Contents

1 Abstract

A misalignment of the absorber with respect to the optical axis defined by circular apertures may give rise to a deformation of the baseline of a Mossbauer spectrum. An idealized situation with a point source and an extended circular source and circular absorber is treated numerically. In the special case of an aligned situation aperture effects still can disturb the base line of the spectrum. Cosine smearing will be observed for all cases with large apertures. The observation of a canted baseline which could be restored by carefully readjusting source-Absorber-apertures to a well defined optical axis initiated simulating such misaligned situations. The program code developed according to the algebra outlined in the following pages could not reproduce a canted baseline.

2 Misalignment

2.1 Absorber out of source-detector axis

The vector $\mathbf{a}$ to the center of the misaligned absorber in the coordinate system fixed at z_0 with unit vectors $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ is (see Fig. 1)

$$\mathbf{a} = H \cdot \mathbf{e}_z + d_{yA} \cdot \mathbf{e}_y \tag{1}$$

and the vectors $\mathbf{c}_A(\varphi)$ of the limiting circle

$$\mathbf{c}_A = A/2 \cdot (sin\varphi \, \mathbf{e}_x + cos\varphi \, \mathbf{e}_y) \tag{2}$$

are the sum $\mathbf{r}_A = \mathbf{a} + \mathbf{c}_A(\varphi)$. The projection of the circle of the absorber

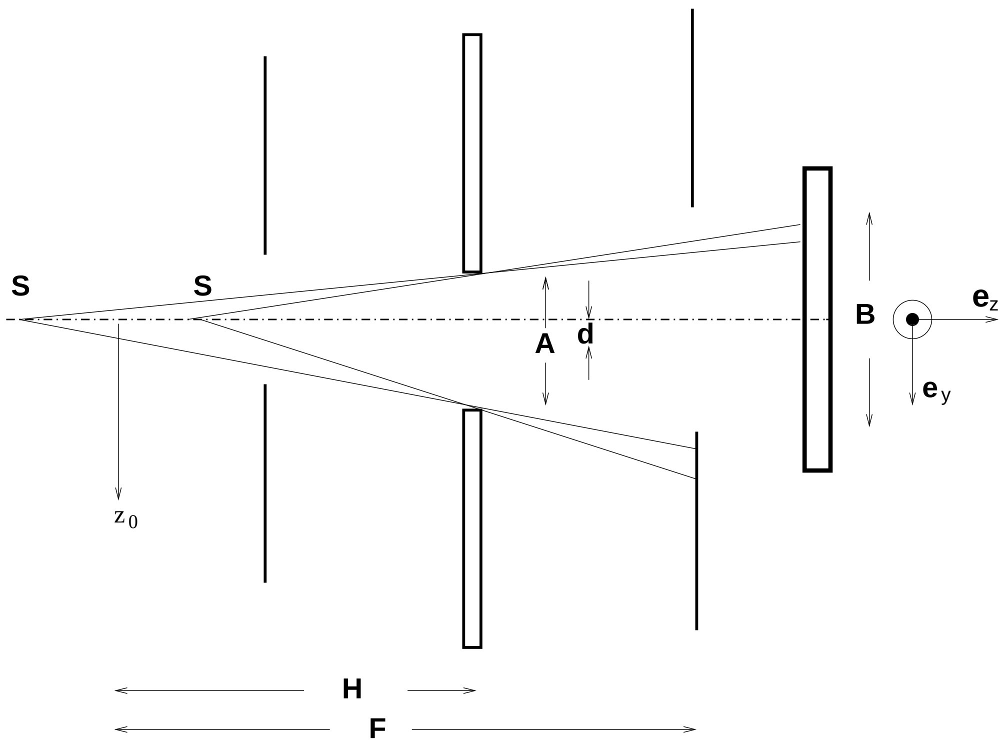

Figure 1: Misaligned absorber of circular shape by a displacement d from the axis (-··-·-). The circular aperture in front and behind the absorber are aligned. The solid angles of idealized point sources S on the axis are shown at two positions. All photons passing the second aperture are counted by the detector with equal probability. A is the diameter of the absorber, w the width of the second aperture. The first aperture in front shall not limit the solid angle. H and F are distances of the Absorber and second aperture from the source position z_0 at maximum velocity.

onto the surface of the second aperture at distance F from the position of the source at $\mathbf{p}_S = s\mathbf{e}_z$ is needed. The vector $\mathbf{k}_A$ from $\mathbf{p}_S$ to the circle of the absorber is the difference $\mathbf{k}_A = \mathbf{r}_A - \mathbf{p}_S$. The projection is obtained by the equation $\mathbf{p}_S + \tau \cdot \mathbf{k}_A = \mathbf{c}_B$ where

$$\mathbf{c}_B = F \cdot \mathbf{e}_z + c_x \cdot \mathbf{e}_x + c_y \cdot \mathbf{e}_y \tag{3}$$

is a point on the surface and τ a length. Comparing the coefficients of the 3 unit vectors

$$\begin{aligned} \tau \cdot A/2\, sin\varphi &= c_x \\ \tau \cdot (d_{yA} + A/2\, cos\varphi) &= c_y \\ \tau(H - s) &= F - s \end{aligned}$$

c_x and c_y is given by

$$\begin{aligned} c_x &= R_B\, sin\varphi \qquad (4) \\ c_y &= d_y + R_B\, cos\varphi \\ R_B(s) &= \frac{A}{2}\tau \qquad d_y = d_{yA}\tau \qquad \tau = \frac{F - s}{H - s} \end{aligned}$$

c_B is again a circle with radius $R_B(s)$. The circle may not be inside of the aperture at F (see Fig. 1).

2.2 Misaligned source

The vector $\mathbf{a}$ to the center of the aligned absorber in the coordinate system fixed at z_0 with unit vectors $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ is (see Fig. 2)

$$\mathbf{a} = H \cdot \mathbf{e}_z \tag{5}$$

and the vectors $\mathbf{c}_A(\varphi)$ of the limiting circle

$$\mathbf{c}_A = A/2 \cdot (sin\varphi\, \mathbf{e}_x + cos\varphi\, \mathbf{e}_y) \tag{6}$$

are the sum $\mathbf{r}_A = \mathbf{a} + \mathbf{c}_A(\varphi)$. The projection of the circle of the absorber onto the surface of the second aperture at distance F from the position of the source at $\mathbf{p}_S = s\mathbf{e}_z + d_{yS}\mathbf{e}_y$ is needed. The vector $\mathbf{k}_A$ from $\mathbf{p}_S$ to the circle of the absorber is the difference $\mathbf{k}_A = \mathbf{r}_A - \mathbf{p}_S$. The projection is obtained by the equation $\mathbf{p}_S + \tau \cdot \mathbf{k}_A = \mathbf{c}_B$ where

$$\mathbf{c}_B = F \cdot \mathbf{e}_z + c_x \cdot \mathbf{e}_x + c_y \cdot \mathbf{e}_y \tag{7}$$

is a point on the surface and τ a length. Comparing the coefficients of the 3 unit vectors

$$\begin{aligned} \tau \cdot A/2\, sin\varphi &= c_x \\ \tau \cdot (-d_{yS} + A/2\, cos\varphi) &= c_y - d \\ \tau(H - s) &= F - s \end{aligned}$$

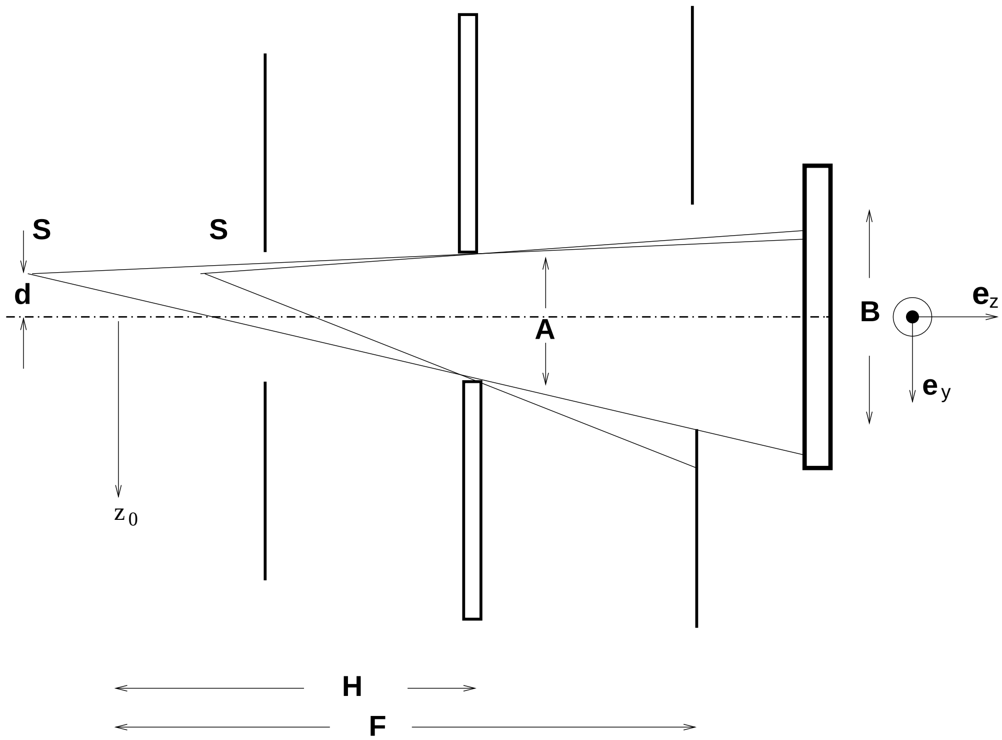

Figure 2: Misaligned absorber of circular shape by a displacement d from the axis (-··-·-). The circular aperture in front and behind the absorber are aligned. The solid angles of idealized point sources S on the axis are shown at two positions. All photons passing the second aperture are counted by the detector with equal probability. A is the diameter of the absorber, w the width of the second aperture. The first aperture in front shall not limit the solid angle. H and F are distances of the Absorber and second aperture from the source position z_0 at maximum velocity.

c_x and c_y is given by

$$\begin{aligned} c_x &= R_B \, sin\varphi && (8)\\ c_y &= d_y + R_B \, cos\varphi && (9)\\ R_B(s) &= \frac{A}{2}\tau \qquad d_y = d_{yS}(1-\tau) \qquad \tau = \frac{F-s}{H-s} && (10) \end{aligned}$$

2.3 Absorber and point source out of axis

2.3.1 Absorber, source and axis are in plane

The vectors $\mathbf{a}/\mathbf{p}_S$ to the center of the misaligned absorber/source in the coordinate system fixed at z_0 with unit vectors $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ are (see Fig. 1)

$$\begin{aligned} \mathbf{a} &= H \cdot \mathbf{e}_z + d_{yA} \cdot \mathbf{e}_y \\ \mathbf{p}_S &= s \cdot \mathbf{e}_z + d_{yS} \cdot \mathbf{e}_y. \end{aligned}$$

The vectors $\mathbf{r}_A$ of limiting circle of the absorber are the sum $\mathbf{r}_A = \mathbf{a} + \mathbf{c}_A(\varphi)$ with $\mathbf{c}_A(\varphi)$

$$\mathbf{c}_A = A/2 \cdot (sin\varphi\, \mathbf{e}_x + cos\varphi\, \mathbf{e}_y). \tag{11}$$

The projection of the circle of the absorber onto the surface of the second aperture at distance F from the position of the source at $\mathbf{p}_S$ is needed. The difference $\mathbf{k}_A = \mathbf{r}_A - \mathbf{p}_S$ is the vector from $\mathbf{p}_S$ to a point $\mathbf{r}_A(\varphi)$ on the circle of the absorber. The projection is obtained by the equation $\mathbf{p}_S + \tau \cdot \mathbf{k}_A = \mathbf{c}_B$ where

$$\mathbf{c}_B = F \cdot \mathbf{e}_z + c_x \cdot \mathbf{e}_x + c_y \cdot \mathbf{e}_y \tag{12}$$

is a point on the surface of the aperture and τ a length. Comparing the coefficients of the 3 unit vectors

$$\begin{aligned} \tau \cdot A/2\, sin\varphi &= c_x \\ d_{yS} + \tau \cdot (d_{yA} - d_{yS} + A/2\, cos\varphi) &= c_y \\ \tau(H - s) &= F - s \end{aligned}$$

c_x and c_y is given by

$$\begin{aligned} c_x &= R_B\, sin\varphi \\ c_y &= d_y + R_B\, cos\varphi \\ R_B(s) &= \frac{A}{2}\tau \qquad d_y = d_{yS} + (d_{yA} - d_{yS})\tau \qquad \tau = \frac{F-s}{H-s} \end{aligned} \tag{13}$$

2.3.2 Source out of plane

The vector $\mathbf{p}_S$ to the center of the misaligned source is extended to

$$\mathbf{p}_S = s \cdot \mathbf{e}_z + d_{xS} \cdot \mathbf{e}_x + d_{yS} \cdot \mathbf{e}_y$$

The comparison of the coefficients of the 3 unit vectors now leads to

$$\begin{aligned} d_{xS} + \tau \cdot (-d_{xS} + A/2\, sin\varphi) &= c_x \\ d_{yS} + \tau \cdot (d_{yA} - d_{yS} + A/2\, cos\varphi) &= c_y \\ \tau(H - s) &= F - s \end{aligned}$$

with c_x, c_y and τ

$$c_x = d_x + R_B\, sin\varphi \tag{14}$$

$$
\begin{aligned}
c_y &= d_y + R_B\, cos\varphi \\
R_B(s) &= \frac{A}{2}\tau \quad d_x = d_{xS}(1-\tau) \quad d_y = d_{yS} + (d_A - d_{yS})\tau \\
\tau &= \frac{F-s}{H-s}
\end{aligned}
$$

Replacing $R_B(s) = \frac{A}{2}\tau$ by $R = r\tau$ $(r \leq A/2)$ gives a general image of the absorber point r, φ for any position (d_{xS}, d_{yS}) of the point source.

2.4 Integration over the aperture/detector

The intensity of the radiation from the source S on the surface of the second aperture is proportional to the solid angle element $d\Omega$ with the

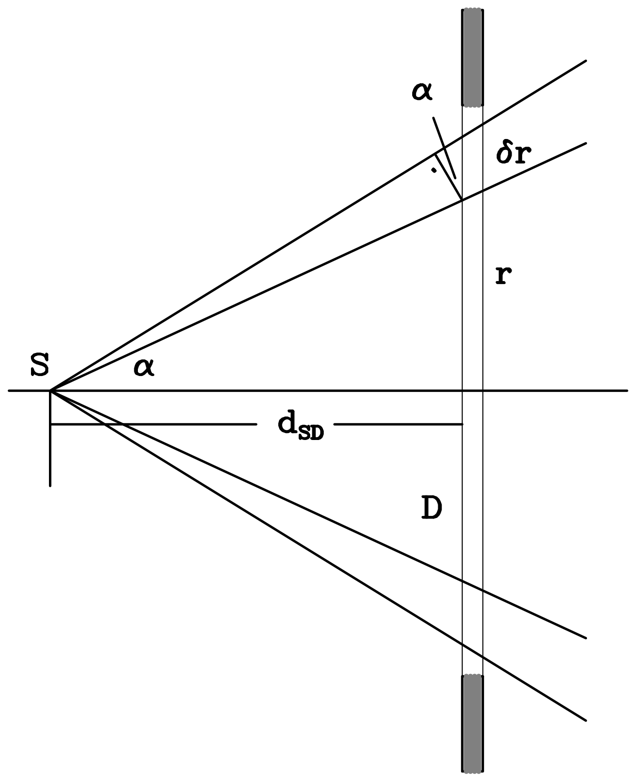

Figure 3: Source at position S, a diaphragm D (=A or B) is centered to an optical axis. The solid angle $d\Omega$ belonging to the surface element at distance r and width δr is equal to the surface $2r\pi\delta r \cdot cos\alpha$ devided by the surface $4\pi\delta^2$ of the sphere of radius δ $(\delta^2 = r^2 + d_{SD}^2)$.

distance δ from $\mathbf{p}_S$ to a point on the surface. When integrating over the surface element dD of the diaphragm the related solid angle $d\Omega$ is smaller by the factor $cos\alpha$ (see Fig. 3).
The vector from the source position $\mathbf{p}_S$ through a point r, φ of the absorber ending at $\mathbf{c}_B$ on the plane of the aperture has the direction

$\mathbf{K} = \mathbf{c}_B - \mathbf{p}_S$.

$$
\begin{aligned}
\mathbf{K} &= (F-s)\mathbf{e}_z + (d_x - d_{xS} + Rsin\varphi)\mathbf{e}_x + (d_y - dyS + Rcos\varphi)\mathbf{e}_y \\
&= (F-s)\mathbf{e}_z + K_x\mathbf{e}_x + K_y\mathbf{e}_y
\end{aligned}
$$

Defining $R = r\tau$ $(r \leq A/2)$ and the vector $\mathbf{k} = (-d_{xS} + rsin\varphi, d_A - d_{yS} + rcos\varphi)$ the distance $\delta = K$ can be written as

$$
\begin{aligned}
\delta^2 &= (F-s)^2 + K_x^2 + K_y^2 \\
&= (F-s)^2\left(1 + g^2\tau^2\left(\frac{k}{F}\right)^2\right)
\end{aligned}
$$

The relations $d_x - dx_S = -dx_S\tau$ and $d_y - d_{yS} = (d_A - d_{yS})\tau$ from Eq.14 have been used. $cos\alpha = \mathbf{K}\mathbf{e}_z/K$ is given by

$$
\begin{aligned}
cos\alpha &= (F-s)/\sqrt{\delta} && (15) \\
&= \frac{1}{\sqrt{1 + g^2\tau^2\left(\frac{k}{F}\right)^2}} && (16) \\
\frac{cos\alpha}{\delta^2} &= \frac{g^2}{F^2}\left(1 + g^2\tau^2\left(\frac{k}{F}\right)^2\right)^{-\frac{3}{2}}
\end{aligned}
$$

The abbreviation $g = F/(F-s)$ is related to the geometry effect (g^2, see chapter 5). The integration over the area of the aperture of radius R_B gives the solid angle Ω which is proportional to the intensity.

$$
\begin{aligned}
\Omega &= \int r_b dr_B d\varphi \frac{1}{(F-s)^2}\left(1 + g^2\tau^2\left(\frac{k(r,\varphi)}{F}\right)^2\right)^{-\frac{3}{2}} && (17) \\
&= \int \tau r d\tau r d\varphi \frac{1}{(F-s)^2}\left(1 + \left(\frac{k(r,\varphi)}{H-s}\right)^2\right)^{-\frac{3}{2}} \\
&= \frac{2\pi}{(H-s)^2}\int_0^{A/2} rdr\left(1 + \left(\frac{k(r,\varphi)}{H-s}\right)^2\right)^{-\frac{3}{2}}
\end{aligned}
$$

The integration runs over those r, φ values of the absorber. The ratio $\Omega(s)/\Omega(s=0)$ establishes the geometry effect.

Intersection with the aperture

A point $\mathbf{p}_B$ inside the aperture with radius B/2 is given by an equation like Eq. 12:

$$\mathbf{p}_B = F \cdot \mathbf{e}_z + p_x \cdot \mathbf{e}_x + p_y \cdot \mathbf{e}_y \tag{18}$$

and $p_x = r_B sin\psi$, $p_y = r_B cos\psi$ and $r_B \leq B/2$. The image of an absorber point (r_A, φ) is according to Eq.14

$$\begin{aligned} \mathbf{c}_B &= F \cdot \mathbf{e}_z + c_x \cdot \mathbf{e}_x + c_y \cdot \mathbf{e}_y \\ c_x &= d_{xS}(1-\tau) + r_A\tau\, sin\varphi \\ c_y &= d_{yS} + (d_A - d_{yS})\tau + r_A\tau\, cos\varphi \\ r_A(s) &\leq \frac{A}{2} \end{aligned} \tag{19}$$

At $r_A = 0$ the center $\mathbf{c}_i$ of the absorber image is obtained:

$$\mathbf{c}_i = F \cdot \mathbf{e}_z + (d_{xS}(1-\tau)) \cdot \mathbf{e}_x + (d_{yS} + (d_A - d_{yS})\tau) \cdot \mathbf{e}_y \tag{20}$$

The difference $\mathbf{\Delta} = \mathbf{p}_B - \mathbf{c}_i$

$$\mathbf{\Delta} = (r_B sin\psi - (d_{xS}(1-\tau))) \cdot \mathbf{e}_x + (r_B cos\psi - (d_{yS} + (d_A - d_{yS})\tau)) \cdot \mathbf{e}_y \tag{21}$$

is the vector from the image of center of the absorber to the point $\mathbf{p}_B$ inside the aperture, so that the condition to be inside the image of the absorber is $|\mathbf{\Delta}| \leq A/2\tau$. For any point $\mathbf{p}_B$ the vector $\mathbf{K} = \mathbf{p}_B - \mathbf{p}_S$ defines the $cos\alpha$ and $\delta = K$ (see previous chapter 2.4).

$$\begin{aligned} K^2 &= (F-s)^2 + (p_x - d_{xS})^2 + (p_y - d_{yS})^2 \\ \frac{\mathbf{K}\mathbf{e}_z}{K} &= \sqrt{1 + g^2 \frac{(p_x - d_{xS})^2 + (p_y - d_{yS})^2}{F^2}}^{-1} \\ \frac{cos\alpha}{\delta^2} &= \frac{g^2}{F^2}\left(1 + g^2 \frac{(p_x - d_{xS})^2 + (p_y - d_{yS})^2}{F^2}\right)^{-3/2} \end{aligned}$$

The other way round is the condition of an image point $\mathbf{c}_B(r_A, \varphi)$ inside the aperture. In the plane of the aperture the image points are the vectors $\mathbf{\Delta} = \mathbf{c}_B - F\mathbf{e}_z$

$$\mathbf{\Delta} = (d_{xS}(1-\tau) + r_A\tau\, sin\varphi) \cdot \mathbf{e}_x + (d_{yS} + (d_A - d_{yS})\tau + r_A\tau\, cos\varphi) \cdot \mathbf{e}_y \tag{22}$$

such that $|\mathbf{\Delta}| \leq B/2$ defines the condition.

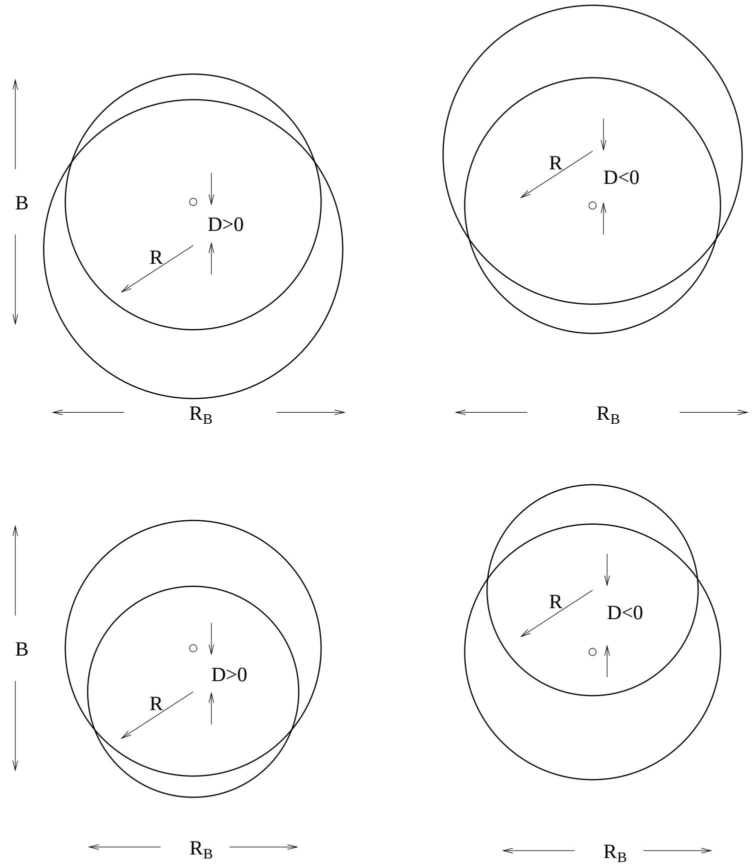

Figure 4: Four situations for the image of the absorber on the plane containing the aperture of diameter B. D is the shift of the center of the circular image of diameter R_B from the center of the aperture. At the top $R_B > B/2$ and at the button the opposite case $R_B < B/2$.

The parameters of the **general situation** $(d_{A,S} \neq 0)$ of Eq. 19 are $d_A, d_S, A,\ B, H, F$. All distances enter the equations in units of F. $\tau = (F-s)/(H-s)$ may be expressed by $g = F/(F-s)$ and H/F.

$$\tau = \left(1 - g\left(1 - \frac{H}{F}\right)\right)^{-1} \tag{23}$$

A,B,H,F shall be known from the experimental set up. The unknown misalignments $d_A/F, d_S/F$ will be fit parameters.
The integration runs over the intersection A_I of the aperture with the image of the absorber area such that $\int\int RdRd\varphi = A_I$. For situations of relative sizes and positions of the aperture and absorber image are shown in Fig. 4. The position of the image of the absorber on the plane of the aperture is characterized by the lowest point of the circle $\mathbf{c}_B$ in $(\varphi = 0)$ y-direction $c_y(+) = d_{yS} + (d_A - d_{yS} + A/2)\tau$ and the highest point $c_y(-) = d_{yS} + (d_A - d_{yS} - A/2)\tau$ at $(\varphi = \pi)$. The decision whether the

integration runs only over a circular intersection (simple case) requires the knowledge whether the image is inside the aperture or vice versa the aperture inside the image. Since the answer depends on $\tau(s(v))$ the minimum and maximum of the image of the absorber from all points of the source has to be considered. In order to make such a decision to be valid for all τ the maximum or minimum of τ has to be inserted dependent on the sign of the pre-factor $(d_A - d_{yS} + A/2)$ and of $\tau_{min}, \tau_{max} > 0$.
The lowest (at $\varphi = 0$) and highest (at $\varphi = \pi$) y-values ($c_y(+)_{max}$ and $c_y(-)_{max}$) are given by:

$$\begin{array}{lll} (d_A - d_{yS} + A/2) > 0 & \Rightarrow & c_y(+) = d_{yS} + (d_A - d_{yS} + A/2)\tau_{max} \\ (d_A - d_{yS} + A/2) < 0 & \Rightarrow & c_y(+) = d_{yS} + (d_A - d_{yS} + A/2)\tau_{min} \end{array}$$

$$\begin{array}{lll} (d_A - d_{yS} - A/2) > 0 & \Rightarrow & c_y(-) = d_{yS} + (d_A - d_{yS} - A/2)\tau_{min} \\ (d_A - d_{yS} - A/2) < 0 & \Rightarrow & c_y(-) = d_{yS} + (d_A - d_{yS} - A/2)\tau_{max} \end{array}$$

The highest (at $\varphi = 0$) and lowest (at $\varphi = \pi$) y-values ($c_y(+)_{min}$ and $c_y(-)_{min}$) are given by replacing τ_{max} by τ_{min} and vice versa:

$$\begin{array}{lll} (d_A - d_{yS} + A/2) > 0 & \Rightarrow & c_y(+) = d_{yS} + (d_A - d_{yS} + A/2)\tau_{min} \\ (d_A - d_{yS} + A/2) < 0 & \Rightarrow & c_y(+) = d_{yS} + (d_A - d_{yS} + A/2)\tau_{max} \end{array}$$

$$\begin{array}{lll} (d_A - d_{yS} - A/2) > 0 & \Rightarrow & c_y(-) = d_{yS} + (d_A - d_{yS} - A/2)\tau_{max} \\ (d_A - d_{yS} - A/2) < 0 & \Rightarrow & c_y(-) = d_{yS} + (d_A - d_{yS} - A/2)\tau_{min} \end{array}$$

τ_{max} and τ_{min} are reached for the points of return at zero velocity where $|s(v = 0)/F| = geo$.

$$\begin{aligned} \tau_{max} &= \frac{1 - geo}{H/F - geo} \\ \tau_{min} &= \frac{1 + geo}{H/F + geo} \end{aligned}$$

The following relations are obvious:

$$\begin{array}{ll} c_y(+)_{min} > \frac{1}{2}B \text{ and } c_y(-)_{min} < -\frac{1}{2}B & \Rightarrow A_I := B \text{ (aperture)} \\ c_y(+)_{max} < \frac{1}{2}B \text{ and } c_y(-)_{max} > -\frac{1}{2}B & \Rightarrow A_I := R_B \text{ (full image)} \end{array}$$

If the intersection changes at some τ-value from full aperture to full absorber image then the intersection has to be calculated. In case of full alignment, however, the decision can be done at any τ-value without a large decision tree. The following cases correspond to Fig 4.

$c_y(+) > \frac{1}{2}B$ and $c_y(-) > -\frac{1}{2}B \quad \Rightarrow A_I$: Fig 4 left
$c_y(+) < \frac{1}{2}B$ and $c_y(-) < -\frac{1}{2}B \quad \Rightarrow A_I$: Fig 4 right

If $c_y(+) < -\frac{1}{2}B$ or $c_y(-) > \frac{1}{2}B$ the image of the absorber has no intersection with the aperture. That means there are velocity regions without any count rate. In the case of complete alignment the conditions above restrict to $c_y(+) = A/2\tau_{max}$ and $c_y(-) = -A/2\tau_{max}$, such that the conditions for complete overlap are simply met.

3 Numerical integration

3.1 Point source

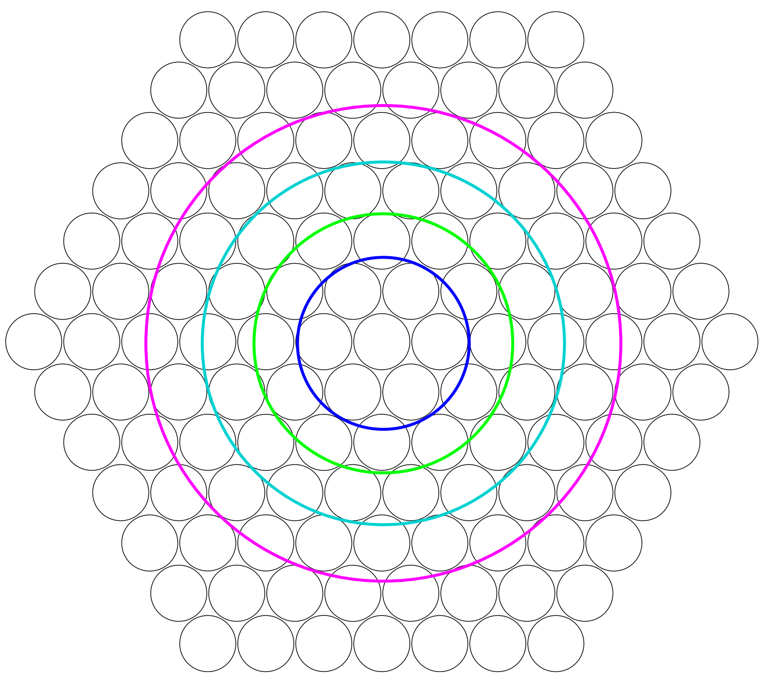

Figure 5: The integration area is covered with small circles of radius ρ which define a R, φ value at the center. The integration area of the large circle of radii 3ρ, $(2\sqrt{3}+1)\rho$, $(2\sqrt{7}+1)\rho$, $(2\sqrt{13}+1)\rho$,... contain 7, 19, 37, 61,... small circles. If the integration runs over the intersection of the aperture and the image the common small circle positions are taken.

Eq. 19 and 15 depend on $s(v)$ and have to be integrated over the aperture in front of the detector for each channel of the spectrum. It is of

course assumed that γ-quanta passing the aperture are detected with the same probability. That means that the efficiency of the detector is independent of the position inside the detector window, a property which typically is not very well fulfilled.
There are several cases defined by the relative sizes of B, D, r_B which are treated separately:

$R_B < B/2$:The image of absorber is inside the aperture
- **alignment** ($(D(d_A, d_S) = 0)$; integration $0 \leq R \leq R_B$ over image of the absorber by surface elements $2\pi R dR$
- **misalignment** $(D(d_A, d_{yS}) > 0)$
  - image R_B is filled with small circles.
  - Intersection A_I with aperture $B/2$.
  - mirror y,z-plane $\Rightarrow$ mirror circles are counted twice

$R_B > B/2$: The image of absorber larger than aperture, aperture inside the image of the absorber
- **alignment** ; integration $0 \leq R \leq B/2$
  - over full aperture by surface elements $2\pi R dR$
- **misalignment** $(D(d_A, d_{yS}) > 0)$
  - aperture $B/2$ is filled with small circles.
  - Intersection A_I with the image of the absorber R_B
  - mirror y,z-plane $\Rightarrow$ mirror circles are counted twice

The integration runs over two variables: R and φ which are the centers of the small circles (see Fig. 5) belonging to the intersection A_I decided by the position of the center of the small circle. The circles related by the mirror plane are counted twice. The general position of the source $d_{xS}, d_{yS} > 0$ and an aligned absorber $d_A = 0$ is equivalent by an appropriate rotation around the z-axis such that the mirror symmetry with respect to the y,z-plane is preserved. The case that also $d_A > 0, d_{yS} > 0$ requires the integration over all image points inside the aperture (this case is not implemented - d_{xS} is not an input parameter).

3.2 Extended source

Two cases are considered, the fully aligned situation and the source displaced by d_{yS}, but absorber and aperture aligned. There are several cases defined by the relative sizes of B, D, r_B which are treated separately:

$R_B < B/2$: aperture larger than image of absorber for any point
(center of the circle) of the source $R_S = Dsource/2 < B/2$
$D = 0$ aligned ; rotational symmetry $\Rightarrow$ integration $0 \leq R \leq R_B$
by surface elements $2\pi RdR$ over the absorber image
from each point $(R, \varphi = 0)$ to all circles of the source area.
mirror y,z-plane $\Rightarrow$ mirror circles are counted twice

$D > 0$ misalignment: y,z-plane is a mirror plane
Source R_S and absorber image R_B are filled with circles.
The y,z-mirror plane is accounted for by counting mirror circles of the absorber image twice (more effective than counting circles inside the source)

$R_B < B/2$: aperture larger than image of absorber
not for all points (center of the circle) of the source
mirror y,z-plane is preserved
$D = 0$ aligned ; integration $0 \leq r_S \leq R_S$
by surface elements $2\pi r_s dr_s$ over the source
from each point $(r_S, \varphi_S = 0)$ to all circles
of the intersection A_I of absorber image and aperture
mirror y,z-plane $\Rightarrow$ mirror circles are counted twice

$D > 0$ misalignment: y,z-plane is a mirror plane
Source R_S and absorber image R_B are filled with circles.
Integration (summation) is restricted to A_I for points of the source with part of the absorber image outside $B/2$
The y,z-mirror plane is accounted for by counting mirror circles of the absorber image twice (more effective than counting circles inside the source)

$R_B > B/2$: image of absorber larger than aperture
$D = 0$ aligned ; rotational symmetry $\Rightarrow$ integration $0 \leq R \leq B/2$
by surface elements $2\pi RdR$ over the aperture
from each point $(R, \varphi = 0)$ to all circles of the source area.
mirror y,z-plane $\Rightarrow$ mirror circles are counted twice

$D > 0$ misalignment
Source R_S and aperture areas are filled with circles.

Summation from each point of the aperture area (A_I) to all circles of the source area.
mirror circles of the aperture are counted twice

The integration runs over two variables for the image/aperture intersection: R and φ and the for the source r_S and φ_S which in the case of no rotational symmetry are the centers of the small circles (see Fig. 5). The y,z-plane is a mirror plane which simplifies again the summation but only for one of the surfaces: aperture or source. In order to minimize the sum the symmetry of the surface with the larger number of circles is used. The larger number is in the aperture plane for source diameters $Dsource < B = Daperture, R_B$.

4 Aligned source, absorber, aperture

The case of a well **aligned situation** $(d_A, d_S = 0)$ simplifies since the integral of Eq. 17 can be executed as k reduces to r:

$$\begin{aligned}\Omega &= \frac{2\pi}{(H-s)^2}\int_0^{A/2} r dr \left(1+\left(\frac{r}{H-s}\right)^2\right)^{-\frac{3}{2}} \qquad (24)\\ &= 2\pi\left(1-\frac{1}{\sqrt{1+\left(\frac{A/2}{H-s}\right)^2}}\right)\end{aligned}$$

Two cases have to be considered depending on the size of the detector defined by the second aperture of diameter B as shown in Fig. 4. B may be larger than $2R_B(s)$ for all positions $(z_S = z_0+s)$ of the source S. Then the integration over the aperture $(RdRd\varphi)$ is obtained by replacing H by F and diameter A by diameter B. The radius of the decisive aperture devided by its distance from the source at s=0 may be denoted by $\epsilon = a/2/H$ or $B/2/F$. The relative position of the source $-s_{max} < s < s_{max}$ devided the distance H or F shall be $\delta = -s/H/\delta = -s/F$. Then the ratio Ω/Ω_0 is expressed as

$$\frac{\Omega}{\Omega_0} = \left(1-\frac{1+\delta}{\sqrt{(1+\delta)^2+\epsilon^2}}\right) / \left(1-\frac{1}{\sqrt{(1+\epsilon^2}}\right) \qquad (25)$$

The geometry effect as realized in the Mossbauer programs is taken in the limit $\epsilon = 0$, such that the diameter of the apertur is not a parameter.

In this case Eq.25 is undefined (0 devided by 0). For small ϵ the ratio is expanded

$$\frac{\Omega}{\Omega_0} = \frac{1}{(1+\delta)^2}\left(1 - \frac{3}{4}\frac{\epsilon^2}{(1+\delta)^2} + ...\right) / \left(1 - \frac{3}{4}\epsilon^2 + ...\right) \tag{26}$$

The dependence of this ratio on s which in turn depends on the velocity of the source is called the geometry effect. For constant acceleration mode with acceleration b and maximum velocity v_{max} the relative position $\delta(v)$ is given by

$$\delta(v) = \pm geo\left(\left(\frac{v}{v_{max}}\right)^2 - 1\right) \tag{27}$$

with the pre-factor $geo = s_{max}/H$ or $= s_{max}/F$. Usually geo is fitted to the baseline of the Mossbauer spectrum. Since s_{max} is known from the frequency and the fitted v_{max} (see 5.1) the value of geo is not a free parameter. If its fitted value differs the geometry of the set up or dead time effects are possible reasons.

5 Velocity scale

Starting at $t = 0$ and $v = -v_{max}$ the acceleration b in the opposite direction decreases the velocity to zero in a quarter of a period $T/4$.

$$v(t) = -v_{max} + bt \tag{28}$$

Integration of $v(t)$ gives

$$\begin{aligned} s(t) &= -v_{max}t + \frac{1}{2}bt^2 & s(t=0) &= 0 \\ s(\frac{T}{4}) &= -v_{max}\frac{T}{4} + \frac{1}{32}bT^2 & s(\frac{T}{2}) &= -v_{max}\frac{T}{2} + \frac{1}{8}bT^2 \end{aligned}$$

At $t = T/4$ the velocity is zero, so that $v_{max} = bT/4$. Inserting T into the equations for $s(t)$ the maximal deviation of $s_{max} = -\frac{1}{2}v_{max}^2/b$ is obtained (see Fig. 6).

The dependency of s on the velocity v is obtained inserting t from Eq. 28 into $s(t)$.

$$\begin{aligned} s(v) &= -v_{max}\frac{v+v_{max}}{b} + \frac{1}{2}b\left(\frac{v+v_{max}}{b}\right)^2 \qquad (29) \\ &= \frac{1}{2b}(v^2 - v_{max}^2) \end{aligned}$$

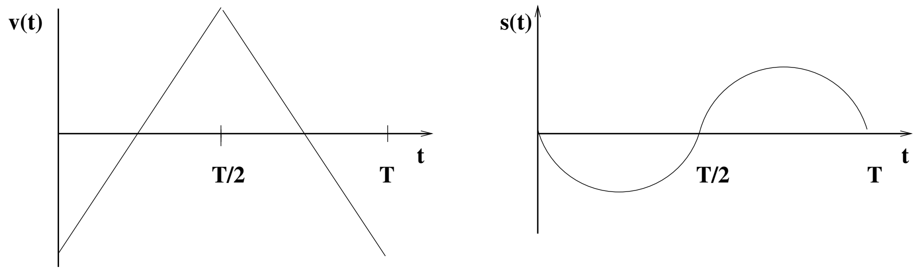

Figure 6: Time dependence of $v(t)$ and $s(t)$ in the range of a full period T for the constant acceleration mode. The $s(t) = \int v(t)dt$ within the two half periods are parabola (here indicated by a segment of a circle).

$$\begin{aligned} \frac{s}{F} &= \pm \frac{v_{max}^2}{2bF}\left(\left(\frac{v}{v_{max}}\right)^2 - 1\right) \\ geo &= \frac{v_{max}^2}{2bF} \\ &= \frac{s_{max}}{F} \end{aligned} \tag{30}$$

The constant geo is the maximal deviation from the zero position of the source divided by the distance source detector (aperture). The $\pm$ sign is introduced in order to cover both halves of the period.

5.1 Maximal deviation s_{max}

The maximal deviation s_{max} is a function of v_{max} and the period time T. In case of constant accellaration $-s_{max} = s(t = 0, v = 0)$ is

$$s(t = 0) = -\frac{v_{max}^2}{2b} \tag{31}$$

The velocity v (see Fig.6) is $-v_{max}$ at $t = 0$, $v = 0$ at $t = T/4$ or v_{max} at $t = T/2$. With $b = (v(t) + v_{max})/t$ from eq.28 the maximal deviation at $v(t = T/4) = -s_{max}$ becomes

$$s_{max} = \frac{v_{max}}{8} \cdot T \tag{32}$$

For sinusoidal velocity mode with $v(t) = A\omega sin(\omega \cdot t)$ the maximal deviation at t=0 is given by $(\omega = 2\pi/T)$

$$s_{max} = \frac{v_{max}}{2\pi} \cdot T \tag{33}$$

5.2 The folded spectrum

The two halfs of a spectrum have different sign of s, such that the simple folding procedure leads to a sum proportional to σ

$$\begin{aligned}\sigma(v) &= \frac{1}{(F+s)^2} + \frac{1}{(F-s)^2} \\ &= \frac{2}{F^2}\left(1 + 3\left(\frac{s}{F}\right)^2 + 5\left(\frac{s}{F}\right)^4 + ...\right)\end{aligned}$$

Neglecting the fourth order term and inserting $s(v)$ gives

$$\sigma(v) = \frac{2}{F^2}\left(1 + 3\left(\frac{s_{max}}{F}\right)^2\left(\left(\frac{v}{v_{max}}\right)^2 - 1\right)^2\right)$$

Again neglecting the fourth order term of v/v_{max} the deviation from a constant baseline is proportinal to a parabola

$$= 1 - 6\left(\frac{s_{max}}{F}\right)^2\left(\frac{v}{v_{max}}\right)^2$$

Taking typical values like $v_{max} = 1mm/s$, a drive frequency of 10Hz and a source-detector(/apertur) distance of 100mm the deviation at v_{max} becomes

$$\begin{aligned}b &= 4v_{max}/T = 400mm/s^2; \qquad s_{max} = \frac{v_{max}^2}{2b} = 1/8mm \\ 6\left(\frac{s_{max}}{F}\right)^2 &= 6\left(\frac{1}{800}\right)^2 \\ &= 0.93 \cdot 10^{-5}\end{aligned}$$

If the baseline has 10^6 counts such that the 1σ-error bars are 10^3 the deviation of $0.93 \cdot 10^{-5} \cdot 10^6 = 9.3$ is neglegible. In case of a drive frequency of 1Hz the deviation is larger by a factor of 10^2 and of the same size as the error bars, so that the parabola is clearly visible.