i}{v_i - v_k}, \quad k = 0, \ldots, 4 \quad T_k = \sum_{i=1}^{m} \frac{y_i v_i^k}{v_i}$$

For the particular choice of equidistant sampling frequencies defined above we get $S_0 = m, S_1 = h(m-1)/2, S_2 = h^2 m(m - 1)/(2m - 1)/6, S_3 = h^3 m(m - 1)/2(2m - 1)/30, S_4 = h^4 m(m - 1)/2(3m - 1)/90$.

The coefficients $a, A, B, \sigma_0^2, \sigma_a^2, \sigma_b^2, \sigma_{ab}^2$ are defined by

$$\sigma_0^2 = \frac{720 a^2}{h^2 m(m - 1)/2(2m - 1)/30}$$

$$\sigma_a^2 = \frac{12(8m - 11)(2m - 1)a^2}{h^2 m(m - 1)/2(2m - 1)/30}$$

with correlation coefficient $\rho_{ab}$ given by

$$\rho_{ab} = \frac{(A - B) - b}{a} = \frac{\sqrt{15(m - 1)^2}{\sqrt{8m - 11)(2m - 1)}}$$

The resonance frequency $v_0$ is calculated as $v_0 = \rho_{ab} / a$ and should be considered as a value of the random variable $Z = B/A$. The distribution of the ratio of two normal distributions has been considered in [34]; a good approximation of the probability density $\phi(z)$ of $Z$ is found there to be

$$\phi(z) = f(z) \frac{1}{\sqrt{2\pi}} \exp(-f(z)^2/2), \quad f(z) = \frac{z - \bar{a}}{\sqrt{\sigma_z^2 + 2 \rho_{z\sigma} \sigma_z \sigma_\bar{a} + \sigma_\bar{a}^2}}$$

i.e. $Z$ is approximately expressed in terms of the normally distributed random variable $T \sim N(0, 1)$ by means of the inverse relation $Z = f^{-1}(T)$, where

$$f^{-1}(t) = \begin{cases} \frac{1}{2} \arctan(t) - t, & t \leq 0 \\ \frac{1}{2} \arctan(t) + t, & t > 0 \end{cases}$$

Similar to the Cauchy probability density, $\phi(z)$ decreases slowly at $z \to \infty$ and the central moment integrals are divergent. Because of this, we define the uncertainty interval $[z_{-\sigma}, z_{+\sigma}]$ around the “most probable value” of $Z, z = \bar{a} / \sigma_\bar{a}$ through the normally distributed variable $T: z_{\pm \sigma} = f^{-1}(\pm \sigma); t$ so that $z \in [z_{-\sigma}, z_{+\sigma}]$ with the same probability as $T \in [-t, t]$. By substituting the explicit expressions of $\sigma_a, \sigma_\bar{a}$,
and $\rho_{\Delta m}$ into Eq. (16), we obtain for the uncertainty
\[ \Delta v_0 = \frac{(m - 1)^2}{4m(m + 1)(m^2 - 4)} \left( \frac{t}{\rho_0} \right)^2 \left( 1 - \frac{(m - 1)^2}{4m(m + 1)(m^2 - 4)} \rho_0^2 \right)^{-1} \times \left( \frac{v_0}{\Gamma} \right)^2 + \left( \frac{m^2 - 4}{15(m - 1)^2} - \frac{3(m - 1)^2}{4m(m + 1)} \rho_0^2 \right)^{1/2}. \]

Here $\Gamma$ is the half width of the scanned frequency interval: $2\Gamma = h(m - 1)$, while $\rho$ is the signal-to-noise ratio at resonance: $\rho = |R(v_0) - R(v_0 + \Gamma)|/\sigma$. The estimate $R(v_0) - R(v_0 + \Gamma) = -dt^2/2$ is obtained by assuming that $v_0$ is close to the center the scanned frequency interval. In the limit $m \gg 1$, Eq. 18 is transformed to Eq. (10).

Note that the relative uncertainty is minimized if the interval of scanned frequencies is symmetric with respect to $v_0$, so that $v_0/\Gamma = 1$; the latter may not hold for non-equidistant sampling frequencies. The parameter $t$ describes how stringent our estimate is supposed to be: the probability that the ratio $Z \in [z, z]$ is given by $\text{erf}(t/\sqrt{2})$. Values of reasonable interest are $t \sim 1$; for such values the terms quadratic in $t/\rho$ can usually be neglected. The relative uncertainty is mainly determined by the number of sampling points $m$ (decreasing as $m^{-1}$) and by the accuracy of the experimental values $\rho$ near resonance.

References

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