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Method to calibrate the NMR system using the water cell

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Abstract

We present briefly the method used to calculate the NMR water calibration constant.

1 The Water Calibration Constant

The signal induced in the pick-up coils by the rotating spins at the resonance and detected by the lock-in amplifier is proportional to the macroscopic magnetization of the sample :

$$S = kM = k\mu nP \tag{1}$$

where :

- S : amplitude of the lock-in amplifier signal (in V)
- k : proportionality constant, taking into account gains, losses in the cables, ... (usually expressed in V.mA^{-1})
- μ : magnetic moment of the sample (in Am^2 or JT^{-1})
- n : density of spins (usually expressed in m^{-3})
- P : polarization of the sample (no unit)

The ratio of the Helium NMR signal height S_{He} to the water NMR signal height S_w can then be written as :

$$\frac{S_{He}}{S_w} = \frac{G_{He}}{G_w}\frac{\mu_{He}}{\mu_p}\frac{n_{He}}{n_p}\frac{P_{He}}{P_w} \tag{2}$$

with the following definitions :

- S_{He} : amplitude of the Helium signal (usually expressed in mV)
- S_w : amplitude of the water signal (usually in μV)
- G_{He} : absolute gain of the pick-up coil preamplifier in the Helium configuration (usually 1)
- G_w : absolute gain of the pick-up coil preamplifier in the water configuration (usually 100 or 200)
- μ_{He} : magnetic moment of the ^{3}He nucleus (in JT^{-1})
- μ_p : magnetic moment of the proton in water (in JT^{-1})
- n_{He} : density of ^{3}He nuclei in the Helium target (usually expressed in Amagats)
- n_p : density of protons in the water target (in Amagats)
- P_{He} : polarization of the Helium target, which needs to be calculated (no unit)

- P_w : polarization of the water sample (no unit)

We recall : 1 Amagat (amg) = $2.689.10^{19}$ cm $^{-3}$. All these constants are known (G_{He}/G_w, μ_{He}/μ_p and P_w) or measured during E94-010 (n_{He}/n_p, S_{He} and S_w), except P_{He}. The previous formula is usually written :

$$P_{He} = c_w \frac{S_{He}}{n_{He}} \tag{3}$$

with :

$$c_w = \frac{1}{S_w} \frac{G_w}{G_{He}} \frac{\mu_p}{\mu_{He}} n_p P_w \tag{4}$$

usually expressed in Amagats per mV.

- S_w is the amplitude of the water signals extracted from the fit of the water NMR data, as explained in E94-010 Technical Note 10.
- G_w and G_{He} are the preamplifier gain and are set by hand once down in the Hall (usually, G_w=100 or 200 and G_{He}=1).
- The ratio μ_p/μ_{He} is known from the literature and equal to $\mu_p/\mu_{He} = 1.313$.
- The density of protons in the water cell is estimated to be $n_p = 6.670.10^{22} \pm 0.005$ cm $^{-3} = 2482 \pm 2$ Amagats at 22^oC [1].
- The value of P_w is calculated from Boltzman statistics :

$$P_w = tanh\left(\frac{\mu_p B}{kT_w}\right) = tanh\left(\frac{h\nu}{2kT_w}\right) \simeq \frac{h\nu}{2kT_w} \tag{5}$$

where μ_p is the magnetic moment of protons in H_2O, $k = 1.380658.10^{-23}$ JK^{-1} is the Boltzman constant, T_w is the water temperature in K, $h = 6.6260755.10^-34$ Js is the Planck constant, $B = H_0 = 2\pi\nu/\gamma_p$ is the resonance holding field, $\nu = 91$ kHz is the RF field frequency, and $\gamma_p = 2.67515255.10^8$ s $^{-1}$ T^{-1} is the gyromagnetic ratio of protons in water. At $22^oC\pm3^oC$, $P_w = 7.400.10^{-9} \pm 0.074.10^{-9}$.

Table 1: *Values of the calibration constant c_w*

G_w	G_{He}	$S_w(\mu V)$	$T_w(^oC)$	c_w (amg.mV^{-1})
100	1	6.59	22	0.366

2 Estimation of the Cell Density

To extract the polarization value of the Helium target, it is then necessary to measure the density $n_{He} \equiv n_t$ in the target chamber of the Helium cell. That density depends on the pumping cell and target cell temperatures.

Its expression is easy to deduce from the "Loi des gaz parfaits" (ideal gas law) : $PV = NkT$, where P stands for the gas pressure, V its volume, N the number of contituents and T for its temperature. Neglecting the volume of the transfer tube between the pumping cell and the target cell and assuming the pressure equilibrium between the pumping chamber (index $_p$) and the target chamber (index $_t$), we have :

$$\frac{N_t k T_t}{V_t} = \frac{N_p k T_p}{V_p} \tag{6}$$

from which we can express N_p :

$$N_p = \frac{V_p}{V_t}\frac{T_t}{T_p} N_t \tag{7}$$

We can introduce the "equilibrium" density of Helium n_0 in the target using :

$$N_p + N_t = n_0 (V_p + V_t) \tag{8}$$

so that we extract N_t:

$$N_t = n_0 (V_p + V_t) - N_p \tag{9}$$

and using the previous expression for N_p :

$$\begin{aligned} N_t &= n_0 (V_p + V_t) - \frac{V_p}{V_t}\frac{T_t}{T_p} N_t && (10) \\ N_t &= n_0 \frac{V_p + V_t}{1 + \frac{V_p}{V_t}\frac{T_t}{T_p}} && (11) \end{aligned}$$

We get the density $n_{He} \equiv n_t = N_t / V_t$ in the target chamber :

$$n_{He} \equiv n_t = n_0 \frac{1 + \frac{V_p}{V_t}}{1 + \frac{V_p}{V_t}\frac{T_t}{T_p}} \tag{12}$$

The values for the equilibrium densities n_0 are given by the Princeton group and may be checked at the internet address : http://www.jlab.org/~incerti/cells.html. The dependence of n_{He} with the temperatures is shown on figure 1.

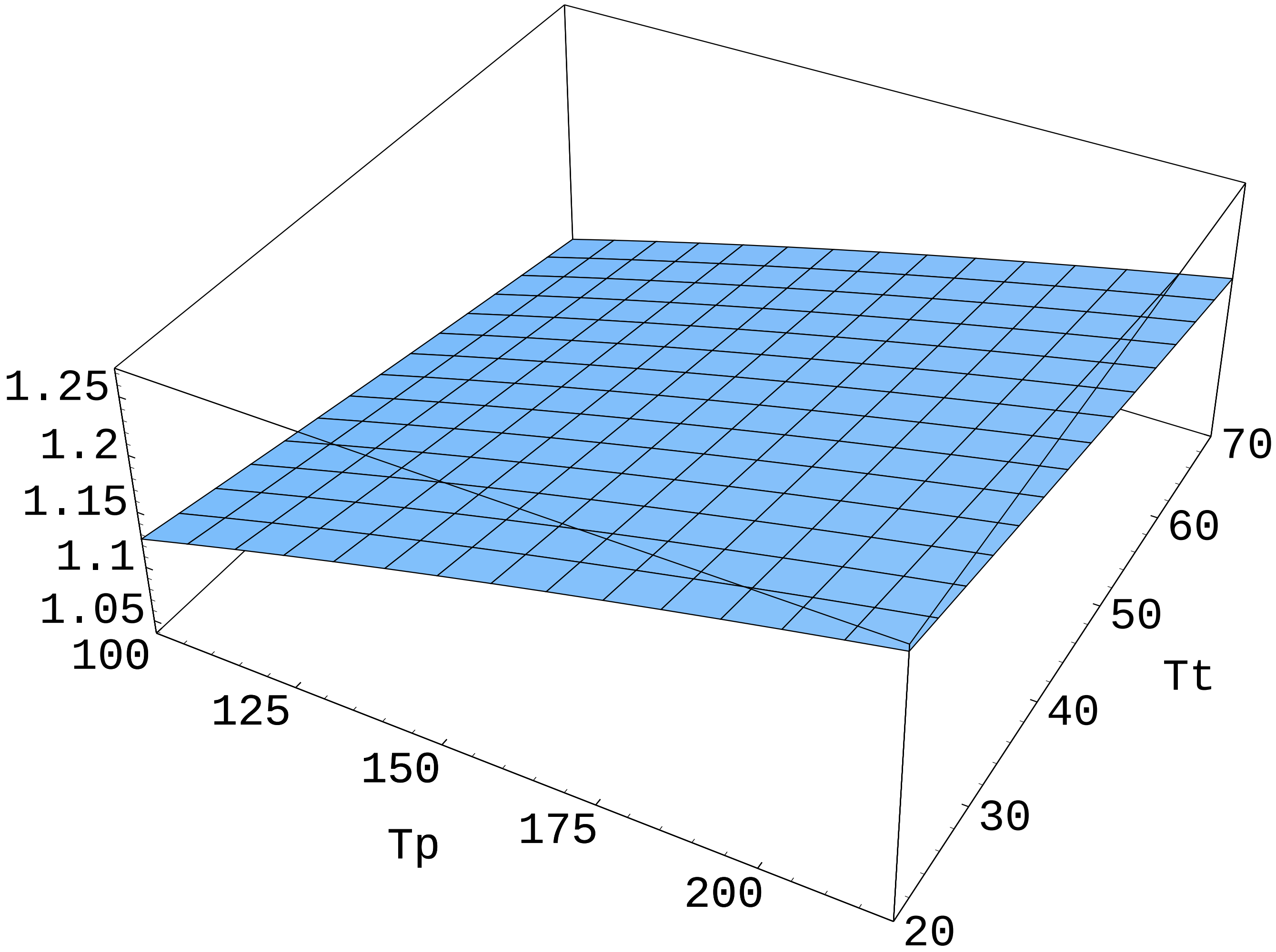

Figure 1: Evolution of n_{He}/n_0 in the target cell, as a function of the temperatures T_t and T_p, expressed in ^{o}C. We have assumed Nepheli target's values for V_p and V_t.

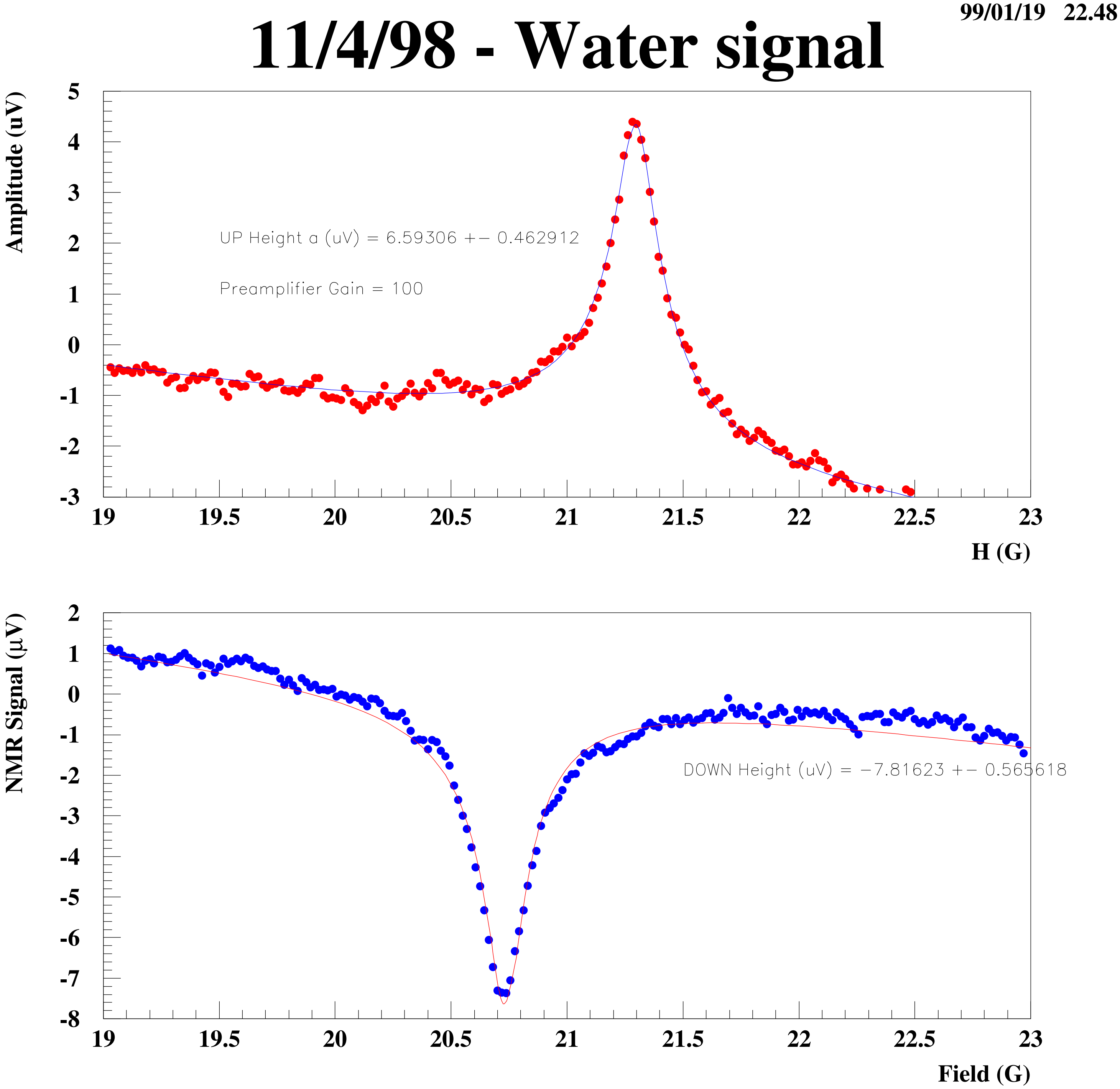

Figure 2: Example of first order averaged water signal obtained after 359 sweeps. For a precise calibration, noisy sweeps should not be taken into account in the average and attention should be payed to magnetic field drifts when performing the average computation. This signal was measured before installing the E94010 Nepheli Helium 3 target and was used to calculate its polarization calibration constant.

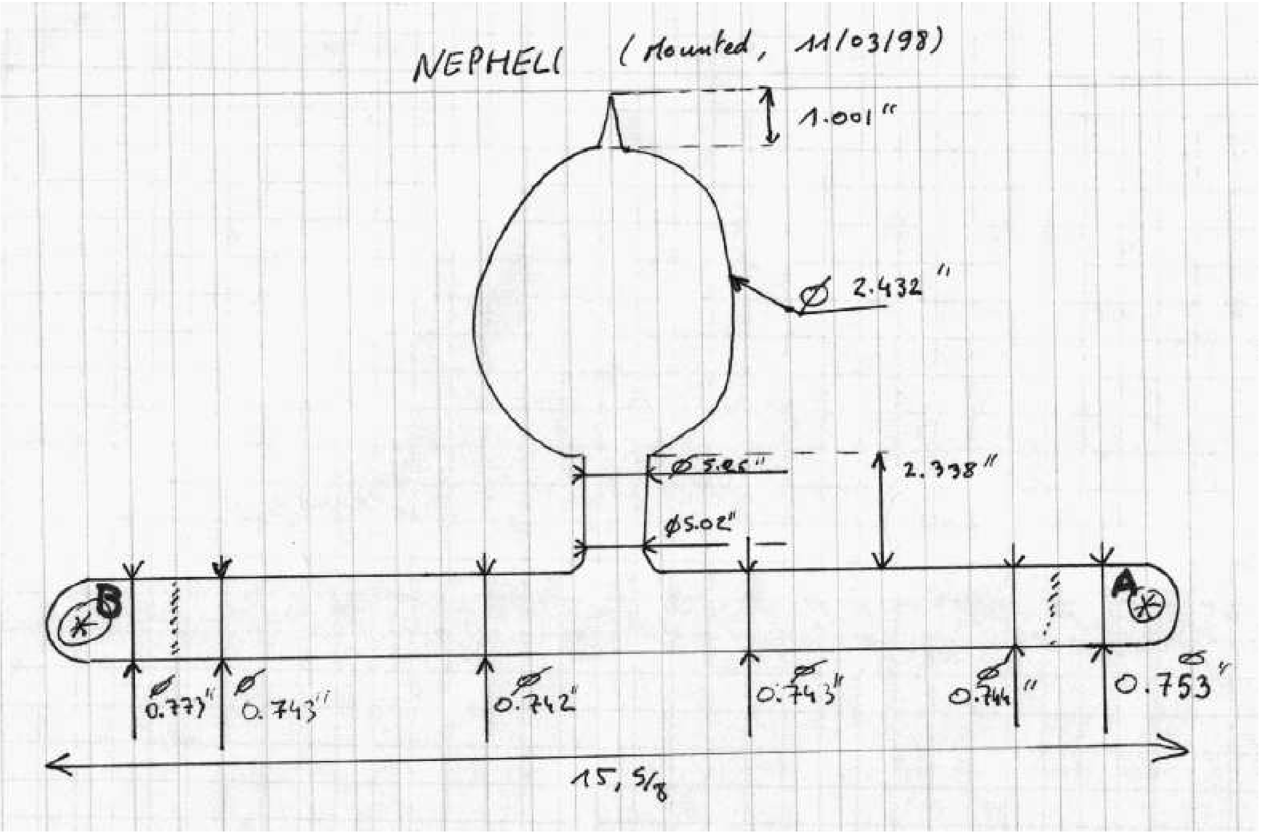

Figure 3: Dimensions of the Nepheli cell in inch (except if specified). Drawing by A. Deur. For information : 1 inch = 2.54 cm.

Table 2: *Values of the ratio P_{He}/S_{He} (in $\%.mV^{-1}$). The temperatures have to be expressed in K. The calibration gives 2.85 % per mV :*

Cell	V_t(cm^{-3})	V_p(cm^{-3})	T_t(^{o}C)	T_p(^{o}C)	n_0(amg)	n_{He}(amg)	P_{He}/S_{He}
Nepheli	113.24	123.46	55	190	10.9	12.85	2.85

3 Influence of the cell temperature

To estimate the effect of the cell temperature changes on the target polarization, we can compute the ratio :

$$\frac{\Delta P_{He}}{P_{He}} = \frac{\Delta n_{He}}{n_{He}} \tag{13}$$

where more explicitely :

$$\Delta P_{He} = P_{He}(T_p + \Delta T_p, T_t + \Delta T_t) - P_{He}(T_p, T_t) \tag{14}$$

$$\Delta n_{He} = n_{He}(T_p + \Delta T_p, T_t + \Delta T_t) - n_{He}(T_p, T_t) \tag{15}$$

We show the evolution of the $\Delta P_{He}/P_{He}$ ratio first as a function of ΔT_p and ΔT_t on figure 4, and as a function of $\Delta T_t = \Delta T_t$ on figure 5. The relative variation $\Delta P_{He}/P_{He}$ reaches 0.2% only if $\Delta T_t = \Delta T_t = 5^o$C. For a polarization of $P_{He} = 35\%$, the absolute change is very small : $\Delta P_{He} = 0.07\%$

References

[1] M. Romalis, “Laser polarized ^{3}He target used for a precision measurement of the neutron spin structure ”, Ph-D Thesis, Princeton University Press (1997)

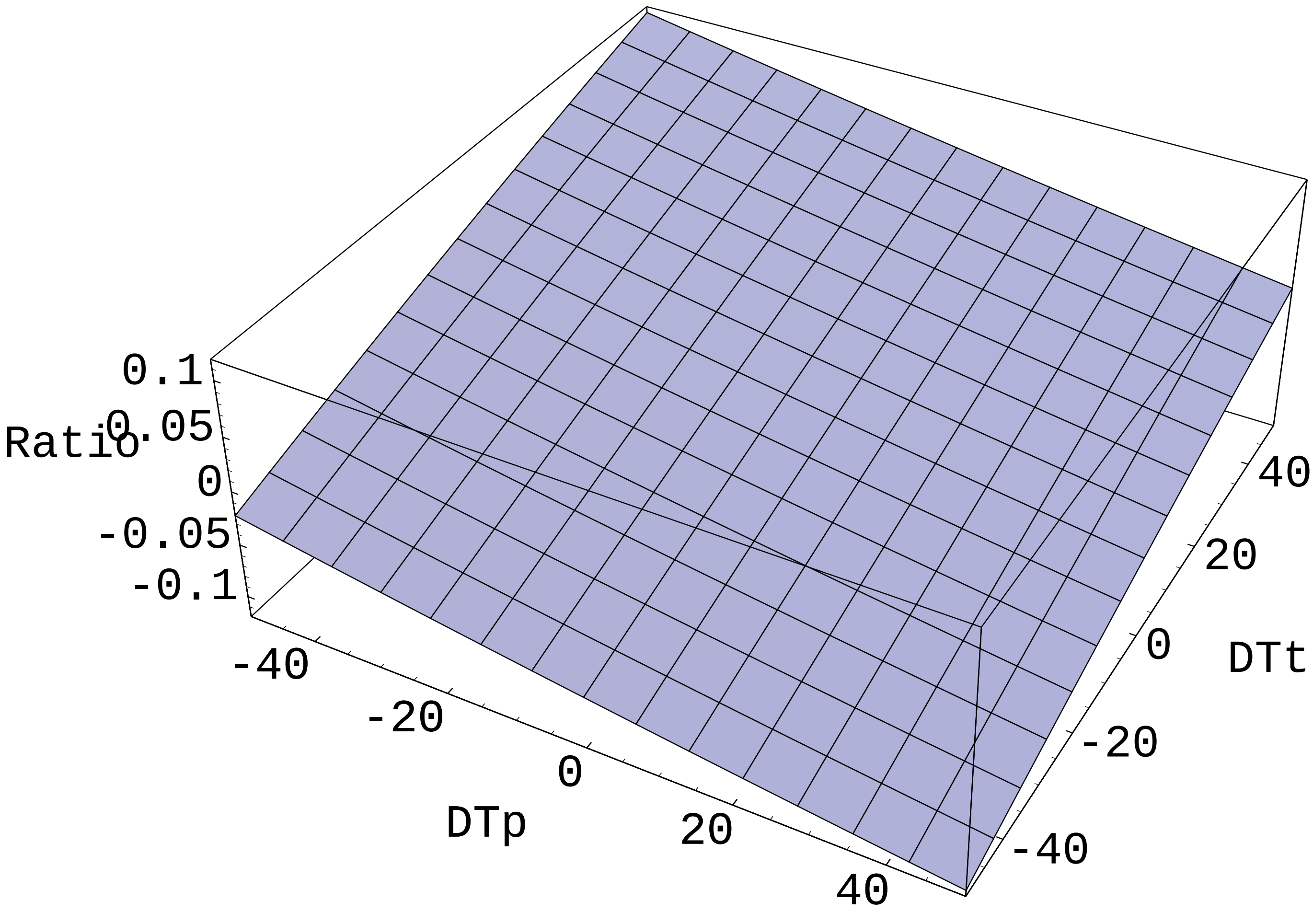

Figure 4: Ratio $\Delta P_{He}/P_{He}$ as a function of ΔT_p and ΔT_t. Those temperature deviations are expressed in ^{o}C.

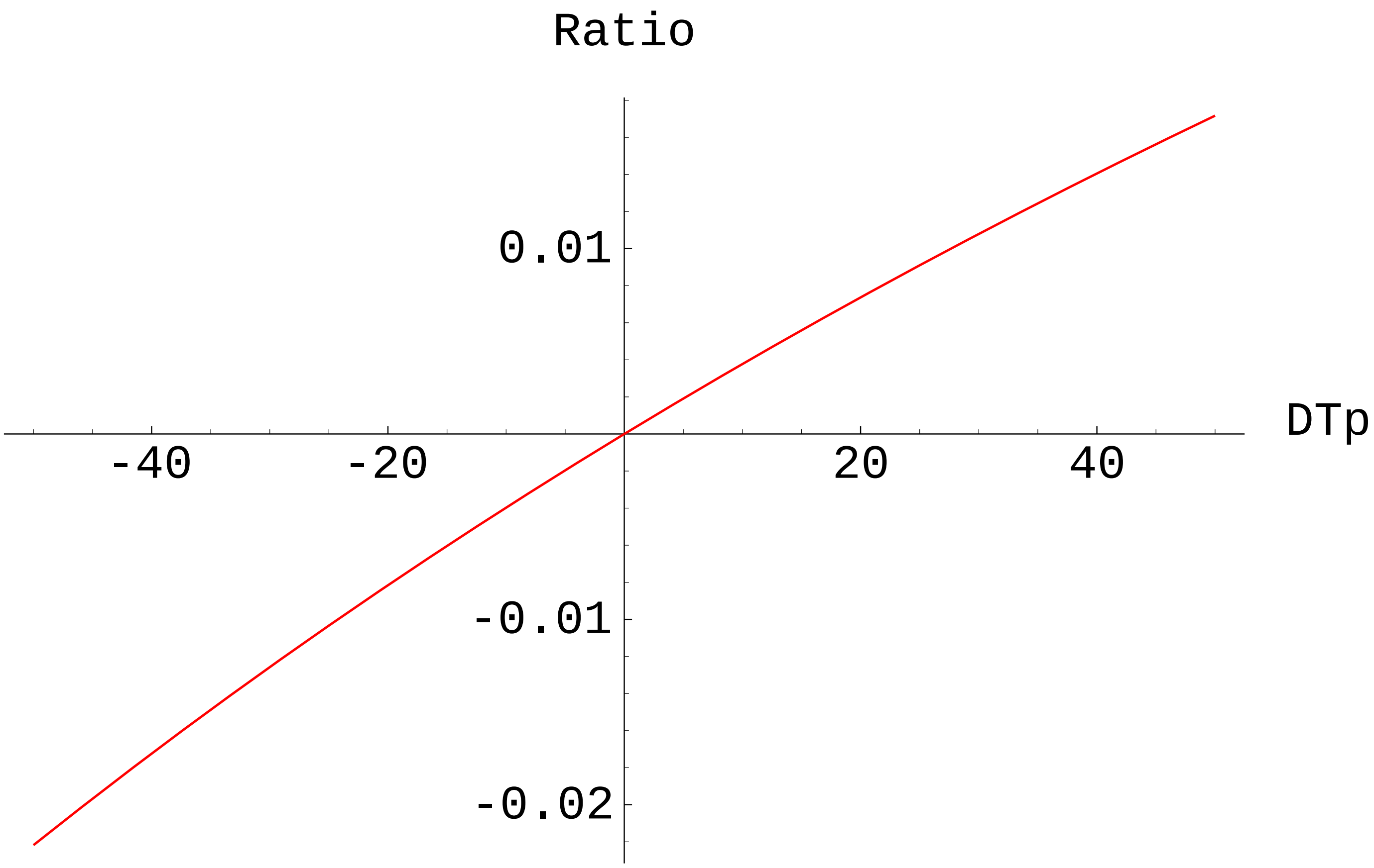

Figure 5: Ratio $\Delta P_{He}/P_{He}$ as a function of $\Delta T_p = \Delta T_t$. This temperature deviation is expressed in ^{o}C.