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Effect of the lock-in time constant on the NMR signal shape

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Abstract

We estimate the correction that has to be applied to the NMR signal height to take into account the effect of the lock-in time constant.

1 The Raw NMR Signal

The time evolution of the raw NMR signal can be ideally described with the parametrization :

$$S_{raw}(t) = \frac{H_1}{\sqrt{H_1^2 + \alpha^2 t^2}} \tag{1}$$

where t stands for the time (in s), H_1 is the RF field rotating component (H_1=90.8 mG) and α is the the sweep speed ($\alpha = 1.2$ G.s^{-1}). We usually include a linear background in the expression to fit the experimental data. The numerical values used are the default values of E94010 given in [1].

2 The NMR Signal Given by the Lock-in Amplifier

The shaping due to the lock-in time constant can be described by the first order differential equation (as seen for the study of the water signal model, cf. [2]) :

$$\frac{dS_{lock-in}(t)}{dt} = \frac{1}{t_c}\left(S_{raw}(t) - S_{lock-in}(t)\right) \tag{2}$$

where t_c is the lock-in time constant. With the initial condition at the time t_i when the sweep starts :

$$\frac{dS_{lock-in}}{dt}(t = t_i) = 0 = \frac{1}{t_c}\left(S_{raw}(t_i) - S_{lock-in}(t_i)\right) \tag{3}$$

The solution is :

$$S_{lock-in}(t) = e^{-(t-t_i)/t_c}\left[S_{raw}(t_i) + \frac{1}{t_c}\int_{t_i}^{t} e^{(u-t_i)/t_c} S_{raw}(u)du\right] \tag{4}$$

Figure 2 shows you the evolution of the signal given by the lock-in when the time constant t_c goes from 10 ms to 100 ms. We clearly see that the height of the lock-in signal decreases when the time constant of the lock-in increases.

3 Height Correction

Using for example H_1=62 mG, the previous differential equation has been solved with Mathematica v3.0. The raw signal and the numerical solution of the differential equation have been represented on Figure 1 (dots). These two signals have then been fitted with Paw using the usual parametrization (cf. [1]) :

$$signal(t) = \frac{h}{\sqrt{1 + \frac{(t-t_{res})^2}{w^2}}} \tag{5}$$

with : width w (in G), resonance time t_{res}(in s) and peak height h (in Arbitrary Unit), as described in [1].

For a RF field value H_1=62 mG, the fits show us that the raw signal is larger than the signal given by the lock-in (ratio raw/lock-in = 1.01) and that the lock-in signal is also delayed by approximately t_c.

For different values of H_1, ranging from 10 mG to 100 mG, we have estimated as previoulsly described the following ratios :

- HEIGHT ratio : ratio of the raw NMR signal height to the lock-in NMR signal height
- WIDTH ratio : ratio of the raw NMR signal width to the lock-in NMR signal width

These ratios are shown on Figure 3. They have been interpolated using Mathematica 3.0. Refer to Figure 4 and to Figure 5. The values of each ratio for values of H_1 ranging from 10 mG to 100 mG by steps of 0.5 mG are given in the numerical tables shown on Figures 6 and 7.

4 Conclusion

For an absolute calibration of the NMR setup, it is necessary to increase the height of the lock-in signals to account for the lock-in time constant effect. This correction is not necessary for the usual relative calibration using the water target, since the AFP conditions and settings (H_1, lock-in, ...) remain the same.

References

[1] S. Incerti "The NMR system of the Hall A polarized Helium 3 target", E94-010 Technical Note 9 (November 1998)

[2] S. Incerti and E. Lakuriqi, "Model of the water signal shape from the Bloch equations", E94-010 Technical Note 10 (November 1998)

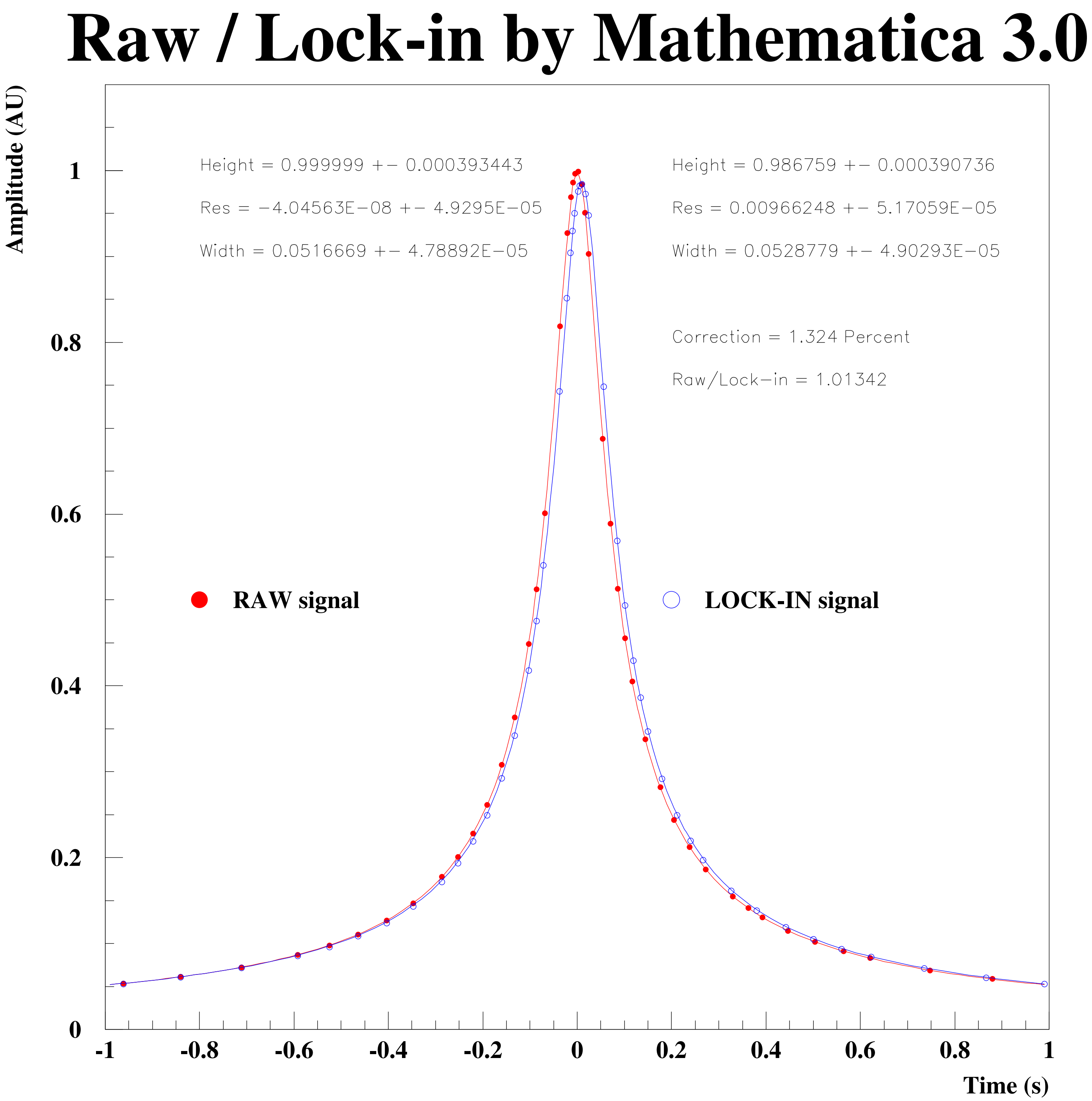

Figure 1: Shape (calculated by Mathematica) and fit (calculated by Paw) of the raw signal (plain circles) and of the signal given by the lock-in (open circles). Height stands for the height given by the fit (called h), Res for t_{res} and Width for w. Vertical scale in arbitrary units.

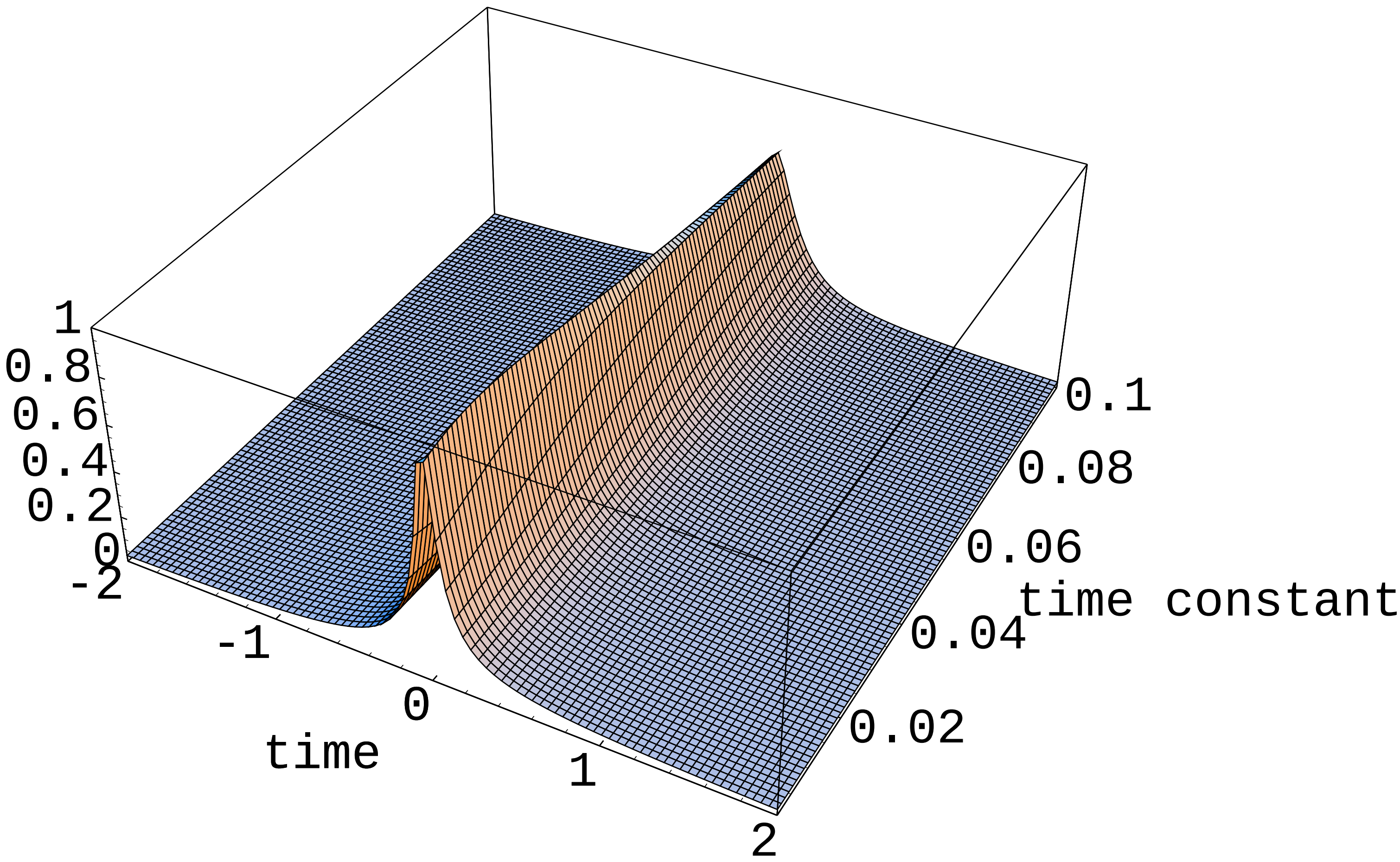

Figure 2: Mathematica modelization of the signal given by the lock-in as a function of time (left axis, from -2 s to 2s) and as a function of the lock-in time constant (right axis, from 10 ms to 100 ms).

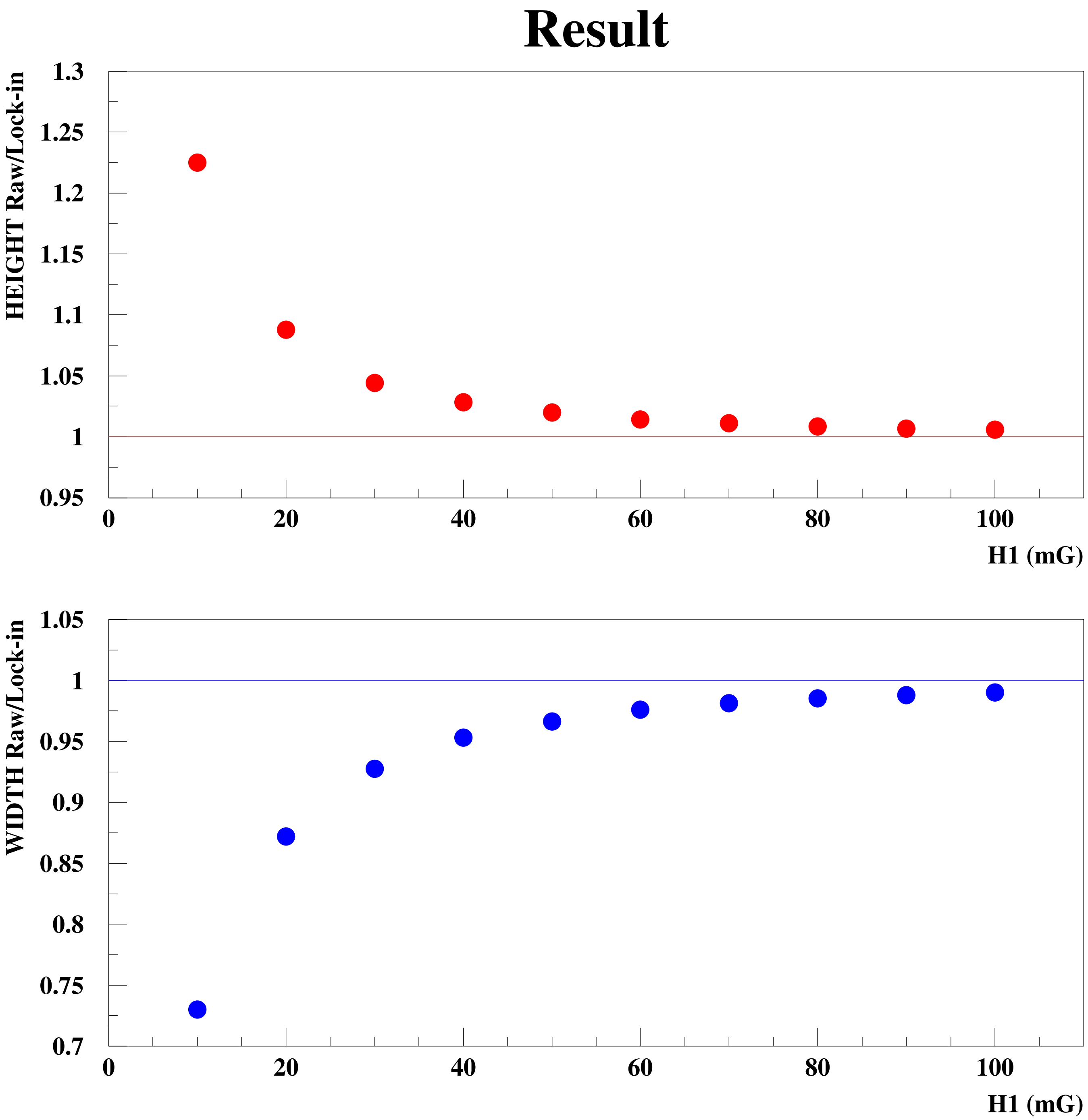

Figure 3: Mathematica modelization of the HEIGHT and WIDTH ratios, as a function of H_1 (mG).

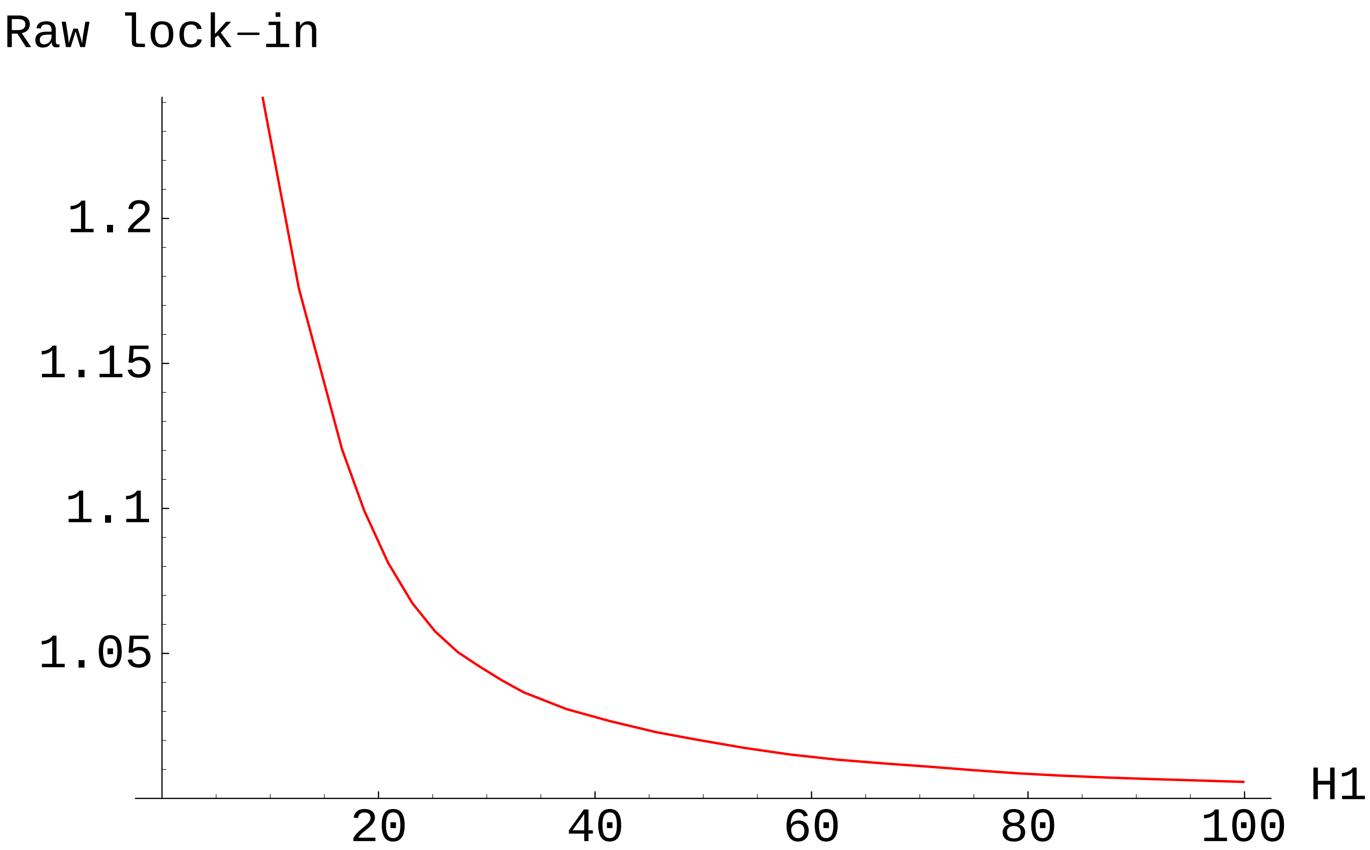

Figure 4: Cubic interpolation of the HEIGHT ratio.

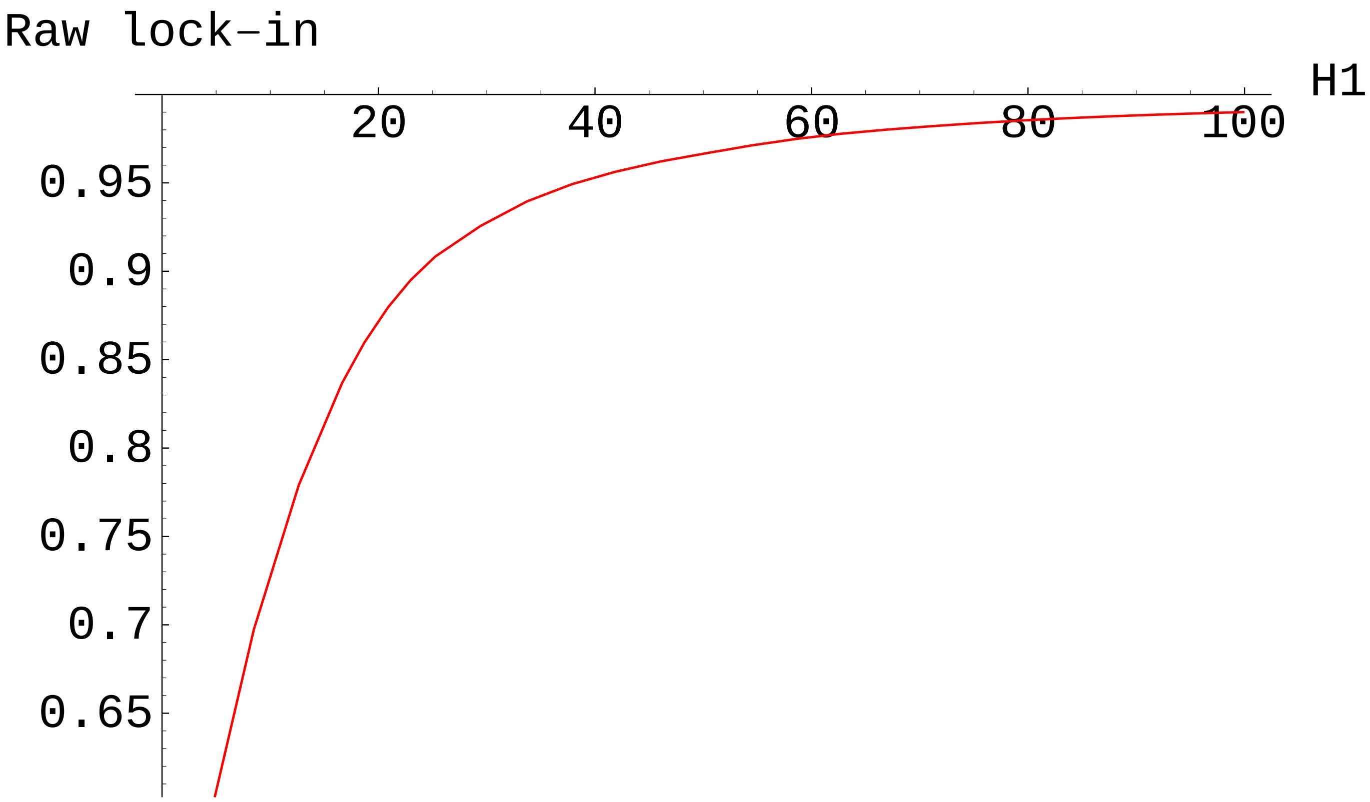

Figure 5: Cubic interpolation of the WIDTH ratio.

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*** CUBIC INTERPOLATION OF HEIGHT RATIO ***

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    1.17825},{13.,1.17005},{13.5,1.1622},{14.,1.15468},{14.5,1.14749},{15.,
    1.14063},{15.5,1.13408},{16.,1.12784},{16.5,1.12189},{17.,1.11624},{17.5,
    1.11086},{18.,1.10576},{18.5,1.10093},{19.,1.09635},{19.5,1.09202},{20.,
    1.08793},{20.5,1.08408},{21.,1.08044},{21.5,1.07703},{22.,1.07382},{22.5,
    1.07082},{23.,1.068},{23.5,1.06537},{24.,1.06292},{24.5,1.06063},{25.,
    1.0585},{25.5,1.05652},{26.,1.05469},{26.5,1.05299},{27.,1.05141},{27.5,
    1.04996},{28.,1.04861},{28.5,1.04737},{29.,1.04622},{29.5,1.04515},{30.,
    1.04417},{30.5,1.04287},{31.,1.04165},{31.5,1.04048},{32.,1.03938},{32.5,
    1.03834},{33.,1.03736},{33.5,1.03643},{34.,1.03555},{34.5,1.03472},{35.,
    1.03394},{35.5,1.0332},{36.,1.0325},{36.5,1.03185},{37.,1.03123},{37.5,
    1.03064},{38.,1.03009},{38.5,1.02957},{39.,1.02907},{39.5,1.02859},{40.,
    1.02814},{40.5,1.02759},{41.,1.02705},{41.5,1.02653},{42.,1.02603},{42.5,
    1.02555},{43.,1.02508},{43.5,1.02463},{44.,1.02419},{44.5,1.02377},{45.,
    1.02336},{45.5,1.02296},{46.,1.02258},{46.5,1.0222},{47.,1.02184},{47.5,
    1.02149},{48.,1.02115},{48.5,1.02082},{49.,1.02049},{49.5,1.02018},{50.,
    1.01987},{50.5,1.01953},{51.,1.01919},{51.5,1.01886},{52.,1.01853},{52.5,
    1.01821},{53.,1.0179},{53.5,1.0176},{54.,1.0173},{54.5,1.01701},{55.,
    1.01672},{55.5,1.01644},{56.,1.01617},{56.5,1.01591},{57.,1.01565},{57.5,
    1.01539},{58.,1.01515},{58.5,1.01491},{59.,1.01468},{59.5,1.01445},{60.,
    1.01423},{60.5,1.01404},{61.,1.01385},{61.5,1.01367},{62.,1.01349},{62.5,
    1.01332},{63.,1.01315},{63.5,1.01299},{64.,1.01284},{64.5,1.01268},{65.,
    1.01253},{65.5,1.01239},{66.,1.01225},{66.5,1.01211},{67.,1.01197},{67.5,
    1.01184},{68.,1.01171},{68.5,1.01158},{69.,1.01145},{69.5,1.01132},{70.,
    1.0112},{70.5,1.01105},{71.,1.01089},{71.5,1.01074},{72.,1.01059},{72.5,
    1.01044},{73.,1.0103},{73.5,1.01015},{74.,1.01001},{74.5,1.00986},{75.,
    1.00972},{75.5,1.00958},{76.,1.00944},{76.5,1.00931},{77.,1.00917},{77.5,
    1.00904},{78.,1.00891},{78.5,1.00879},{79.,1.00866},{79.5,1.00854},{80.,
    1.00842},{80.5,1.00832},{81.,1.00822},{81.5,1.00813},{82.,1.00804},{82.5,
    1.00795},{83.,1.00786},{83.5,1.00777},{84.,1.00769},{84.5,1.00761},{85.,
    1.00753},{85.5,1.00746},{86.,1.00738},{86.5,1.00731},{87.,1.00724},{87.5,
    1.00717},{88.,1.0071},{88.5,1.00704},{89.,1.00697},{89.5,1.00691},{90.,
    1.00685},{90.5,1.00678},{91.,1.00672},{91.5,1.00666},{92.,1.00661},{92.5,
    1.00655},{93.,1.00649},{93.5,1.00643},{94.,1.00638},{94.5,1.00632},{95.,
    1.00626},{95.5,1.00621},{96.,1.00615},{96.5,1.00609},{97.,1.00604},{97.5,
    1.00598},{98.,1.00592},{98.5,1.00586},{99.,1.0058},{99.5,1.00574},{100.,
    1.00568}}
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Figure 6: Numerical table of the interpolated values of the HEIGHT ratio.

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*** CUBIC INTERPOLATION OF WIDTH RATIO ***

{{10,0.729992},{10.5,0.740034},{11.,0.749724},{11.5,0.759069},{12.,0.768076},{
    12.5,0.776753},{13.,0.785107},{13.5,0.793144},{14.,0.800872},{14.5,
    0.808297},{15.,0.815428},{15.5,0.822271},{16.,0.828833},{16.5,0.835122},{
    17.,0.841144},{17.5,0.846906},{18.,0.852417},{18.5,0.857682},{19.,
    0.862709},{19.5,0.867505},{20.,0.872077},{20.5,0.876432},{21.,0.880578},{
    21.5,0.884521},{22.,0.888269},{22.5,0.891829},{23.,0.895208},{23.5,
    0.898412},{24.,0.901449},{24.5,0.904327},{25.,0.907052},{25.5,0.909631},{
    26.,0.912072},{26.5,0.914382},{27.,0.916567},{27.5,0.918635},{28.,
    0.920593},{28.5,0.922449},{29.,0.924208},{29.5,0.925879},{30.,0.927468},{
    30.5,0.92931},{31.,0.93108},{31.5,0.932779},{32.,0.934411},{32.5,
    0.935977},{33.,0.93748},{33.5,0.938921},{34.,0.940303},{34.5,0.941629},{
    35.,0.942899},{35.5,0.944117},{36.,0.945285},{36.5,0.946405},{37.,
    0.947478},{37.5,0.948508},{38.,0.949497},{38.5,0.950446},{39.,0.951358},{
    39.5,0.952235},{40.,0.953079},{40.5,0.953969},{41.,0.954829},{41.5,
    0.955661},{42.,0.956466},{42.5,0.957244},{43.,0.957996},{43.5,0.958725},{
    44.,0.95943},{44.5,0.960113},{45.,0.960775},{45.5,0.961417},{46.,
    0.962039},{46.5,0.962644},{47.,0.963231},{47.5,0.963803},{48.,0.96436},{
    48.5,0.964903},{49.,0.965433},{49.5,0.965951},{50.,0.966459},{50.5,
    0.967027},{51.,0.967586},{51.5,0.968134},{52.,0.968674},{52.5,0.969203},{
    53.,0.969723},{53.5,0.970233},{54.,0.970733},{54.5,0.971224},{55.,
    0.971704},{55.5,0.972175},{56.,0.972637},{56.5,0.973088},{57.,0.97353},{
    57.5,0.973962},{58.,0.974384},{58.5,0.974796},{59.,0.975199},{59.5,
    0.975591},{60.,0.975974},{60.5,0.976327},{61.,0.97667},{61.5,0.977004},{
    62.,0.97733},{62.5,0.977646},{63.,0.977954},{63.5,0.978254},{64.,
    0.978546},{64.5,0.978831},{65.,0.979108},{65.5,0.979378},{66.,0.979642},{
    66.5,0.979899},{67.,0.98015},{67.5,0.980396},{68.,0.980636},{68.5,
    0.98087},{69.,0.9811},{69.5,0.981325},{70.,0.981546},{70.5,0.981779},{71.,
    0.982007},{71.5,0.982232},{72.,0.982453},{72.5,0.98267},{73.,0.982883},{
    73.5,0.983093},{74.,0.983298},{74.5,0.9835},{75.,0.983699},{75.5,
    0.983894},{76.,0.984085},{76.5,0.984272},{77.,0.984457},{77.5,0.984638},{
    78.,0.984815},{78.5,0.984989},{79.,0.98516},{79.5,0.985328},{80.,
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    82.5,0.986267},{83.,0.986413},{83.5,0.986556},{84.,0.986697},{84.5,
    0.986835},{85.,0.98697},{85.5,0.987102},{86.,0.987232},{86.5,0.98736},{
    87.,0.987485},{87.5,0.987608},{88.,0.987728},{88.5,0.987846},{89.,
    0.987962},{89.5,0.988076},{90.,0.988187},{90.5,0.988297},{91.,0.988404},{
    91.5,0.98851},{92.,0.988613},{92.5,0.988715},{93.,0.988815},{93.5,
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    96.,0.989379},{96.5,0.989468},{97.,0.989556},{97.5,0.989642},{98.,
    0.989727},{98.5,0.98981},{99.,0.989893},{99.5,0.989974},{100.,0.990054}}
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Figure 7: Numerical table of the interpolated values of the WIDTH ratio.