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EDM Technical Note: Sensitivity of the Liquid He EDM Experiment as Derived from Least Squares Fitting of Pseudo-Data and Comparisons to the Heisenberg-Uncertainty Principle

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Abstract

The results in the EDM proposal[1], chapter 5H, for the sensitivity of the EDM experiment have been checked using pseudo data and least squares fitting techniques. The applicability of the formula in Chibane *et al.*[2] has been tested for the case of small backgrounds. The role of the phase factor in the fitting is clarified. In the case of EDM pseudo-data, the sensitivity is mapped as a function of the efficiency for identifying and vetoing the UCN beta decays, with a factor-of-two improvement found if all beta decays are removed. Finally, the sensitivity of the experiment is determined to be twice the limit given by the Heisenberg Uncertainty-Principle when beta decays are not identified and equal to the limit when they are removed from the data stream. The Uncertainty-Principle limit is found to be optimally small at a different measuring time than in the EDM proposal, *i.e.* 2000 s.

I. Introduction

The electric-dipole-moment (EDM) experiment proposal[1] states that the scintillation rate from neutron absorption on ^{3}He is given by

$$\Phi = \Phi_B + N e^{-\Gamma_{AVE} t}\left[\frac{1}{\tau_\beta} + \frac{1}{\tau_3}\left[1 - P_3 P_n e^{-\Gamma_p t}\cos(\omega_r t + \phi)\right]\right], \qquad (1)$$

Eq. V.H.1 of the proposal, where Φ_B is the background rate, N is the initial number of ultra-cold neutrons (UCN), and Γ_{AVE} is the decay width. The β-decay lifetime is τ_β and the absorption lifetime is τ_3. P_3 is the ^{3}He polarization, P_n is the neutron polarization, Γ_p is the polarization-decay width, and ϕ is an arbitrary phase. The precision that the frequency $f = \omega_r/2\pi$ may be determined is given by

$$(\Delta f)^2 = \frac{6\bar{I}}{(\pi A)^2 T_m^3}, \qquad (2)$$

Eq. V.H.2 of the proposal, where A is the magnitude of the oscillatory term, $\bar{I}$ is the magnitude of the background term, and T_m is the measurement time. Equation (2) is derived in Chibane *et al*[2] based on least squares fitting of a function closely related to Eq. (1) with certain assumptions about its form. This study addresses a number of points by doing least-squares fits to pseudo-data and extracting the value of $(\Delta f)^2$:

- Does Eq. (2) give the proper value for the standard deviation of *f* when applied to Eq. (1).
- Equation (2) is derived under the assumption that $\bar{I}$>>*A*. This assumption is not satisfied in Eq. (1); is there a consequence?
- Equation (2) has a natural time range that starts at 0, when the measurement begins, and ends at T_m, when the measurement ends. Chibane *et al*[2] used the range [-T_m/2, T_m/2]. Does the time range make a difference?
- Equation (1) assumes no suppression of the β decays via particle identification. How much improvement in sensitivity arises from identifying the β decays?
- How are the errors, Δf=$\sigma(f)$, affected by the other free parameters in Eq. (1)?
- How do the uncertainties, Δf, from fitting the pseudo-data, compare to the optimal expectation from the Heisenberg-Uncertainty Principle?
- Does the Heisenberg-Uncertainty Principle guide us to better parameters than those in the proposal?

It is convenient to rewrite Eq. (1) as

$$\Phi = \frac{1}{2\tau}\mathrm{N}e^{-\frac{t}{\tau}}\left[\varepsilon_\beta + \varepsilon_3\left[1-\cos(2\pi \mathrm{f}t+\phi)\right]\right], \tag{3}$$

where it is assumed that there is no constant background and the two species remain 100% polarized throughout the measurement. The factor ε_β is introduced to measure the efficiency for observing the β decays and for eliminating them. It is further assumed that the efficiency for detecting the absorption is unity (except when ε_3 is treated as a variable in a fit) and that τ_3=τ_β=2τ. For convenience, τ_3 is taken to be 1000 s. The quantity Γ_{AVE} becomes

$$\Gamma_{\mathrm{AVE}} = \frac{1}{\tau_\beta} + \frac{1}{\tau_3} = \frac{1}{\tau} \tag{4}$$

because the β decays are still happening even if they are suppressed in the signal measurement. The assumptions in Eq. (3) are the same as made in the EDM proposal[1].

Section II is devoted to understanding the fitting of periodic functions as done in Chibane *et al.*[2] Section III discusses how the pseudo-data is produced and the effects of some of the caveats. Section IV gives the results that address the questions above, and Section V summarizes the conclusions.

II. Fitting Periodic Functions

Equation (2) is derived as a result for fitting the function

$$\begin{aligned} &\mathrm{I} = 0 && \text{for } |t| > \mathrm{T_m}/2 \\ &\mathrm{I} = \bar{\mathrm{I}} + \mathrm{A}\sin(2\pi \mathrm{f}_0 t + \phi) && \text{for } |t| \le \mathrm{T}_{m/2}, \end{aligned} \tag{5}$$

which is closely related to Eq. (3) except for the normalization, the exponential decay, and the β decays. The Chibane *et al.*[2] assumption of $\bar{I}$>>A is used below.

Drawing on the standard development for least squares fitting described in Bevington,[3] the best estimator for parameters of a function determined by fitting data is given by minimizing the χ^2 per degree of freedom

$$\frac{\chi^2}{\nu} = \frac{1}{\nu}\sum\frac{1}{\sigma_i^2}\left(y_i - g_i(x_j)\right)^2 \tag{6}$$

as a function of the parameters x_j, where y_i is a measured data point, σ_i is the standard error in y_i, and $g_i(x_j)$ is the value of the function evaluated at i. In the case that g_i is non-linear in the parameters x_j, g_i can be expanded around the solution and the minimum is found via iteration. This work utilizes the CURVFIT method described in Bevington.[3] The minimization requires the calculation of the curvature matrix

$$\alpha_{jk} = \sum\frac{1}{\sigma_i^2}\frac{\partial g_i}{\partial x_j}\frac{\partial g_i}{\partial x_k}\,. \tag{7}$$

Then the variance of x_j is

$$\mathrm{var}(x_j) = \left(\alpha^{-1}\right)_{jj}. \tag{8}$$

In the case where the measured data has normal errors,

$$\sigma_i = \sqrt{y_i}\,. \tag{9}$$

The number of counts in a bin of width Δt is $\Phi\Delta t$. For the case of the first parameter (j=1) selected to be f_0,

$$\alpha_{11} = \frac{\sum(2\pi A t_i \Delta t\cos(2\pi f_0 t_i + \phi))^2}{\bar{I}\Delta t} = \frac{(2\pi A)^2}{\bar{I}}\int dt\left(t^2\cos^2(2\pi f_0 t + \phi)\right)$$

$$\alpha_{11} = \frac{(2\pi A)^2}{\bar{I}}\int dt\left(\frac{t^2}{2}(1+\cos(4\pi f_0 t + 2\phi))\right) \tag{10}$$

If $T_m >> (2\pi f_0)^{-1}$, the oscillatory term will integrate to zero with high accuracy, and

$$\alpha_{11} = \frac{(2\pi A)^2}{6\bar{I}}t^3 \tag{11}$$

evaluated over the range $[-T_m/2, T_m/2]$. The result is

$$\alpha_{11} = \frac{(\pi A)^2 T_m^3}{6\bar{I}}, \tag{12}$$

which is the inverse of Eq. (2).

The natural time range for a measurement with a decaying species is $[0,T_m]$. If Eq. (11) is evaluated over this range, the result for α_{11} is 4 times larger, and thus Δf_0 is twice as small. This result is unphysical because the change in range only corresponds to a shift in phase. If the fitting process is expanded to include two variables, f_0 (j=1) and ϕ (j=2), the α matrix can be shown, by methods very similar to those used to get Eq. (10), to be

$$\alpha = \frac{(2\pi A)^2}{\bar{I}}\begin{pmatrix} \frac{t^3}{6} & \frac{t^2}{4} \\ \frac{t^2}{4} & \frac{t}{2} \end{pmatrix} \tag{13}$$

with each matrix element evaluated over an arbitrary starting time t_0 and of length T_m, *i.e.* $[t_0, t_0+Tm]$. The inverse of α is

$$\alpha^{-1} = \frac{\bar{I}}{(\pi A)^2 T_m^3}\begin{pmatrix} 6 & -6t_0 - 3T_m \\ -6t_0 - 3T_m & 6t_0^2 + 6t_0 T_m + T_m^2 \end{pmatrix}. \tag{14}$$

The $(\alpha^{-1})_{11}$ element, the square of the standard error $\sigma(f_0)$, is independent of t_0 and equal to Eq. (2). By including ϕ into the fitting, a physical result is obtained. The choice of Chibane *et al.*,[2] $t_0=-T_m/2$, makes Eq. (14) diagonal and explains why those authors did not need to consider the simultaneous fitting of ϕ. This choice of t_0 also gives the minimum value for $(\alpha^{-1})_{22}$, the square of the standard error $\sigma(\phi)$. The error in ϕ depends on t_0 for reasons that are not understood.

The technique used to generate pseudo data will be described in the next section. When the fitting program is used to evaluate $\sigma(f_0)$ from pseudo data, the result is 4.23 for $\bar{I}=27000$, $A=2700$ and $T_m=500$s. The value from Eq. (2) is 4.24 and provides a useful check of the program. The units of $\sigma(f_0)$ are unnatural because Eq. (5) is not normalized; note that Eq. (3) is normalized to the initial number of UCN.

III. The Generation of Pseudo Data

The program produces sets of pseudo-data, the y_i in Eq. (6), that depend on the random number seeds. The initial values for the y_i are $\Phi\Delta t$, where Φ comes from Eq. (3) and Δt is 1/90 s. Whereas f is taken to be 3 Hz as in the EDM proposal,[1] each cycle is broken into 30 bins. The choice to use a large number of bins per cycle removes inaccuracies associated with the size of the time bins. The total number of bins is $30fT_m=45{,}000$ for $T_m=500$ s. The values of the other parameters in Eq. (3) are taken to be the same as in the EDM proposal[1], namely $\tau=500$ s and $N=2\text{x}10^6$; the value of $\phi=0.2-\pi/2$ is picked arbitrarily.

The initial value of σ_i is the square root of y_i, with the special case that σ_i is 0.7 when y_i is 0. The final value of y_i is derived from the initial value by adding a random number selected from a Gaussian distribution characterized by σ_i; y_i is set to the closest integer or zero in the case of a negative value. The final value of σ_i is the square root of y_i, again with the special case that σ_i is 0.7 when y_i is 0.

Although the choice of Gaussian statistics is adequate for this study, it produces some problems that should be taken into account in detailed studies. Firstly, the errors σ_I and the data values y_i should be picked according to Poisson statistics. Secondly, the fitting expression, Eq. (6), should be modified to match Poisson statistics. The consequences of choosing Gaussian statistics are that the central values of the fits for some of the parameters, *e.g.* τ, come out slightly off the generating value and χ^2/ν is somewhat greater than 1. An examination of the contributions to χ^2/ν at each data point shows that the biggest contributions come where Φ is near zero, exactly where Gaussian statistics break down.

The CURVFIT[3] algorithm uses a parameter λ to switch between the gradient method and the method of steepest decent. The diagonal elements of the α matrix are multiplied by $(1+\lambda)$. As the program iterates toward a minimum in χ^2 space, the value of λ is increased by a factor of 10 when χ^2 gets worse and is decreased by a factor of 10 when χ^2 improves. The search is stopped without solution if λ exceeded 10^4. The search is stopped successfully when χ^2/ν improves by less than 10^{-6}. Experience indicates that the search converges if the initial parameters are within about 10 standard deviations of the final values.

IV Results and Comparison to the Uncertainty Priciple

The computer program for solving for the parameters of Eq. (3) has been checked in two ways when f and ϕ are varied simultaneously. Firstly, Eq. (7) can be evaluated analytically, in much the same way as Eq. (14) was derived, for the case when ε_β=0. The analytic solution gave a value of 1.35 μHz, while the program gave 1.42 μHz. The small difference is attributed to type of statistics assumed in generation of the pseudo data.

Secondly, the value of $\sigma(f)$ from the program is compared to the distribution of central values obtained for a number of different pseudo-data sets. The pseudo-data sets are produced by changing the initial random number seeds for each set. The results for 40 data sets with ε_β=1 are shown in Fig. 1. The mean for the distribution is –0.02 μHz, and the standard deviation is 2.8 μHz. The standard deviation compares well to $\sigma(f)$=2.7 μHz from the program. The curve in Fig. 1 is a Gaussian normalized to 40 data sets in bins of 0.4 μHz with an offset of –0.02 μHz and a standard deviation of 2.7 μHz, *i.e.* with the parameters of the data sets except for the standard deviation that comes from the program.

Table 1 shows how $\sigma(f)$ varies as the number of free parameters in the fits is increased beyond f and ϕ. The decrease in accuracy is very slow because all of the added variables are determined from distinct aspects of Eq. (3). If the variables were not statistically independent, complicated contributions to the signal function would degrade the experiment. This note does not treat the case where there are other exponential contributions as might arise from cold-neutron activation betas.

The value of $\sigma(f)$ has been calculated as a function of ε_β when only f and ϕ are free parameters. The result is plotted in Fig. 2. There is nearly a factor-of-two improvement in the error when all the β-decays are removed from the sample by particle identification. The value calculated in the EDM proposal[1] is shown also as the solid point at ε_β=1; the point falls on the curve within the round-off accuracy of the calculation in the proposal. Empirically, the assumption that $\bar{I}>>A$, *i.e.* the background is large, does not seem to have been required for this case to get an accurate answer.

The results in Fig. 2 can be compared to limit imposed by the Heisenberg-Uncertainty Principle. The principle states that

$$\Delta E \Delta t \geq \frac{\hbar}{2}, \tag{15}$$

or

$$\Delta f \Delta t \geq \frac{1}{4\pi}. \tag{16}$$

The Δ symbol means root-mean square error in this application. Thus $\Delta t = t/\sqrt{12}$. It is interesting to understand the best measurement that can be made, i.e. when the equal symbol is appropriate. The evaluation of Eq. (16) is experiment dependent. For the

EDM proposal,[1] the expression for N initial neutrons in a single cycle over the time t becomes

$$\Delta f = \sigma(f[t]) = \frac{1}{4\pi t}\sqrt{\frac{12}{\frac{\tau}{\tau_3}N(t)}}, \tag{17}$$

where

$$N(t) = \frac{N e^{-\frac{t}{\tau}}\Delta t}{\tau} \tag{18}$$

in a time bin Δt. The initial number of neutrons is reduced to those absorbed by the ^{3}He. The contributions to the error is integrated from all the time bins as

$$\frac{1}{\sigma^2(f)} = \frac{(4\pi)^2 N}{12\tau_3}\int_0^{T_m} dt\cdot t^2 e^{-\frac{t}{\tau}}. \tag{19}$$

Thus

$$\sigma(f) = \frac{1}{4\pi}\sqrt{\frac{12\tau_3}{N\tau\left(2\tau^2 - \left[T_m^2 + 2\tau T_m + 2\tau^2\right]e^{-\frac{T_m}{\tau}}\right)}}. \tag{20}$$

When Eq. (20) is evaluated for the conditions assumed in the EDM proposal,[1] the result is $\sigma(f)$=1.38 μHz and is shown as the dashed line in Fig. 2. This result is 2.0 times smaller than the EDM proposal[1] and equal to what can be achieved with perfect particle identification of the neutron β-decays. The no-background limit, ε_β=0, is the best that can be done with this technique and these parameters.

The proposal implicitly assumes a UCN-fill time T_F of 1000 s. The initial number of neutrons N in the cell is then

$$N = PV\tau\left(1 - e^{-\frac{T_F}{\tau}}\right), \tag{21}$$

where P is the specific-production rate (1/cc/s) and V is the volume (4x10^3 cc) of one measuring cell. If the experiment runs for a total time T, say 100 d=8.64x10^6 s, then the measurement of $\sigma(f)$ is repeated $T/(T_m+T_F)$ times. Hence, the ultimate result will be

$$\sigma_T(f) = \frac{1}{4\pi}\sqrt{\frac{12\tau_3(T_m+T_F)}{PV\left(1-e^{-\frac{T_F}{\tau}}\right)T\tau^2\left(2\tau^2 - \left[T_m^2 + 2\tau T_m + 2\tau^2\right]e^{-\frac{T_m}{\tau}}\right)}}. \tag{22}$$

If evaluated at the standard values, $\sigma_T(f)$ is 19.5 nHz. The quantity $\sigma_T(f)$ can be optimized as a function of T_m, T_F and τ_3, *i.e.* the ^{3}He concentration. A simple grid search of Eq. (22) yields a minimum value for $\sigma_T(f)$ of 8.2 nHz with T_m=2850 s, T_F=1375 s and τ_3=2000 s. The minimum value varies quite slowly, and for the more familiar values of T_m=2000 s, T_F=1000 s and τ_3=1000 s, $\sigma_T(f)$=9.0 nHz. The optimization yields a factor-of-two improvement. The biggest contribution comes from a longer measuring time. It is assumed but not demonstrated that the least-squares fitting of no-background pseudo-data will track these results. A similar examination of the equations on page 142 of the proposal, where β decay provides a background, seems to indicate that adjusting the times only leads to a 20% improvement in the limit. Hence eliminating the β decays is even more important if it allows for a better parameter optimization. The various combinations of times and backgrounds are the subject for further study. For reference, a 9.0-nHz measurement in each of two cells corresponds to a two-sigma limit on the neutron EDM of $2.4\text{x}10^{-28}$ e•cm with a 50-kV/cm applied electric field.

If the neutron EDM is measured via the Ramsey method of separated-oscillatory fields,[4] all the surviving neutrons are measured at the same time, there is no ^{3}He absorption, and Eq.(22) is replaced by

$$\sigma_T(f)=\frac{1}{4\pi}\sqrt{\frac{12\left(T_m+T_F\right)}{PV\left(1-e^{-\frac{T_F}{\tau}}\right)\tau T T_m^2 e^{-\frac{T_m}{\tau}}}}\,. \tag{23}$$

Here τ is a constant equal to τ_β. The value for $\sigma_T(f)$ in Eq. (23) is 5.9 nHz for the proposal parameters. For identical conditions, the Ramsey method is roughly a factor of 3.3 times better than the superfluid-He method. However, Eq. (23) may also be optimized as a function of T_m and T_F. The optimum is at T_m=T_F=1500 s. In this case, $\sigma_T(f)$=4.1 nHz. If each type if measurement is made at its optimum parameters, the Ramsey method is better by a factor of 2.0. Presumably, the proposal conditions are farther from optimal for the superfluid-He method.

In superfluid He, the UCN lifetime τ may be 500 s, but the best value for τ in the latest EDM measurement with the Ramsey technique[5] is roughly 100 s due to wall losses. Under these circumstances, the superfluid-He method gives the better result.

V. Conclusions

Least-squares fitting programs, applied to EDM pseudo data, give the same result for error in the extracted frequency as derived by Chibane *et al.*[2] and presented in Eq. (2) so long as both f and ϕ are treated as varied parameters. For this case, the assumption that the background must dominate the oscillatory signal does not seem to be relevant. If the neutron β-decays can be identified and removed from the data sample, up to a factor of two in sensitivity may be gained. Besides the ϕ parameter, other free variables in the fitting function do not appear to degrade the uncertainty in f. The limits that can be set by the EDM experiment are 2.0 times the value calculated for the Heisenberg-Uncertainty Principle and equal to the calculation when the β-decays are removed from the data. By optimizing the measuring time T_m, the cell loading time T_F and the absorption lifetime t_3, a minimum in the calculation of the limit from the Heisenberg Uncertainty Principle is found at 2000, 1000 and 1000 s, respectively. That is another factor of two better than the value at T_m=500 s when the β-decay background is eliminated.

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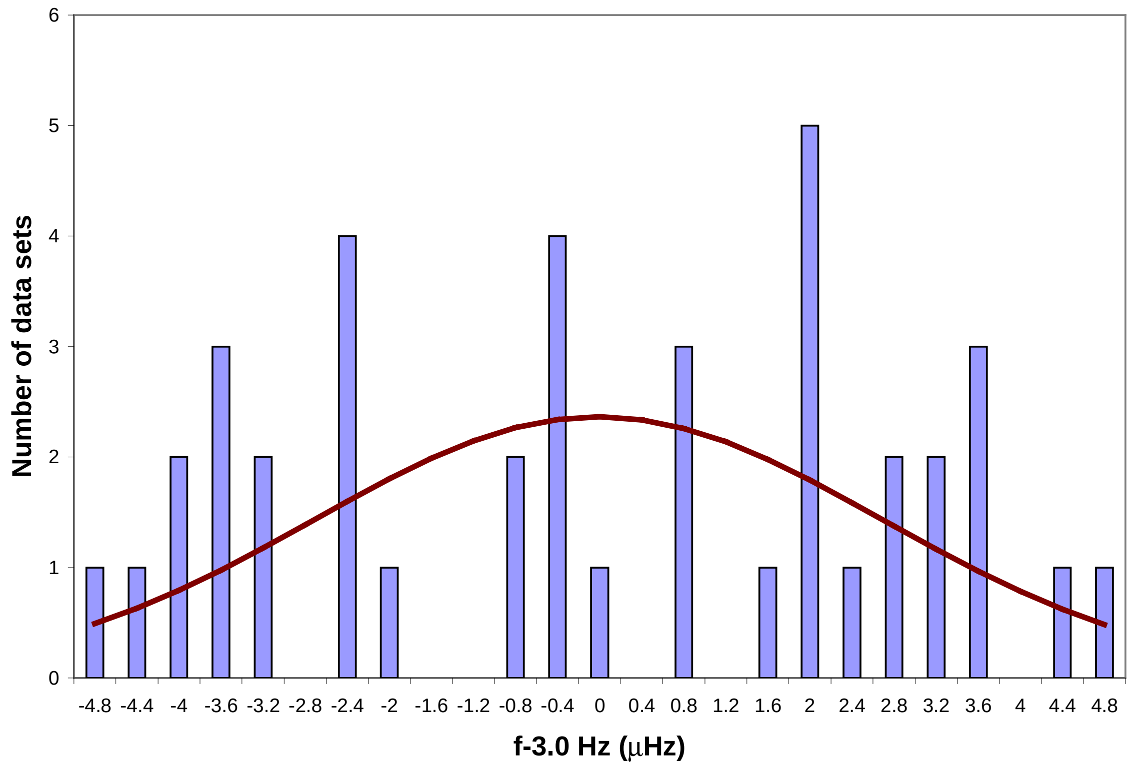

Figure 1: The number of data sets that have *f* offset from 3 Hz in 0.4 μHz bins. The histogram has an offset of –0.02 μHz and a $\sigma(f)$ of 2.8 μHz. The solid curve is a properly normalized Gaussian with the value of $\sigma(f)$ set to 2.7 μHz as predicted by the fitting program.

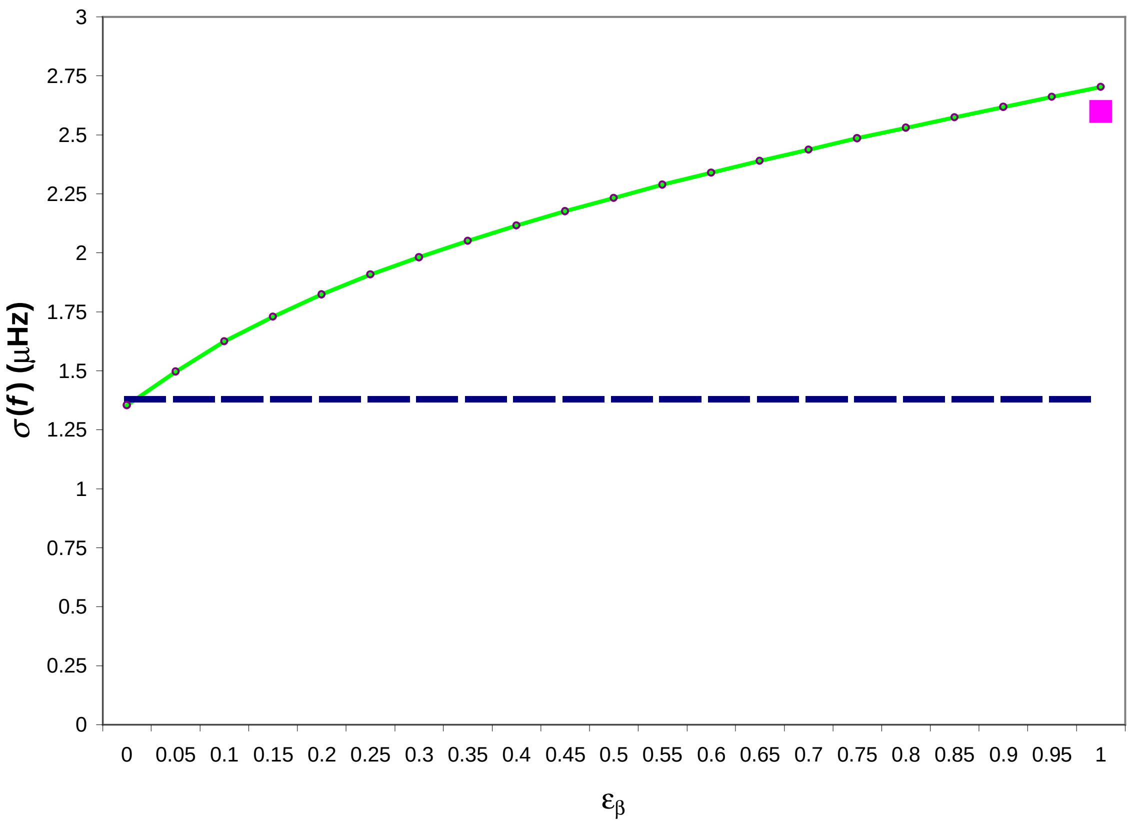

Figure 2. The value of $\sigma(f)$ plotted versus the efficiency of observing β decays ε_β after they are vetoed. The solid curve runs from ε_β=0, no remaining β decays, to ε_β=1, no detection of β decays. The solid point at ε_β=1 is the value from the EDM proposal.[1] The dashed line is the limit imposed by the Heisenberg-Uncertainty Principle on this method of measurement.

Variables	$\sigma(f)$ (μHz)
f, ϕ	2.70
f, ϕ, τ	2.77
f, ϕ, τ, ε_3	2.77
f, ϕ, τ, ε_3, ε_β	2.77

Table 1: The variations in $\sigma(f)$ as the number of variables in the fit are changed.