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OPTIMIZATION OF FEL PARAMETERS FOR THE MUH EXPERIMENT (SPECTROSCOPY OF MUONIC HYDROGEN)

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Abstract

Recently an experimental proposal has been put forward to observe and measure the level shifts in muonic hydrogen. The experiment requires a powerful tuneable microwave source in the FIR range, and given these requirements a Free Electron Laser (FEL) turns out to be the only suitable device. Unfortunately FEL's are very expensive devices, and it is important to establish the exact working conditions to accomodate the FEL to tight experimental budgets. Therefore it is important to maximize the expected data rate keeping costs reasonably low.

1. Introduction

Recently an experimental proposal has been put forward to observe and measure the level shifts in muonic hydrogen [1]. The experiment requires a powerful, tuneable pulsed microwave source in the range $\approx$ 400 GHz - 1700 GHz, with peak power near 1MW, triggerable within $\approx$ 2μs and with a high average repetition rate (> 100Hz). The only source that satisfies these requirements is a Free Electron Laser (FEL). Unfortunately FEL's are still in their infancy, and most existing FEL's are large experimental setups. The ENEA researchers who participate to the MUH Collaboration, have been studying small, compact FEL's for a few years and plan to build a machine with the size of a CO_2 laser with similar power output.

However even a small machine can be very expensive, therefore FEL parameters must be optimized to reduce costs without sacrificing the physics goals. This note reports on the optimization procedure (while the transition frequencies and the transition probabilities have already been discussed in other notes [2,3]).

The FEL parameters affect the final experimental accuracy in a very complicated way. All the calculations reported here have been done for the $3D^7{}_{5/2}$->$3P^5{}_{3/2}$ transition at 1288 GHz, and to simplify the optimization of the parameters I have decided to decouple the problem in two parts.

I assume at first that the following quantities are given:

- background event rate,
- number of measurement points (DATAPOINTS),
- range of measurement points (MAXDEV),
- signal-to-background ratio (SB),
- relative LASER linewidth (LASERwidth).

Since the SB ratio is at most of the order of 0.1, the total data-taking time is determined by the background event rate and by the number of measurement points. The measurement range is determined by the number of measurements and by the "natural" tuning step of the FEL (which is fixed by the operating frequency of the FEL klystron, i.e. 3 GHz).

A direct analytic evaluation of the experimental accuracy is unfeasible. Therefore I have written a simulation program (in the *Mathematica* symbolic manipulation language) and have run it repeatedly with different values for the SB ratio, etc.

The program (with its output) with parameters that are approximately those given in the experimental proposal is listed in appendix A. The χ^2 minimization routine uses the Levenberg-Marquardt adaptive algorithm.

The other part of the optimization is the evaluation of the SB ratio from the FEL parameters. To do this I have written another program (also in *Mathematica*) that implements the transition probability calculations of Peter Hauser [2]. The program (with output) is listed in appendix 2. The parameters in the listing are once again approximately those given in the proposal.

The tables that follow have been obtained by running these two programs repeatedly with different parameters (listed in the heading of each table)

2. Computed experimental accuracy (from program listed in Appendix A)

The following table lists the relative accuracy on the position of the mean value of the fitting Lorentzian, and has been computed with

LASERwidth = 0.005;
DATAPOINTS = 11;
LOOPS = 100;
Separation between datapoints = 3 GHz.

Table 1

SB EVENTS	0.025	0.050	0.075	0.100
$0.5 \cdot 10^5$	$6.9 \cdot 10^{-4}$	$3.8 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$
$1.0 \cdot 10^5$	$5.4 \cdot 10^{-4}$	$2.6 \cdot 10^{-4}$	$1.7 \cdot 10^{-4}$	$1.4 \cdot 10^{-4}$
$1.5 \cdot 10^5$	$4.1 \cdot 10^{-4}$	$2.0 \cdot 10^{-4}$	$1.4 \cdot 10^{-4}$	$1.1 \cdot 10^{-4}$
$2.0 \cdot 10^5$	$3.9 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	$1.2 \cdot 10^{-4}$	$1.0 \cdot 10^{-4}$

In some cases the χ^2 in the fit procedure had a rather shallow minimum and because of this the minimization algorithm stopped after reaching the maximum number of iterations (a normal stop would result after reaching the algorithmic accuracy requirement). A careful inspection shows that this is not usually a problem (and the numbers in the table are upper bounds to the obtainable accuracy). The relative error on the reported accuracies is approximately 10%.

The following table lists the accuracy as a function of the SB ratio and of the laser linewidth. The other parameters are fixed at

EVENTS = 1.5•10⁵;
DATAPOINTS = 11;
LOOPS = 100;
Separation between datapoints = 3 GHz.

Table 2

SB WIDTH	0.025	0.050	0.075	0.100
0.0025	3.6•10⁻⁴	1.9•10⁻⁴	1.2•10⁻⁴	0.9•10⁻⁴
0.0050	4.2•10⁻⁴	2.1•10⁻⁴	1.4•10⁻⁴	1.2•10⁻⁴
0.0075	5.1•10⁻⁴	2.5•10⁻⁴	1.5•10⁻⁴	1.3•10⁻⁴
0.0100	5.7•10⁻⁴	2.7•10⁻⁴	1.8•10⁻⁴	1.3•10⁻⁴

The next table lists the accuracy as a function of the SB ratio and of the number of datapoints. The other parameters are fixed at

EVENTS = 1.5•10⁵;
LASERWidth = 0.005;
DATAPOINTS = 11;
LOOPS = 100;

while the separation between datapoints is different in the two cases so that the frequency range is nearly the same in both cases.

Table 3

SB POINTS	0.025	0.050	0.075	0.100
5 (Δf = 6 GHz)	29.•10⁻⁴	17.•10⁻⁴	10.•10⁻⁴	8.5•10⁻⁴
11 (Δf = 3 GHz)	4.7•10⁻⁴	2.2•10⁻⁴	1.3•10⁻⁴	1.2•10⁻⁴

It is clear that 5 points are not enough. The total measurement time depends on the parameters given at the beginning of the next section and is approximately 57 hours for 150000 events, and therefore the total measurement time is approximately 26 full days with 11 measurement points.

3. The Signal-to-Background ratio for some combinations of the FEL parameters.

There are some parameters which affect the final data-taking time but which are not well known at present. I fix these parameters (the names are self-explaining and are those given in the program in Appendix B) as follows:

CavityFactor = 50;   Cavity enhancement factor (in practice it
                                                 may turn out to be as small as 10)

TargetArea = 1 cm²;   This depends on our ability to steer the
                                                 muon beam in the PSC

TriggerQuality = 0.5*exp(-TriggerDelay/2.2μs);

TriggerDelay = 2μs;   Time between trigger at PSC entrance and
                                                 FEL firing

DetectorEfficiency = 50%;   May be much higher with different
                                                 CCD's

DetectorSolidAngleFraction = 40%;   This may also be much higher

The FEL parameters are:

AverageMacroPulsePower
Repetition rate (fixed at 200 Hz)
MicroPulseLength
MacroPulseLength (non relevant for these calculations)
RFFrequency (fixed at 3 GHz)

Figure 1 shows the SB ratio as a function of the MicroPulseLength in ps. There are different curves that correspond to different values of AverageMacroPulsePower. (The curves range in power from 5 KW to 30 KW, in steps of 5KW. Obviously, the SB ratio increases as the power increases, and the lowest curve corresponds to 5KW). The average power is referred to MicroPulseLength = 100 ps, and scales with the actual pulse length.
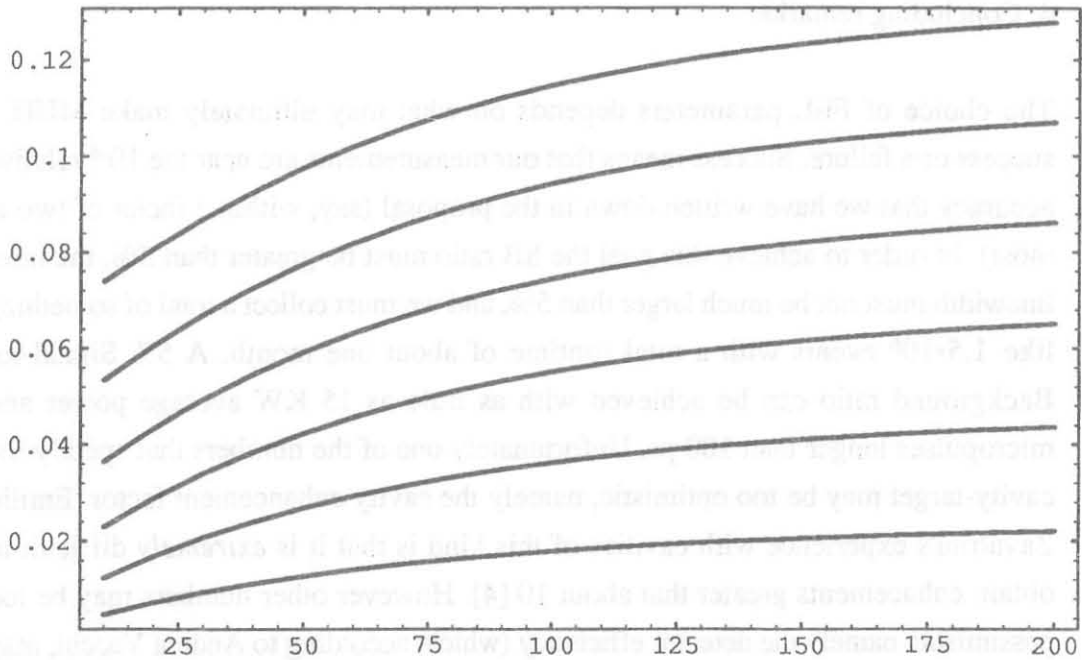
Figure 1: The Signal-toBackground rattio vs. the micropulse length (ps). The curves shown represent different FEL power outputs that range from 5 KW (lowest curve) to 30 KW. Steps are of 5KW, an the nominal power is reached for 100 ps micropulses, and is scaled linearly for longer and shorter micropulses.
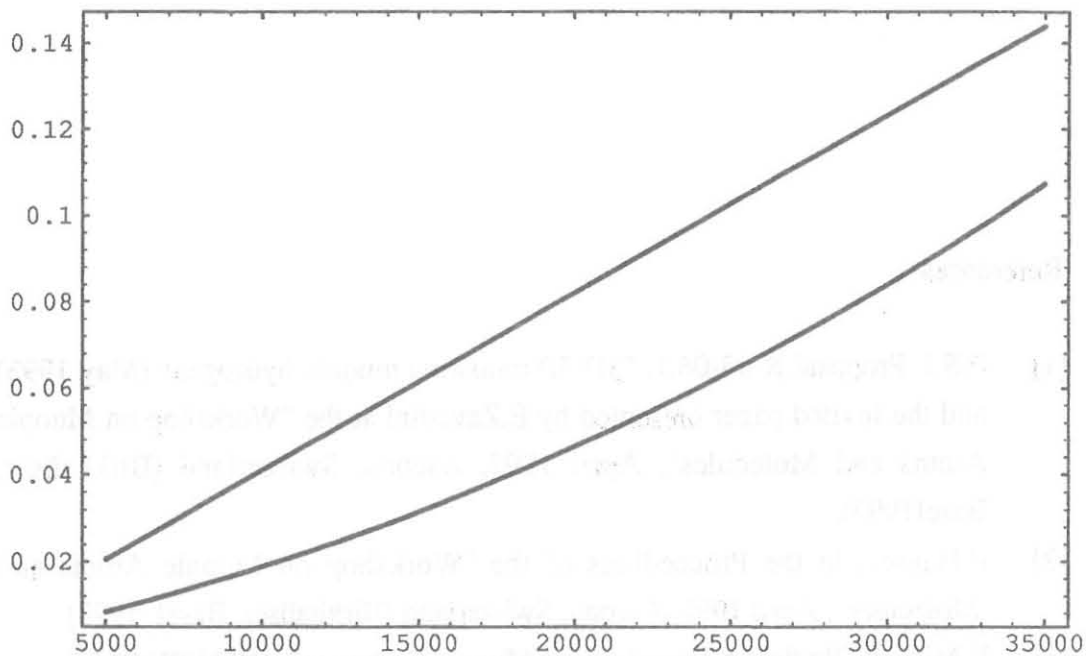

Figure 2: Signal-to-Background ratio vs. output power for two extreme values of the micropulse length 25 ps (lower curve) and 150 ps. Nominal power referred to 100 ps micropulses, as above.

4. Concluding remarks.

The choice of FEL parameters depends on what may ultimately make MUH a success or a failure. Success means that our measurements are near the 10^{-4} relative accuracy that we have written down in the proposal (say, within a factor of two at most). In order to achieve this goal the SB ratio must be greater than 5%, the laser linewidth must not be much larger than 5%, and we must collect a total of something like $1.5 \cdot 10^6$ events with a total runtime of about one month. A 5% Signal-to-Background ratio can be achieved with as little as 15 KW average power and micropulses longer than 100 ps. Unfortunately one of the numbers that specify the cavity-target may be too optimistic, namely the cavity enhancement factor. Emilio Zavattini's experience with cavities of this kind is that it is *extremely* difficult to obtain enhacements greater that about 10 [4]. However other numbers may be too pessimistic, namely the detector efficiency (which, according to Andrea Vacchi, may be almost 100% in "thicker" detectors [5]) and the fraction of solid angle covered by the detectors (it may be reasonable to expect that we are able to cover something like 80% of the solid angle). Taking these factors into account we would almost be back to were we started, and it might say that a 20 KW FEL suffices to reach the experimental goal. It is however quite clear that a 35 KW average pulse power (as in the proposal) would be a safer choice.

References

[1]   P.S.I. Proposal R-93-06.1, "3D-3P transition muonic hydrogen" (May 1993) and the invited paper presented by E.Zavattini at the "Workshop on Muonic Atoms and Molecules", April 1992, Ascona, Switzerland (Birkhaüser, Basel1993).

[2]   P.Hauser, in the Proceedings of the "Workshop on Muonic Atoms and Molecules", April 1992, Ascona, Switzerland (Birkhaüser, Basel 1993).

[3]   E.Milotti: "Radiative Transitions in Muonic Hydrogen", INFN/BE-93/05.

[4]   E.Zavattini, private communication.

[5]   A.Vacchi, private communication.

Appendix A: Monte Carlo program to compute the expected experimental accuracy.

```
<<Statistics`ContinuousDistributions`

<<Statistics`NonlinearFit`

<<Statistics`DescriptiveStatistics`

SB = 0.1; (* SignalToBackground ratio *)
LASERWidth = 0.005; (* relative laser linewidth *)

freq = 1.288*10^12 //N; (* Hertz *) (* frequency of 3D->3P transition *)
df = 3.*10^9/freq //N ; (* relative size of frequency steps *)
Width3D = 1.203*10^10; (* Hertz *)
Width3P = 3.534*10^10; (* Hertz *)
LINEWidth = (Width3D+Width3P)/(2*Pi*freq) //N;
TOTALWidth = LASERWidth+LINEWidth; (* total relative width *)
Clear[TransitionShape];
TransitionShape[f_] := SB*(TOTALWidth^2/4)/((1.-f)^2+TOTALWidth^2/4)+1.;
Print["Relative frequency step: ",df];
Print["Lifetime 3D (ps): ",1.*10^12/(Width3D)//N];
Print["Lifetime 3P (ps): ",1.*10^12/(Width3P)//N];
Print["LINEWidth: ",LINEWidth];
Print["LASERWidth: ",LASERWidth];
Print["TOTALWidth: ",TOTALWidth];

Relative frequency step: 0.00232919
Lifetime 3D (ps): 83.1255
Lifetime 3P (ps): 28.2965
LINEWidth: 0.00585339
LASERWidth: 0.005
TOTALWidth: 0.0108534

(* The main loop follows: the results of measurements are simulated at DATAPOINTS
points, with a total number of approximately EVENTS*DATAPOINTS events. Then the
measurements are fit with a Lorentzian shape. The fitting procedure is a
Levenberg-Marquardt adaptive fit (which is the standard fit routine in the
Mathematica NonlinearFit package). The simulation is repeated LOOPS times: this
generates LOOPS values for the fit mean value of the Lorentzian. The standard
deviation of the fit mean value is the measurement accuracy. The loop prints out
the results of the fits, and outputs the following plots:

- datapoints for the first fit
- fitting Lorentzian for the first fit
- superposition of the two previous plots
- all datapoints generated *)

EVENTS = 1.2*10^5; (* events per point *)
DATAPOINTS = 11;
MAXDEV = (DATAPOINTS-1)*df; (* relative range of frequency scan *)
LOOPS = 10;

Print["Relative range of frequency scan: ±",0.5*MAXDEV];

For[l=1; ListOfAverages={}; DataList={}, l<=LOOPS,

        For[ld=1; f=1.-0.5*MAXDEV+(Random[]-0.5)*df; data={}, ld<=DATAPOINTS,
            dist = NormalDistribution[TransitionShape[f]*EVENTS,
                                Sqrt[TransitionShape[f]*EVENTS]];
            AppendTo[data,{f,Random[dist]}];
            f += df;
            ld++];

        AppendTo[DataList,data];
```

```
    If[l==1,dataplot=ListPlot[data,PlotStyle->{PointSize[0.02]},
                      PlotRange->{{1.-0.55*MAXDEV,1.+0.55*MAXDEV},
                      {0.9*EVENTS,1.2*EVENTS}},
                      Frame->True, Axes->False]];

    fitparameters = NonlinearFit[data,a+b/((c-x)^2+d^2),x,
                      {{a,EVENTS},{b,SB*EVENTS*(TOTALWidth/2)^2},
                      {c,1.},{d,TOTALWidth/2}},
                      AccuracyGoal->1,PrecisionGoal->2];

    If[l==1,fitplot=Plot[(a+b/((c-x)^2+d^2)/.fitparameters),
                      {x,1.-0.55*MAXDEV,1.+0.55*MAXDEV},Frame->True, Axes->False];
                      Show[fitplot,dataplot,Frame->True, Axes->False]];

    average = c/.fitparameters;

    Print["Iteration\t",l,"\tmean = ",average];

    AppendTo[ListOfAverages,average];

    l++];

Print["\n"];

Print["Average position of mean :",Mean[ListOfAverages]];
Print["Standard deviation of mean :",StandardDeviation[ListOfAverages]];

ListPlot[Flatten[DataList,1],Frame->True, Axes->False];
```

```
Relative range of frequency scan: ±0.011646
Iteration    1       mean = 1.00009
Iteration    2       mean = 1.00025
Iteration    3       mean = 1.00005
Iteration    4       mean = 1.00017
Iteration    5       mean = 0.999999
Iteration    6       mean = 0.999823
Iteration    7       mean = 1.00006
Iteration    8       mean = 0.999662
Iteration    9       mean = 0.99995
Iteration   10       mean = 0.999817


Average position of mean :0.999988
Standard deviation of mean :0.000178884
```
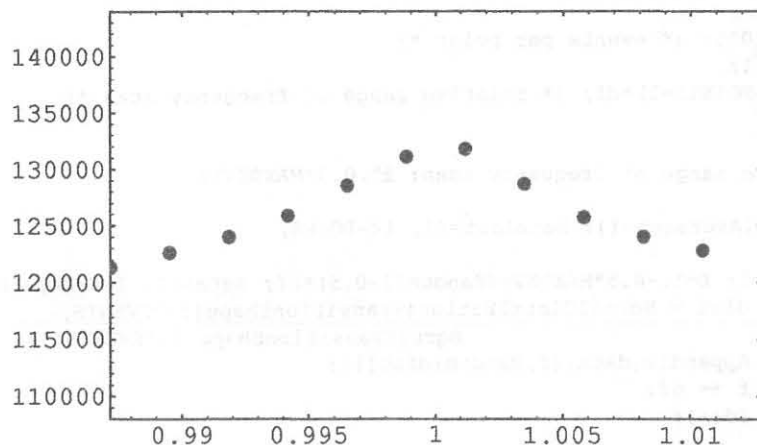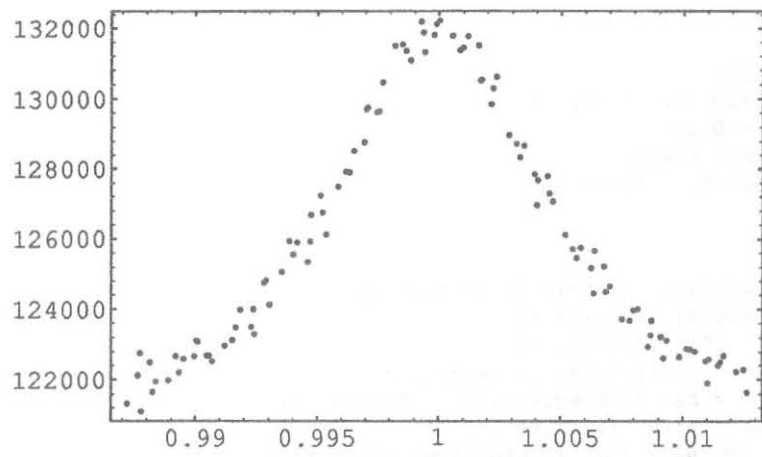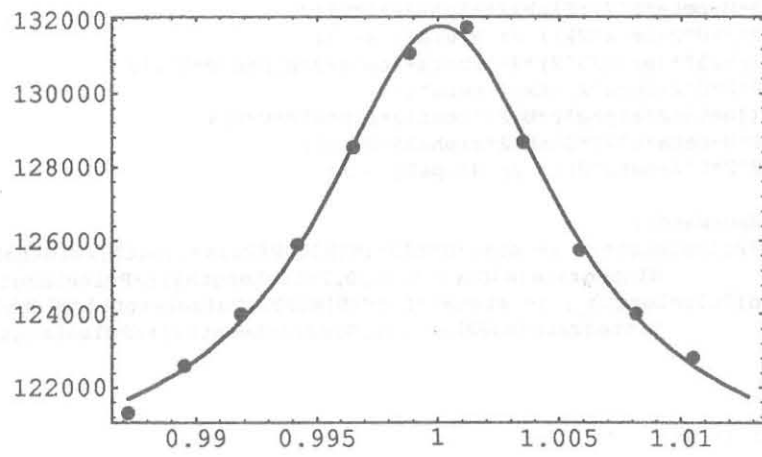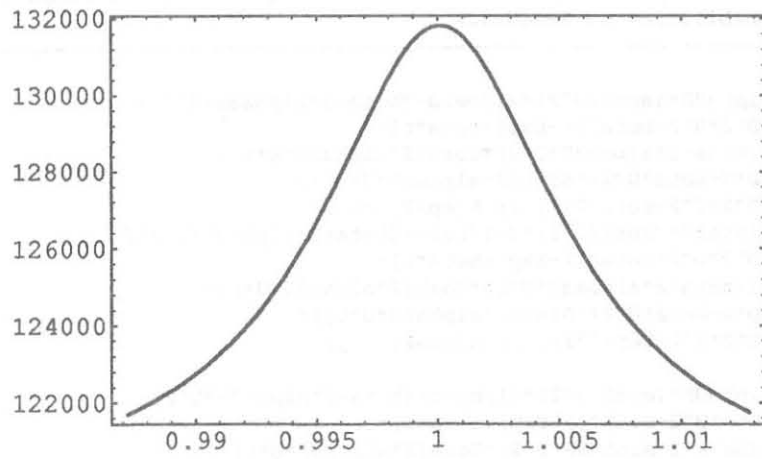
Appendix B: Program to compute the Signal-to-Background ratio.

```
<<Miscellaneous`PhysicalConstants`

(* ----------------------------------------------------------------------
What follows is an implementation of Peter Hauser's formulas to compute the
transition probabilities ON RESONANCE
   ----------------------------------------------------------------------- *)

W3D3P[t_] := alpha3D*(eps2/U^2)*(1/beta+(beta-2*alpha3D*U^2)/
      (4*alpha3D^2*U^2-beta^2)-Exp[-beta*t]*
      (1/beta+((beta-2*alpha3D*U^2)*Cosh[2*alpha3D*U*t]+
      (2*alpha3D*U-beta*U^2)*Sinh[2*alpha3D*U*t])/
      (4*alpha3D^2*U^2-beta^2))) /; N[eps2] <= 1;
W3D3P[t_] := alpha3D*(eps2/U^2)*(-1/beta+(beta+2*alpha3D*U^2)/
      (4*alpha3D^2*U^2+beta^2)-Exp[-beta*t]*
      (-1/beta+((beta+2*alpha3D*U^2)*Cosh[2*alpha3D*U*t]+
      (2*alpha3D*U-beta*U^2)*Sinh[2*alpha3D*U*t])/
      (4*alpha3D^2*U^2+beta^2))) /; N[eps2] > 1;

W3P3D[t_] := alpha3P*(eps2/U^2)*(1/beta+(beta-2*alpha3P*U^2)/
      (4*alpha3P^2*U^2-beta^2)-Exp[-beta*t]*
      (1/beta+((beta-2*alpha3P*U^2)*Cosh[2*alpha3P*U*t]+
      (2*alpha3P*U-beta*U^2)*Sinh[2*alpha3P*U*t])/
      (4*alpha3P^2*U^2-beta^2))) /; N[eps2] <= 1;
W3P3D[t_] := alpha3P*(eps2/U^2)*(-1/beta+(beta+2*alpha3P*U^2)/
      (4*alpha3P^2*U^2+beta^2)-Exp[-beta*t]*
      (-1/beta+((beta+2*alpha3P*U^2)*Cosh[2*alpha3P*U*t]+
      (2*alpha3P*U-beta*U^2)*Sinh[2*alpha3P*U*t])/
      (4*alpha3P^2*U^2+beta^2))) /; N[eps2] > 1;

Clear[Forward,Backward];
      Forward[PulseLength_] := stat3D*f3D*(N[W3D3P[PulseLength]/Width3D] +
                  NIntegrate[W3D3P[t],{t,0,PulseLength}])/PulseLength;
      Backward[PulseLength_] := stat3P*f3P*(N[W3P3D[PulseLength]/Width3P] +
                  NIntegrate[W3P3D[t],{t,0,PulseLength}])/PulseLength;

(* Beam *)

MuonRate = 240; (* Hertz *)

(* Target *)

CavityFactor = 50;
TargetArea = 1.*10^-4; (* m^2 *)
TriggerQuality = 0.5;
DetectorEfficiency = 0.5;
DetectorSolidAngleFraction = 0.4;

(* FEL *)

AverageMacroPulsePower = 0.5*10^4; (* Watt *)
RFFrequency = 3*10^9; (* Hertz *)
RepetitionRate = 200; (* Hertz *)
MicroPulseLength = 100*10^-12; (* Secondi *)
MicroPulsePeriod = N[1./RFFrequency]; (* Secondi *)
MacroPulseLength = 3*10^-6; (* Secondi *)
DutyCycle = (MicroPulseLength/MicroPulsePeriod) //N;
AveragePower = AverageMacroPulsePower*(RepetitionRate*MacroPulseLength) //N;
AveragePulseIntensity = AverageMacroPulsePower/TargetArea //N;
Intensity = CavityFactor*AveragePulseIntensity/DutyCycle //N;
TriggerDelay = 2.*10^-6;
TriggerQuality = TriggerQuality*Exp[-TriggerDelay/(2.2*10^-6)] //N;

(* physics of the 3D-3P transition *)

BohrRadius = 2.85*10^-13; (* m *)
DipoleMatrixElement = Sqrt[13.5]*BohrRadius;
```

```
                              (* matrix element for the transition 3D(7,5/2)->3P(5,3/2) *)
f3D = 0.38;  (* 3D fraction at 20 mbar *)
f3P = 0.1;   (* 3P fraction at 20 mbar *)
stat3D = 0.35;  (* statistical 3D(7,5/2) population *)
stat3P = 0.417;  (* statistical 3P(5,3/2) population *)
Width3D = 1.33*10^10;  (* Hertz *)
Width3P = 3.85*10^10;  (* Hertz *)
BR2STo1S = 0.134;  (* Branching ratio Width(3P->2S)/Width(3P->1S) *)
Omega0 = 2*Pi*1.288*10^12 //N;  (* Hertz *) (* angular frequency *)
V = (Sqrt[PlanckConstant/(Joule*Second)*FineStructureConstant*Intensity]
                   *DipoleMatrixElement);  (* |V|^2 in Peter's formulas *)
GR = 4*(V^2)/((PlanckConstantReduced/(Joule*Second))^2 * (Width3D+Width3P))//N;
RelativeKBetaIntensity = 0.09;


(* ------------------------------------------------------------------------ *)


Print["AveragePower (W): ", AveragePower];
Print["DutyCycle: ",DutyCycle//N];
Print["AveragePulseIntensity (MW/cm2): ",AveragePulseIntensity*10^-6];
Print["Intensity (MW/cm2): ",Intensity*10^-6];
Print["DipoleMatrixElement: ", DipoleMatrixElement];
Print["V:\t",V//N];
Print["Transition rate from Golden Rule: ",GR];
Print["Total forward transition prob in 100ps from Golden Rule:
", (GR/(GR+Width3D))*(1-Exp[-(GR+Width3D)*(10^-10)])];
Print["Total backward transition prob in 100ps from Golden Rule:
", (GR/(GR+Width3P))*(1-Exp[-(GR+Width3P)*(10^-10)])];
Print["Asymptotic forward transition prob from Golden Rule: ",(GR/(GR+Width3D))];
Print["Asymptotic backward transition prob from Golden Rule: ",(GR/(GR+Width3P))];


(* ------------------------------------------------------------------------ *)



omega = Omega0;

eps2 = 4*V^2 / ((PlanckConstantReduced/(Joule*Second))^2 * ((Width3D-
Width3P)/2)^2);
U = Sqrt[1-eps2];
alpha3D = 0.25*(Width3D-Width3P);
alpha3P = -alpha3D;
beta = 0.5*(Width3D+Width3P);

AveragePower (W): 3.
DutyCycle: 0.3
AveragePulseIntensity (MW/cm2): 50.
Intensity (MW/cm2): 8333.33
                                    -12
DipoleMatrixElement: 1.04716 10
                  -25
V:     2.102 10
                                         8
Transition rate from Golden Rule: 3.0679 10
Total forward transition prob in 100ps from Golden Rule: 0.0167639
Total backward transition prob in 100ps from Golden Rule: 0.00774243
Asymptotic forward transition prob from Golden Rule: 0.0225468
Asymptotic backward transition prob from Golden Rule: 0.00790558

(* SB ratio for t = MicroPulseLength *)

SignalToBackgroundRatio = (Forward[MicroPulseLength]-
                           Backward[MicroPulseLength])/f3P
0.0178516

(* table of SB values vs. t at this FEL output power *)
```

```
SBtable = Table[{PulseLength*10^12,(Forward[PulseLength]-
            Backward[PulseLength])/f3P},
         {PulseLength,10.*10^-12,200.*10^-12,10.*10^-12}];

plot05 = ListPlot[SBtable,Frame->True,PlotRange->All,Axes->False,PlotJoined->True]
```