Contents

1 Abstract

The influence of the detector deadtime and dwelltime at a channel given by the sweep frequency of the tranducer on the Mossbauer absorption spectrum shall be studied by Monte Carlo simulation. Deadtime effects distort the shape of the absorption lines since the count rate depends on the channel number. In the limit of infinite long dwelltimes the deadtime effect is calculated. The influence of the dwelltime on the lineshape is an unsolved problem.

2 Interval distribution

The pulse train of the radioactive source reaching the detector follows the Poisson statistic the distribution of intervals Δt is given by the exponential:

$$f(\Delta t) = \lambda * exp(-\lambda * \Delta t) \tag{1}$$

where λ is the counting rate. Time intervals are simulated by a random number generator using the cumulative distribution function (cdf) obtained by integrating from 0 to Δt.

$$\begin{aligned} F(\Delta t) &= \int_0^{\Delta t} f(x)dx \\ &= 1 - exp(-\lambda * \Delta t) \end{aligned} \tag{2}$$

F(Δt) is set equal to the cdf of the uniform random number F(Δt)=u to obtain Δt from the uniform number u=[0,1).

$$\Delta t = -\frac{1}{\lambda} ln(1-u) \tag{3}$$

The Fig.1 is calculated with the fortran code where RAND denotes the random number generator and k=100 channels for time unit 1.

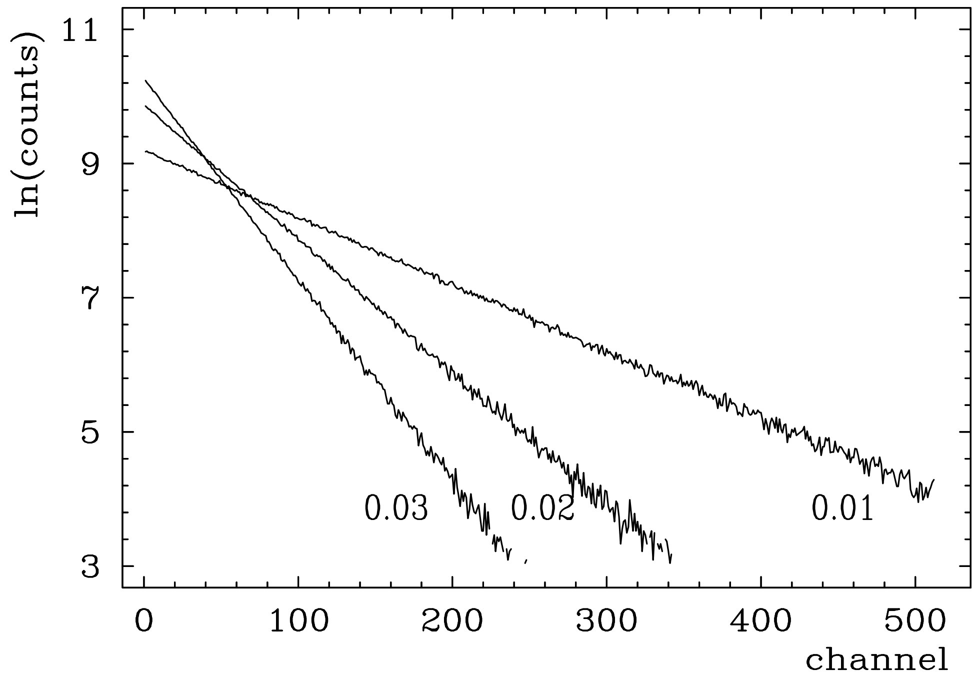

Figure 1: The logarithm of the simulated counts give a straight line. The time intervals in arbitrary units of 0.01 per channels are plotted for three values of $\lambda = 10^2$, 200, and 300. The total number of counts is $N = 10^6$.

```
ix=RAND(iseed)
do i=1,N
ix=-alog(1.-RAND(0))/lambda*k
if(ix.le.512) channel(ix)=channel(ix)+1
end do
```

The following observation has not been analytically derived. The code asking for a shorter Δt by the iy line

```
do i=1,N
ix=-alog(1.-RAND(0))/lambda*k
iy=-alog(1.-RAND(0))/lambda*k; if(iy.lt.ix)ix=iy
if(ix.le.512) channel(ix)=channel(ix)+1
end do
```

gives the same straight line as $\lambda = 2 \cdot 10^2$. Asking again for a shorter Δt by adding the line

```
iz=-alog(1.-RAND(0))/lambda*k; if(iz.lt.ix)ix=iz
```

the result is not again equivalent with the double rate (which could have been expected) of 400, but coincides with the straigt line of rate 300.

3 Single line Mossbauer spectrum in the limit of infinite dwelltime

Single line spectra (natural linewidths of ^{57}Co source and fictive absorber of 1mg natural iron/cm^2 and f-factor 1, back ground fraction zero) with 10^4 counts in the baseline are simulated. The event train of the γ-quanta passing the absorber has rates proportional to the value of the theoretical curve at each channel number. The rates are multiplied by 1 at large velocities (channels 0, 512, 1024) and by 0.75 at

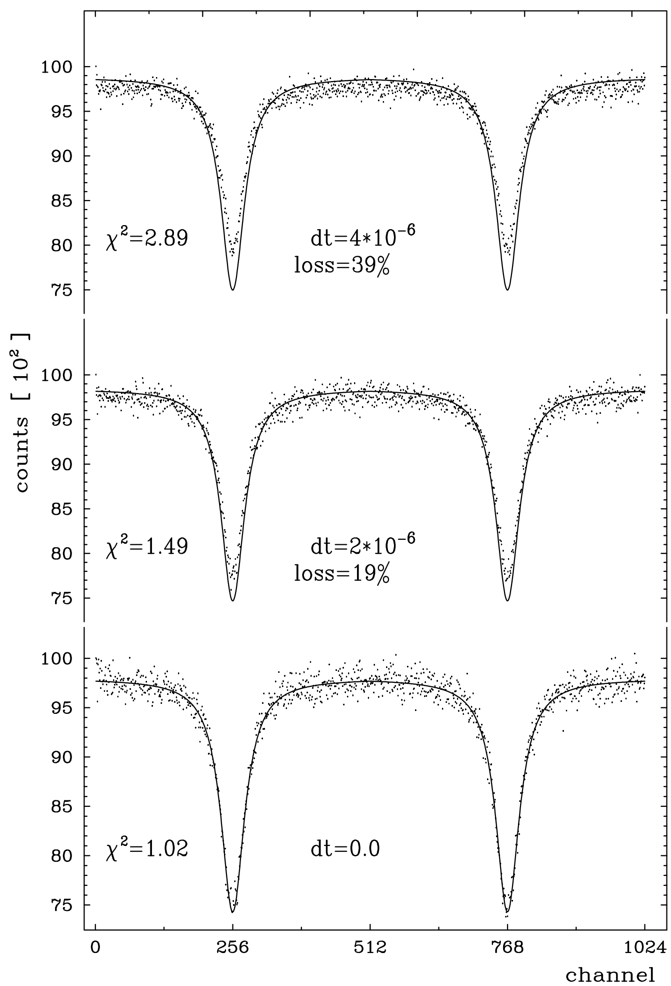

Figure 2: The single line spetra ($\pm 1mm/s$ are simulated with 10^5 counts per time unit and a sweep frequency of $\omega = 10^{-1}$ ($(\omega * nu\_channels)^{-1} \sim 10^{-2}$ time units duration time per channel), so that in average 10^3 events are collected in a channel each period. After about 10 periods 10^4 counts are reached. The simulation when omitting events with time distance $\Delta t < dt$, deadtime dt (events during dt do not start a new deadtime -non-paralyzable deadtime) is shown for $dt \cdot \lambda = 10^{-1}$ and $dt \cdot \lambda = 2 \cdot 10^{-1}$, corresponding to a count loss of 10% and 19%, respectively. The zero velocity channel are 256 and 768.

zero velocity, so that the loss of counts is less around zero velocity. This behaviour is demonstrated in Fig.2, clearly seen in the upper spectrum by the missing counts at zero velocity.

The C-code is again quite simple.

```
ichannel=0;        srandom(*iseed);
lastevent=0.0;
while(isimul[0] < counts){
  eventtime=-log(1.-frand())/(lambda*theo[ichannel]);
  lastevent=lastevent+eventtime;
  if(lastevent > deadtime){isimul[ichannel]++; lastevent=0.0;
   }else{iloss++;}
  totaltime=totaltime+eventtime;
  ichannel= totaltime/dwelltime;
  i=ichannel/nu_channel; ichannel=ichannel-i*nu_channel;
}
```

This simulation can be used to study the influence of deadtime effects on the fit-parameters like intensities, line broadening, thickness etc.

4 Finite dwelltime

In case of finite dwelltime the count rate change from channel to the next channel comes into play. The time Δt between events becomes larger than the dwelltime dt, so that a channel may be reached during Δt with a quite different rate. If e.g. larger time distances Δt_0 are given by the average rate at zero velocity, the next event far from zero velocity has a higher rate so that the probability to have an event earlier than Δt_0 is not accounted for. The pulse train seen by the detector cannot be simulated correctly by the code given above.

The result of the code is shown in Fig.3 for three different sweep frequencies ω. Lets take the usual time unit [s:second]. At $\omega = 10^3 s^{-1}$, which is 10^4 times larger than the value taken as small enough to simulate infinite dwelltime the simulated single line is shifted to higher channels.

There seems to be no solution for an event train in case of a time dependent average rate. A first guess is to compare the time interval Δt_0 at the present channel with interval Δt_1 at the channel reached in time Δt_0. If Δt_0 is larger than Δt_1 (to many channels are jumped over) the shorter time Δt_1 could be taken to proceed to the next channel. The rate λ is a function of time. Such a Poisson process is called non-

homogeneous (NHPP) (see e.g. [1]). Here $\lambda(t) = \lambda \cdot$theo[ichannel] with ichannel= int(dwelltime$\cdot$ t) modulo nu_channel.
One possibility to handle NHPP is simulating by thinning/rejection of events according to its probability.

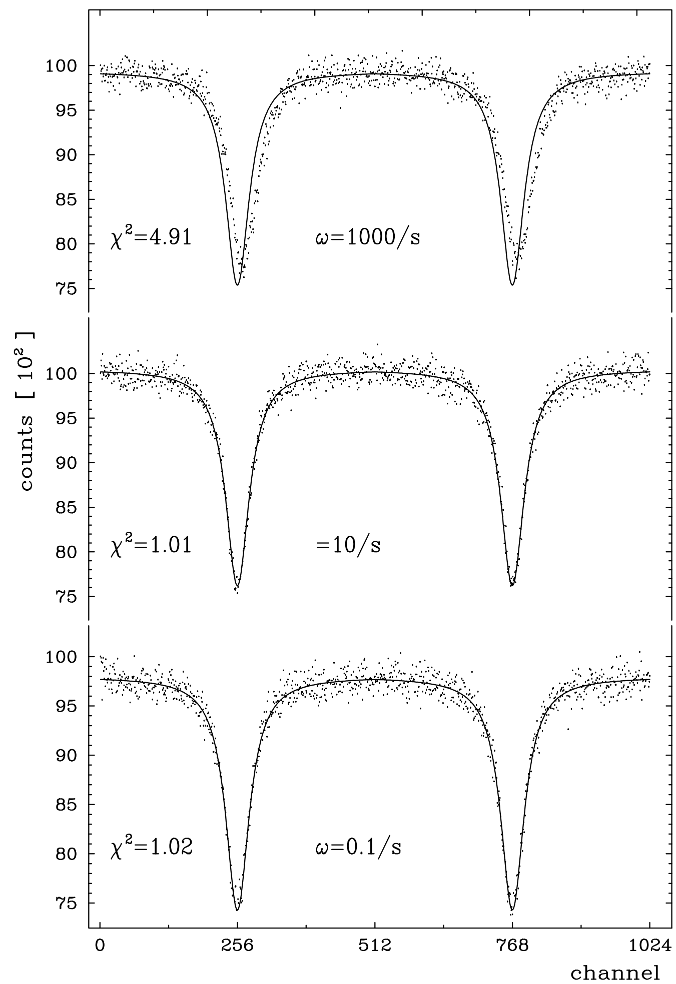

Figure 3: The single line spetra of Fig.2 are simulated with $10^5 s^{-1}$ count rate, zero deadtime and three sweep frequencies $\omega = 10^{-1}, 10, 1000s^{-1}$ such that the dwelltime $dt = (\omega * nu\_channels)^{-1}$ takes values of $10^{-2}s, 10^{-4}s$ and $10^{-6}s$. The finite dwelltime leads to a shift of the lines to higher channels (which tendency is remakable at $\omega = 100s^{-1}$ by the χ^2 value - not shown) und obvious at $\omega = 10^3 s^{-1}$. 10^5 counts per s means in average 10 sweeps are neccessary to collect 1 count.

Starting from the constant rate of the source and its exponential distribution of time intervals the spectrum is obtained by the probability at each channel to pass the absorber. This probability shall be close to 1 at v_{max} (channel 1) and less than 1 at resonance. By the rejection condition u > theo[ichannel] (u $\subset$ (0,1]) for channel number ichannel low count rates are obtained according to the absorption profile. The following code collects the eventtime stored in totaltime, which by the dwelltime determines the next channel number until a γ passes the rejection condition at the current channel.

```
step:
eventtime=-log(1.-frand())/lambda; icall++;
// of source
jch=ichannel;
totaltime=totaltime+eventtime;
lastevent=lastevent+eventtime;
ichannel= totaltime/dwelltime;
i=ichannel/nu_channel; ichannel=ichannel-i*nu_channel;
if(frand() > theo[jch])goto step;
```

Passing this code the current channel is incremented if the last event is later than the deadtime.

```
if(lastevent > deadtime){
isimul[jch]++; lastevent=0.0; icount++;
}else{iloss++;}
```

This code is quite different from the code (I) above (long dwelltime). The simulated spectra at $\omega = 10^{-1}$ are the same.
For higher sweep frequencies (finite dwelltimes) one can only rely on the second code(II). Its behaviour is quite different. With zero deadtime the simulated spectra do not or rather very weak depend on the sweep frequency. the χ^2-values are different although the random number generator starts with the same seed number. The pairs of values (ω, χ^2) are (10^3, 0.91), (10^2, 1.01), (10^1, 1.03), (10^0, 1.06), (10^{-1}, 0.99). The last pair for code(I) reads (10^{-1}, 1.02), which is obviously the same.

(Fig.4 shows the dependence of the simulated counts at constant deadtime of $dt = 4.0 \cdot 10^{-5}s$ and rate $\lambda = 10^5/s$ and 3 sweep frequencies. At $dt \cdot \lambda = 4$ the code misses 38% of counts. At $\omega = 0.1/s$ the two codes have the same result. The deadtime is most effective in the region of high rates (baseline). Around zero velocity the rate is lower such that less counts are rejected by the deadtime condition. At large sweep frequencies this effect decreases and at $\omega = 1000/s$ which corresponds to a dwelltime of $1/1.024 \cdot 10^{-6}s$ a shift to the left is observed. This behaviour questions the validity of the code for all ω although an approximation is not obvious from the logic of the code.

Fig.5 shows a fit including the intensity, which means the underlying theory is changed and adapted to the distorted spectrum (for $\omega = 0.1/s$ the two codes give the same result - see above). The decrase of χ^2 to values much smaller than 1 is a typical deadtime effect. The intensity of 0.67 instead of 1 demonstrates the misin-

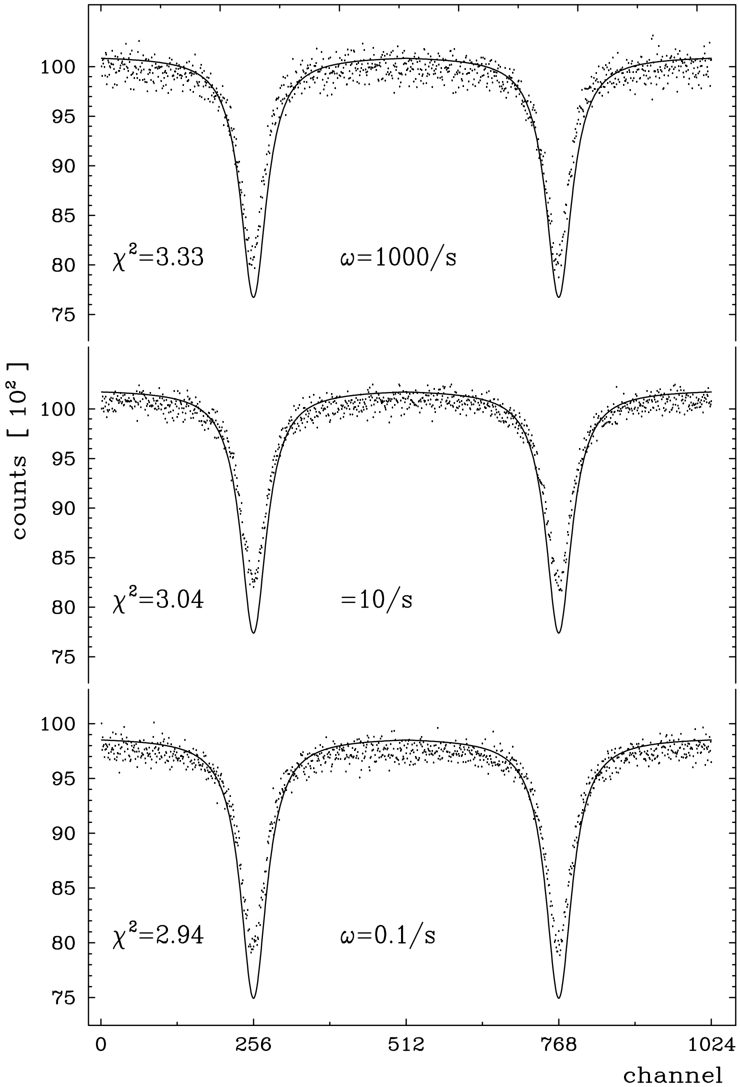

Figure 4: The single line spetra with sweep frequency fixed rate $\lambda = 10^5/s$ and deadtime $dt = 4 \cdot 10^{-5}$ at different sweep frequencies.

terpretation of spectra if deadtime effect are present.

5 Conclusion

Three times/timescale are important for the realibility of a measured spectrum: sweepfrequency, total counts entering the detector/measurering system and the deadtime of the measurering system. The simulation shall serve to estimate the quality of the spectra to be measured.

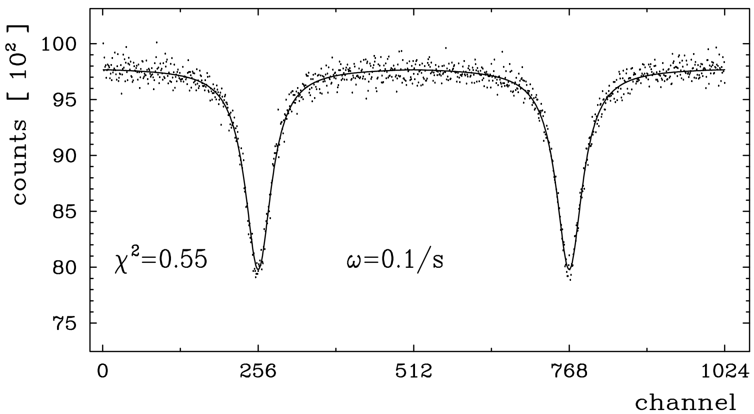

Figure 5: The single line spetra of Fig.4 at $\omega = 0.1/s$ has a $\chi^2 = 0.55$ much less than 1. The fit includes the intensity with a value of 0.72 instead of 1 as a result of the large deadtime.

References

[1] Krzysztof Burnecki, Simulation of counting processes, http://prac.im.pwr.edu.pl/~burnecki/Simulation_of_counting_processes.pdf, Hugo Steinhaus Center Wroclaw University of Technology.