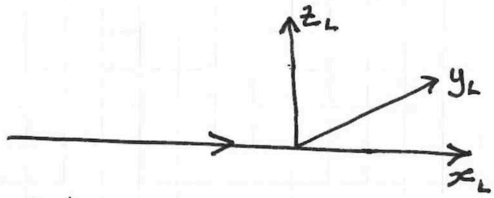
Coordinate frame conventions

18/3/19

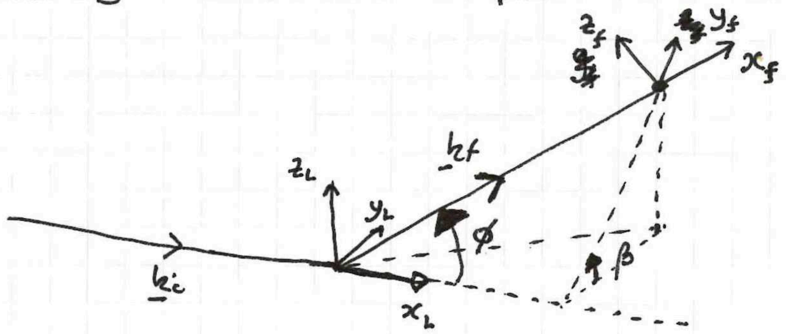
"Spectrometer frame" }
"Laboratory frame" } coordinate frame defined by incident beam direction



$x_L \parallel \underline{k}_i$
z_L vertical upwards
y_L forms rh coordinate frame

" Secondary spectrometer frame"
" final wavevector frame" }
" $\underline{k}_f$ frame" } coordinate frame defined by final beam direction

[Previously called "detector frame" prior to March 2019]



Note: This frame is a similar twist on the conventional spherical coordinates frame. The reasons to stick with it are:
- permeates so many existing functions, and the possibility of error are huge if combine many functions with different conventions
- in the case of instrument equatorial plane, it naturally has x-y pair of axes

$x_f \parallel \underline{k}_f$

y_f plane of $\underline{k}_i$ & $\underline{k}_f$ radially outwards

z_f forms rh coordinate frame

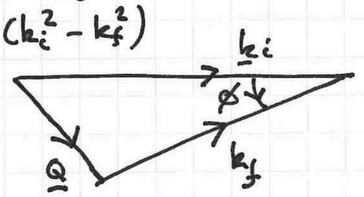
This convention	spherical polar
x_L	z
y_L	x
z_L	y
ϕ	θ
β	ϕ

note: in original .par file the convention had the opposite sign

consistent with common scattering triangle convention

Wavector and energy transfer

$$\underline{Q} = \underline{k}_i - \underline{k}_f$$
$$\mathcal{E} = \frac{\hbar^2}{2m}(k_i^2 - k_f^2)$$



In laboratory frame:

$$\underline{k}_i = (k_i, 0, 0)$$

$$\underline{k}_f = (k_f\cos\phi, \ k_f\sin\phi\cos\beta, \ k_f\sin\phi\sin\beta)$$

$$\Rightarrow \quad \underline{Q} = (k_i - k_f\cos\phi, \ -k_f\sin\phi\overset{\cos}{\cancel{\sin}}\beta, \ -k_f\sin\phi\sin\beta)$$

Small deviations

In resolution function calculations, we will generally deal in small deviations, and have expressed $\delta\underline{k}_i$ in the laboratory frame and $\delta\underline{k}_f$ in the $\underline{k}_f$ frame.

Now, $\quad x_i^f = F_{ij} \cdot x_j^L$, so therefore: — see definition of matrix F in "Detector coordinate frames"

$$\Rightarrow \quad \delta Q_i^L = (\delta k_i^L)_i - F^{-1}_{ij}(\delta k_f^f)_j$$
$$= (\delta k_i^L)_i - F_{ji}(\delta k_f^f)_j \qquad \text{as } F^{-1} = F^T$$

Also
$$\delta\mathcal{E} = \frac{\hbar}{m}\left(k_I(\delta k_i^L)_1 - k_f(\delta k_f^f)_1\right)$$

So we can write in general:

$$\begin{pmatrix}\delta Q_1^L \\ \delta Q_2^L \\ \delta Q_3^L \\ \delta\omega\end{pmatrix} = \begin{pmatrix} \boxed{\quad I \quad} & \boxed{\quad F^T \quad} \\ \frac{\hbar}{m}k_I \quad \cdot \quad \cdot & \frac{\hbar}{m}k_f \quad \cdot \quad \cdot \end{pmatrix} \begin{pmatrix}(\delta k_i^L)_1 \\ (\delta k_i^L)_2 \\ (\delta k_i^L)_3 \\ (\delta k_f^f)_1 \\ (\delta k_f^f)_2 \\ (\delta k_f^f)_3\end{pmatrix}$$

Time bin width

want to relate time bin width to an energy transfer width for direct geometry instrument.

If t = time of absorbtion in the detector
t_s = " " arrival in the sample
l_2 = sample - detector distance

$$v_f = \frac{l_2}{t - t_s}$$

$$\varepsilon = E_i - E_f$$
$$= E_i - C v_f^2$$

$$\Rightarrow \quad \delta\varepsilon = -2 C v_f \, \delta v_f$$

but $$\delta v_f = \frac{-l_2 \, \delta t}{(t - t_s)^2}$$

$$\Rightarrow \quad \delta\varepsilon = 2 C v_f \frac{l_2}{(t - t_s)^2} \delta t$$
$$= 2 E_f \frac{v_f}{l_2} \delta t$$

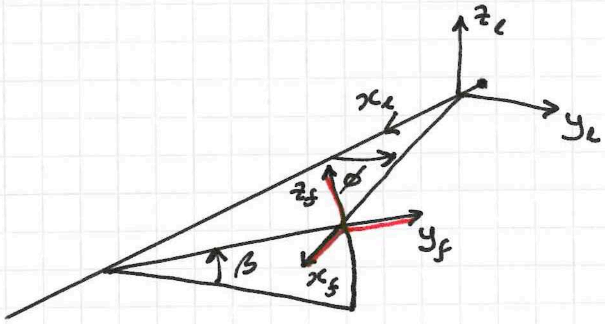
Can write as

$$\frac{\delta\varepsilon}{E_f} = 2 \frac{\delta t}{(t - t_s)}$$

or $$\delta t = A \frac{l_2}{k_f^3} \delta\varepsilon$$ where $A = 3.832 \times 10^{-4}$ if k_f : Å^{-1}
t : s
l : m

Detector coordinate frames

convert coords from $\underline{k}_f$ - frame to lab frame.



Define matrix F s.t. a vector ~~x~~ in lab frame ~~x~~ ~~x~~ has components x_i^l and in $\underline{k}_f$-frame has components x_i^f :

$$\boxed{x^f_i = F_{ij}\, x_j^L} \quad \text{Definition}$$

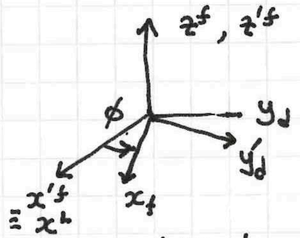
$$\begin{pmatrix} x^f \\ y^f \\ z^f \end{pmatrix} = \begin{pmatrix} C_\phi & C_\beta S_\phi & S_\beta S_\phi \\ -S_\phi & C_\beta C_\phi & S_\beta C_\phi \\ \cdot & -S_\beta & C_\beta \end{pmatrix} \begin{pmatrix} x^L \\ y^L \\ z^L \end{pmatrix}$$

$\left(\begin{array}{l} \text{where} \\ C_\phi = \cos\phi \\ S_\phi = \sin\phi \\ \text{\& sim. } C_\beta, S_\beta \end{array} \right)$

Note: $F^{-1} = F^T$ (as a rotation matrix)

To show this:

(I) get conversion matrix to relate x_i in $\underline{k}_f$-frame to one where rotate about ~~x~~ z^f until x is $\parallel x^L$ ie by $-\phi$:



(II) then conversion matrix to relate $x_i'^f$ to x_i^L by rotating by $-\beta$ about $x'^f \equiv x^L$

$$\Rightarrow \begin{pmatrix} x^l_i \\ y^l_i \\ z^l \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & C_\beta & -S_\beta \\ \cdot & S_\beta & C_\beta \end{pmatrix} \begin{pmatrix} C_\phi & -S_\phi & \cdot \\ S_\phi & C_\phi & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}}_{\begin{pmatrix} C_\phi & -S_\phi & \cdot \\ C_\beta S_\phi & C_\beta C_\phi & -S_\beta \\ S_\beta S_\phi & S_\beta C_\phi & C_\beta \end{pmatrix}} \begin{pmatrix} x^f \\ y^f \\ z^f \end{pmatrix}$$

Then invert by taking the transpose

Proof of transpose ≡ inverse for rotation

if $x_i' = O_{ij}\, x_j$, $x_i' x_i' = O_{ij}\, O_{ik}\, x_j x_k$, but we have invariance of length, so $x_i' x_i' = x_i x_i$

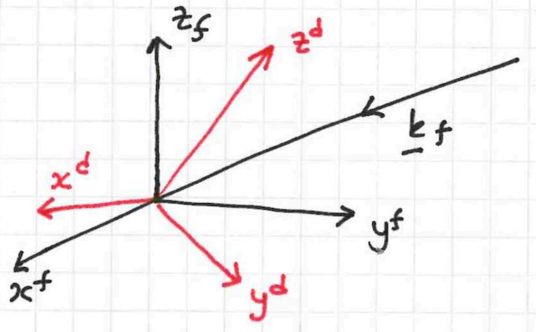
$\Rightarrow O_{ij}\, O_{ik} = \delta_{jk}$

ie $O^T_{ji}\, O_{ik} = \delta_{jk}$ Q.E.D.

Now relate the $\underline{k}_f$ - frame to a convenient frame in the detector geometry

(eg) cylindrical curtain of p.s.d. detectors the z-axis naturally lies along the cylinder axis, and the x - axis lies in the plane of the cylinder axis and $\underline{k}_f$

(eg) scintillator detector, z - axis lies along the normal to the flat scintillator surface.



Define the matrix D s.t. components are related by:

$$\boxed{x_i^f = D_{ij}\, x_j^d}$$ Definition

The form of D will depend on the detector convention for different detector types.

So we have overall,

$$x_i^d = D_{ij}^{-1} F_{jk}\, x_k^L$$

Note that $D^{-1} = D^T$ as it is a rotation matrix

Neutron flight path in detector frame

Neutron flight direction in detector frame: want to know ~~coords of~~ components of $\underline{e}_i^f$ in $\underline{e}_i^d$: from discussion of coordinate frames, where

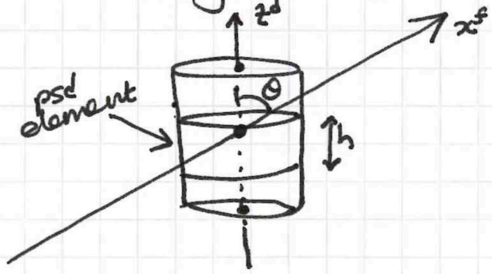
$$x_i' = \begin{pmatrix} \underline{e}_1' \text{ in } \underline{e} \\ \underline{e}_2' \text{ in } \underline{e} \\ \underline{e}_3' \text{ in } \underline{e} \end{pmatrix}_{ij} x_j$$

$\Rightarrow$ neutron path is D_{ij}

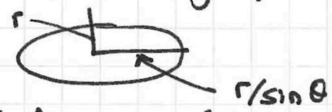
Detector depth variance, mean of flight-path variance & mean

The values of $\langle x_d \rangle \langle y_d \rangle \langle z_d \rangle$ and $\langle w \rangle$, where w is the distance in the detector along the neutron flight path, are not simply related by a matrix transformation.

- Consider a cylindrical detector 3He psd tube:



This neutron path has a flightpath that emerges from the top of the pixel element. A neutron that is absorbed near the ~~top~~ end of the path in the tube is strictly in the adjacent pixel.
We compute flight path in the ellipse



to get the mean flight path & variance in the tube.

We have $\langle x \rangle = \langle w \rangle \sin\theta$
However, it is not the case that $\langle z \rangle = \langle w \rangle \cos\theta$, because there is an equivalent neutron that entered the pixel beneath and was absorbed in our pixel under consideration. In fact, it is the case that $\langle z \rangle = 0$, and $\sigma_z^2 = h^2/12$ ie as for a hat function (ignoring the charge cloud width).

In general, algorithms will have to return $\langle w \rangle$, σ_w^2 for timing, and $\langle \underline{x}_d \rangle$, $\mathrm{cov}(\underline{x}_d)$ for any calculations that involve distances (eg $S k_f/k_f$ calculations, for example. We will require that these quantities are the same as would be computed from random point sampling.

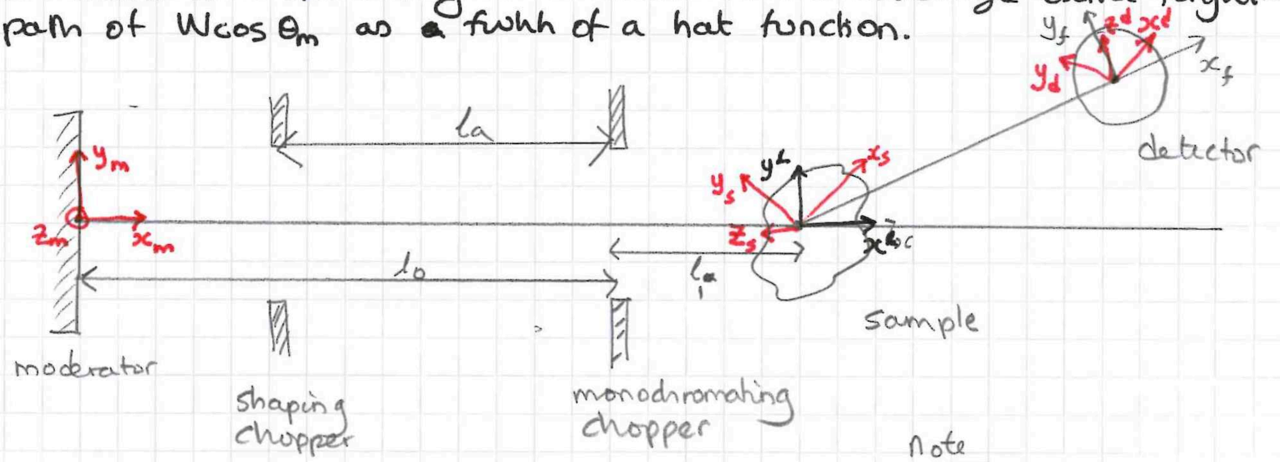
This means that calculations will in general need to know $\underline{\underline{D}}$ in the relation $x_i^f = D_{ij} x_j^d$. (eg) gas tube we need $\sin\theta$

We will get this information from D_{ij}. In fact, the path of the neutron in the detector frame is given by the unit vector D_{1j}

Tobyfit formalism for a disk chopper spectrometer

The primary approximation is that we can decouple the time and angular correlations. This is justified on the basis of the number of bounces down the beamline from the guide walls.

On the same basis, we treat the moderator face as being perpendicular to the beam line. We may have to consider the moderator as having an extra time broadening to account for the average extra flight-path of $W\cos\theta_m$ as a fwhh of a hat function.



Note
sometimes have used
$l_c \equiv l_1$
$l_m = l_0 + l_1$

Matricies btwn frames:

$$x^L_i = S_{ij}\, x^s_j$$
$$x^f_i = F_{ij}\, x^L_j$$
$$x^f_i = D_{ij}\, x^d_j$$

$(x^L, x^s, x^f, x^d$ here illustrate the matrix definitions, but are not the specific deviations in the figure. confusing!)

- Time of arrival at sample:

$$T_s = t_m + \left(\frac{l_0 + l_1 + S_{ij}\, x^s_j}{v_i}\right)$$

- Time of arrival at the detector: using $x^f_i = F_{ij}\, S_{jk}\, x^s_k$

$$T_d = T_s + \left(\frac{l_2 + x^f_1 - F_{1j}\, S_{jk}\, x^s_k}{v_f}\right)$$

- Independent variables are t_m, t_{ch}, t_d : t_m & t_{ch} together define the time origin and $|k_i|$; t_d then defines $|k_f|$

Small ~~angle~~ deviations approximation:

$$v_i = v_I + \delta v_i \quad \Rightarrow \quad \frac{1}{v_i} = \frac{1}{v_I}\left(1 - \frac{\delta v_i}{v_I}\right)$$

$$v_f = v_F + \delta v_f \quad \Rightarrow \quad \frac{1}{v_f} = \frac{1}{v_F}\left(1 - \frac{\delta v_f}{v_F}\right)$$

Substitute these first in expression for T_s:

$$T_s = t_m + \frac{1}{v_I}\left(1 - \frac{\delta v_i}{v_I}\right)\left(l_0 + l_1 + S_{ij}\, x_j^s\right)$$

$$= \left(\frac{l_0 + l_1}{v_I}\right) + t_m - \frac{(l_0 + l_1)}{v_I^2}\,\delta v_i + \frac{S_{1j}\, x_j^s}{v_I}$$

Use this together with expression for $1/v_f$ in the expression for T_d

$$T_d = T_s + \frac{1}{v_F}\left(1 - \frac{\delta v_f}{v_F}\right)\left(\underline{l_2 + x^f_1 - F_{1j} S_{jk} x^s_k}\right)$$

$$= \underbrace{\left(\frac{l_0 + l_1}{v_I} + \frac{l_2}{v_F}\right)} + t_m - \left(\frac{l_0+l_1}{v_I^2}\right)\delta v_i - l_2 \frac{\delta v_f}{v_F^2} + \frac{S_{1j} x^s_j}{v_I}$$

$$- \frac{F_{1j} S_{jk} x^s_k}{v_F} + \frac{x^f_1}{v_F}$$

The nominal time of flight to the time of absorption in the detector

So therefore the deviation in time of arrival from nominal neutron is given by:

$$t_d = t_m - \left(\frac{l_0 + l_1}{v_I^2}\right)\delta v_i - l_2 \frac{\delta v_f}{v_F^2} + \frac{S_{1j} x^s_j}{v_I} - \frac{F_{1j} S_{jk} x^s_k}{v_F} + \frac{x^f_1}{v_F}$$

We have t_m, t_{ch}, t_d, x^s_i & x^f_i (actually x^d_i) as the independent degrees of freedom, so we write δv_i & δv_f in terms of these indep. d.o.f. Actually, we write them as $\frac{\delta k_i}{k_I} \equiv \frac{\delta v_i}{v_I}$ & $\frac{\delta k_f}{k_F} \equiv \frac{\delta v_f}{v_F}$.

$$v_i = l_0 \Big/ \left(\frac{l_0}{v_I} + t_{ch} - t_m\right)$$

$$\therefore \frac{v_i}{v_I} = \frac{1}{1 + \frac{t_{ch} - t_m}{T_0}} \qquad \text{where } T_0 = l_0/v_I$$

$$\therefore \frac{\delta v_i}{v_I} = \frac{t_m}{T_0} - \frac{t_{ch}}{T_0}$$

Substitute in the expression for t_d, bring $\delta v_f/v_F \equiv \delta k_f/k_F$ to l.h.s.

$$\left(\frac{l_0}{v_I}\right)\frac{\delta k_i}{k_I} = t_m - t_{ch}$$

$$\left(\frac{l_2}{v_F}\right)\frac{\delta k_f}{k_F} = -\left(\frac{l_{01}}{l_0}\right) t_m + \left(\frac{l_0 + l_1}{l_0}\right) t_{ch} + \left(\frac{S_{1k}}{v_I} - \frac{F_{1j} S_{jk}}{v_F}\right) x^s_k + \frac{x^f_1}{v_F} - t_d$$

$$\delta E = \frac{\hbar^2}{m}\left(k_i \delta k_i - k_f \delta k_f\right)$$

and

$$\left.\begin{aligned} \frac{\delta k_{iy}}{k_I} &= \frac{S_{2j} x^s_j - y^m}{l_0 + l_1} \\ \frac{\delta k_{iz}}{k_I} &= \frac{S_{3j} x^s_j - z^m}{(l_0 + l_1)} \end{aligned}\right\}$$

We'll just replace these with the divergence lookup tables

$y^m \equiv x^m_2$

$$\left.\begin{aligned} \frac{\delta k_{fy}}{k_F} &= \frac{y^f - F_{2j} S_{jk} x^s_k}{l_2} \\ \frac{\delta k_{fz}}{k_F} &= \frac{z^f - F_{3j} S_{jk} x^s_k}{l_2} \end{aligned}\right\}$$

These are the deviations in the frame of $\underline{k_f}$

$y^f \equiv x^f_2$

We want to write the deviations in the detector in the detector frame, not the k_f-frame, as x_i^d will be more naturally computable. We use $x_i^f = D_{ij} x_j^d$, to get the final result

$$\left(\frac{l_0}{v_I}\right) \cdot \frac{\delta k_i}{k_I} = t_m - t_{ch}$$

$$\left(\frac{l_2}{v_F}\right) \cdot \frac{\delta k_f}{k_F} = -\left(\frac{l_1}{l_0}\right) t_m + \left(\frac{l_0 + l_1}{l_0}\right) t_{ch} + \left(\frac{S_{1k}}{v_I} - \frac{F_{1j} S_{jk}}{v_F}\right) x_k^s + \frac{D_{1k} x_k^d}{v_F} -$$

$$\delta \varepsilon = \frac{\hbar^2}{m} \left(k_I \delta k_i - k_F \delta k_f\right)$$

and

$$\frac{\delta k_{iy}}{k_I} = \frac{S_{2j} x_j^s - x_2^m}{(l_0 + l_1)}$$

$$\frac{\delta k_{iz}}{k_I} = \frac{S_{3j} x_j^s - x_3^m}{(l_0 + l_1)}$$

will replace with deviations from divergence look up t

$$\frac{\delta k_{fy}}{k_F} = \frac{D_{2k} x_k^d - F_{2j} S_{jk} x_k^s}{l_2}$$

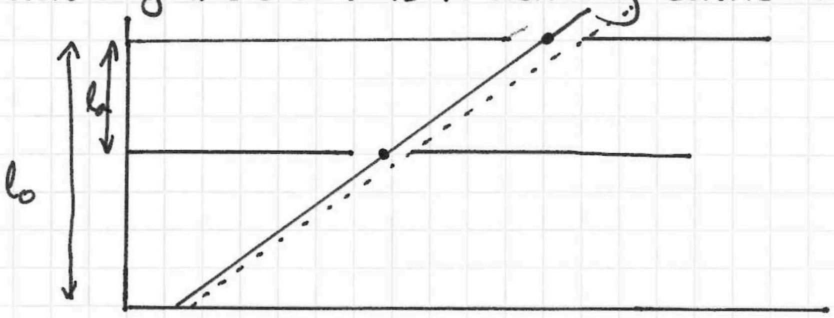
$$\frac{\delta k_{fz}}{k_F} = \frac{D_{3k} x_k^d - F_{3j} S_{jk} x_k^s}{l_2}$$

recall these deviat are in the k_f fra

Paradox: moderator shaping chopper as defining mod. pulse

There is an apparent paradox: in the calculation for δk_i & δk_f we can replace $t_m \Rightarrow t_{sh}$ and $l_0 \rightarrow l_a$ and the expressions should be equally valid.

Is this actually the case? Is it actually consistent?



The key is to note that

$$t_{sh} = t_m + \frac{(l_0 - l_a)}{l_0}(t_{ch} - t_m)$$

ie $$t_{sh} = \left(\frac{l_a}{l_0}\right) t_m + \left(\frac{l_0 - l_a}{l_0}\right) t_{ch}$$

Substitute in the expression for δk_i

$$\left(\frac{l_0}{v_I}\right)\frac{\delta k_i}{k_I} = t_m - t_{ch}$$

$$= \left(\left(\frac{l_0}{l_a}\right) t_{sh} - \left(\frac{l_0 - l_a}{l_a}\right) t_{ch}\right) - t_{ch}$$

$$= \left(\frac{l_0}{l_a}\right) t_{sh} - \left(\frac{l_0}{l_a}\right) t_{ch}$$

$$\therefore \quad \left(\frac{l_a}{v_I}\right)\frac{\delta k_i}{k_I} = t_{sh} - t_{ch}$$ $\Longleftarrow$ ie same form with $l_0 \Rightarrow l_a$ and $t_m \Rightarrow t_{sh}$

Similarly, for δk_f. Below just write out the t_m & t_{ch} terms. We similarly expect this to work out, as ultimately t_m & t_{ch} coefficients come from the time of arrival at the sample and that comes from the primary spectrometer ie δk_i. However, it is nice to see that it does:

$$\left(\frac{l_2}{k_F}\right)\frac{\delta k_f}{k_F} = -\left(\frac{l_1}{l_0}\right) t_m + \left(\frac{l_0 + l_1}{l_0}\right) t_{ch}$$

$$= -\left(\frac{l_1}{l_0}\right)\left(\left(\frac{l_0}{l_a}\right) t_{sh} - \left(\frac{l_0 - l_a}{l_a}\right) t_{ch}\right) + \left(\frac{l_0 + l_1}{l_0}\right) t_{ch}$$

$$= -\left(\frac{l_1}{l_a}\right) t_{sh} + \left(\left(\frac{l_1}{l_0}\right)\left(\frac{l_0 - l_a}{l_a}\right) + \left(\frac{l_0 + l_1}{l_0}\right)\right) t_{ch}$$

$$= -\left(\frac{l_1}{l_a}\right) t_{sh} + \left(\frac{l_1(l_0 - l_a) + l_a(l_0 + l_1)}{l_0 l_a}\right) t_{ch}$$

$$= -\left(\frac{l_1}{l_a}\right) t_{sh} + \left(\frac{l_a + l_1}{l_a}\right)$$ $\Longleftarrow$ ie same with $l_0 \Rightarrow l_a$ & $t_m \Rightarrow t_{sh}$

Dropping time-angle correlations

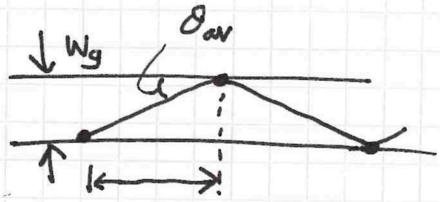
Rob Bewley says that the moderator face is angled at 15° to the beam direction on LET (which way?)

For a guide:

$$\theta^{deg}_{max} = 0.1\, m\, \lambda_{Å} \quad \leftarrow \text{critical angle}$$

so the average bounce angle

$$\theta^{deg}_{av} \approx 0.05\, m \lambda_{Å}$$



LET: width of guide $W_g = 4$ cm

$\Rightarrow$ typical distance between bounces is

$$L \approx \frac{W_g}{\theta_{av}} = \frac{W_g}{0.05\, m \lambda_{Å}} \cdot \frac{180}{\pi}$$

$$m=3\,(?): \quad L = \frac{15.3}{\lambda_{Å}}$$

length of instrument ≈ 25m

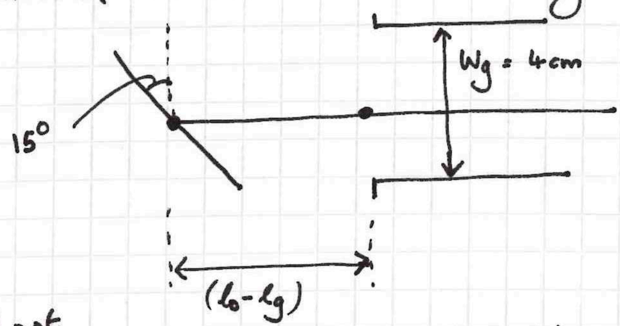
$E_i : 20$meV $\lambda = 2$ Å $\Rightarrow L : 7.6$m $\Rightarrow \sim 3$ bounces

$E_i : 3.3$meV $\lambda = 5$ Å $\Rightarrow L : 3.1$m $\Rightarrow \sim 8$ bounces

Essentially this blurs out the assymmetries of the angled moderator face i.e. no time correlation with position in the beam area at the sample, and no time correlations with angle.

Queries

(1) Ward appear to add an extra moderator broadening that is the convolution of the moderator lineshape with a hat function FWHM equal to the time to travel the distance of the projection of the moderator face along the beam direction



If $l_0 - l_g \sim 1$m (no idea what it is)

at 5Å $\Rightarrow$ 1.3cm

2Å $\Rightarrow$ 0.5cm

So non-trivial

- should not ~~ignore~~ the extra width of $\theta_{av} \cdot (l_0 - l_g)$
- projection is ~ 4cm at 15° = 1cm

$\lambda = 2$ Å ≈ 2000 m/s $\Rightarrow$ 5 μs

$\lambda = 5$ Å ≈ 800 m/s $\Rightarrow$ 12.5 μs

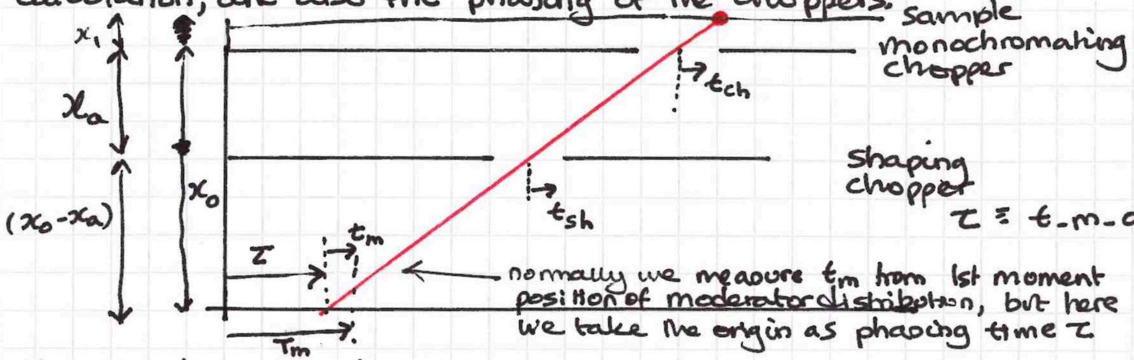
non-trivial.

* Really emphasises the need to compare with Monte Carlo simulations

(2) Not obvious how the bounces average out the divergence profile as a function of position in the beam area at the sample.

Dealing with the moderator-choppers correlation - phasing

The fact that the trio of moderator, shaping chopper, and monochromating chopper define just two degrees of freedom means we have to carefully handle the first moments in the resolution calculation, and also the phasing of the choppers.



How to phase the choppers:
- the gradient defines v_I
- the offset is chosen to maximise the intensity.

At the sample: intensity — transmission functions for choppers

$$I(\tau) = \iint dv\, dT_s\ \ m(t_m+\tau, v)\ s(t_{sh})\ c(t_{ch})$$

In the usual way perform small deviations approximation:

(i) $m(t_m, v) \Rightarrow m(t_m)$ at v_I — $m(t)$ is measured w.r.t. proton pulse

(ii) $t_m = t_s + \frac{(x_0+x_1)}{v_I^2}\delta v$ etc. — ie $m(t) = 0 \quad t \leq 0$

~~We can re-express this as an integral just over T_s, as $\int dv$ is trivial if we ignore~~

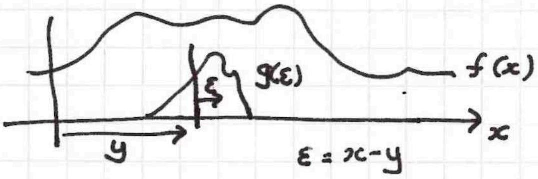
Change integration variables to t_m and δv: the small deviations approx. means the Jacobian is constant, so we ignore it as only care about relative intensities

$$I(\tau) = \iint d\delta v\, dt_m\ \ m(t_m+\tau)\, s\left(t_m - \frac{(x_0-x_a)}{v_I^2}\delta v\right) c\left(t_{ch} - \frac{x_0}{v_I^2}\delta v\right)$$

Looks very much like a convolution, as $\int d\delta v$ only over s & c.

$$h(y) = \int g(x-y)\, f(x)\, dx$$

$$= \int g(x) f(x+y)\, dx$$



- We'd like to think of an integral over $m(T_m)$, with the phase τ being a quantity that slides the view of the choppers over the moderator profile. $\Rightarrow$ transform from $t_m \to T_m = t_m + \tau$
- we also want to recast $\int d\delta v$ so that we clearly have a convolution in standard form over s and c $\Rightarrow$ transform to $t_{ch} = t_m - \frac{x_0}{v_I^2}\delta v$

$$\Rightarrow \quad I(\tau) = \int dT_m\ m(T_m) \int dt_{ch}\ s\left((T_m-\tau)\left(\frac{x_a}{x_0}\right) + t_{ch}\left(\frac{x_0-x_a}{x_0}\right)\right) c(t_{ch})$$

$$= \int dT_m\ m(T_m)\ g(T_m-\tau)$$

where

$$g(t) = \int dt_{ch}\ s\left(t\left(\frac{x_a}{x_0}\right) + t_{ch}\left(\frac{x_0-x_a}{x_0}\right)\right) c(t_{ch})$$

Not yet quite in the form we want: to be a multiple convolution we want

$$g(t) = \int d\varepsilon\, \tilde{s}(t-\varepsilon)\,\tilde{c}(\varepsilon)$$

- rescale function s such that $\tilde{s}(t) = s\left(\left(\frac{x_a}{x_o}\right)t\right)$
- change integration variable to $\varepsilon = -t_{ch}\left(\frac{x_o-x_a}{x_o}\right)\left(\frac{x_o}{x_a}\right) = t_{ch}\left(\frac{x_o-x_a}{x_a}\right)$
- rescale function c such that $\tilde{c}(t) = c\left(\left(\frac{-x_a}{x_o-x_a}\right)t\right)$

Reasons:
- The first means we have $\int s\left(t\left(\frac{x_a}{x_o}\right)\ldots\right)\ldots \Rightarrow \int \tilde{s}(t\ldots)\ldots$
- The second means $t\left(\frac{x_a}{x_o}\right) + t_{ch}\left(\frac{x_o-x_a}{x_o}\right) = \left(\frac{x_a}{x_o}\right)\left(t + t_{ch}\left(\frac{x_o-x_a}{x_a}\right)\right) \Rightarrow \left(\frac{x_a}{x_o}\right)(t-\varepsilon)$
- The third means $\int \ldots c\left(\left(\frac{-x_a}{x_o-x_a}\right)\varepsilon\right) \Rightarrow \int \ldots \tilde{c}(\varepsilon)$

So finally we have, to within a constant of proportionality:

$$I(\tau) = \int dT_m\, m(T_m)\, g(T_m-\tau)$$

where:

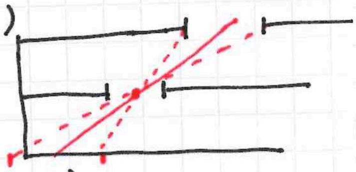
$$g(t) = \int d\varepsilon\, \tilde{s}(t-\varepsilon)\,\tilde{c}(\varepsilon)$$

$$\tilde{s}(t) = s\left(\left(\frac{x_a}{x_o}\right)t\right)$$

$$\tilde{c}(t) = c\left(\left(\frac{x_a}{x_o-x_a}\right)t\right)$$ ⇐ only because symmetric function.

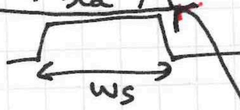
Getting $g(t)$: for speed can use straightforward array convolution
And then do the same again to get convolution with $m(T_m)$.
Choice of time interval

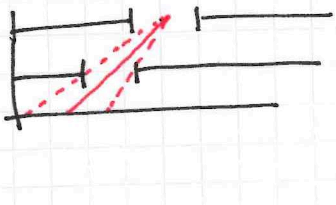
- $\tilde{c}(t)$: if W_c = full width  of $c(t)$



full width of $\tilde{c}(t)$ is $W_c\left(\frac{x_o-x_a}{x_a}\right)$

so take $\boxed{\Delta t_{ch} = \alpha W_c\left(\frac{x_o-x_a}{x_a}\right)}$ ($\alpha = 0.01$, say)

- $\tilde{s}(t)$: If W_s = full width  of $s(t)$



full width of $\tilde{s}(t)$ is $W_s\left(\frac{x_o}{x_a}\right)$

so take $\boxed{\text{time step} = \alpha W_s\left(\frac{x_o}{x_a}\right)}$

- $m(T_m)$: Range over which to convolute:

$g(t)$ width: $W_{Tot} = W_s\left(\frac{x_o}{x_a}\right) + W_c\left(\frac{x_o-x_a}{x_a}\right)$

Then take full 'convolution' range as:

half-heights $\pm\, W_{Tot}$

$\boxed{\text{Time step} = \alpha\, \text{FWHM}_{mod}}$

take step in time as minimum of these three.

A special case is when the monochromating chopper is infinitesimally wide i.e. $c(t) = \delta(t)$

in this case $g(t) \approx \tilde{s}(t)$ (within a constant of proportionality), so

$$\boxed{\begin{aligned} I(\tau) &= \int dT_m \, m(E_m) \, \tilde{s}(T_m - \tau) \\ \tilde{s}(t) &= s\left(\left(\frac{x_a}{x_0}\right) t\right) \end{aligned}}$$

The cases where only one ~~(or neither)~~ of the moderator and shaping chopper are present is straightforward

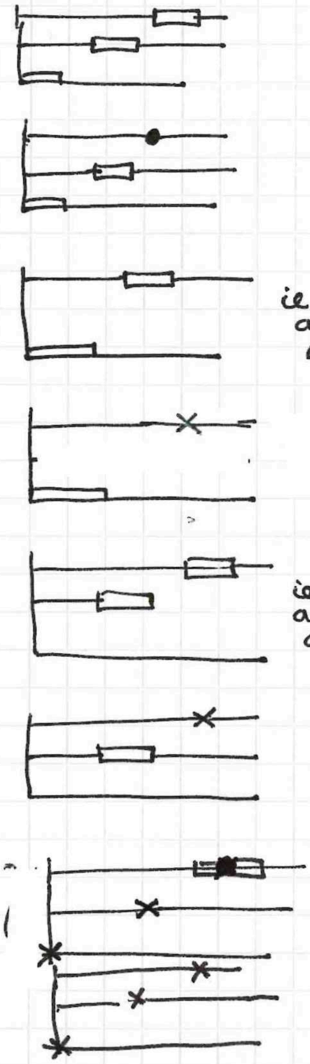
Summary

mod	shape	mono		
1	1	1	τ determined by double convolution & finding maximum flux	
1	1	0	τ determined by single convolution & finding maximum flux	
1	0	1	$\tau = \langle T_m \rangle$	(shaping chopper open all the time)
1	0	1	$\tau = \langle T_m \rangle$	"
0	1	1	$\tau = 0$ (actually, $\tau =$ NaN)	In both cases, the moderator is ∞ wide so that τ is irrelevant
0	1	0		
0	0	1	$\tau = 0$	In both cases moderator is a δ function, which by convention is at $T_m = 0$
0	0	0		

Correcting time origins of distributions, & covariance, in moderator - shaper - monochromator

The cases to consider:

mod	shape	mono	
1	1	1	
1	1	0	
1	0	1	ie shaper assumed ∞ wide
1	0	0	"
0	1	1	ie moderator assumed ∞ wide
0	1	0	"
0	0	1	
0	0	0	



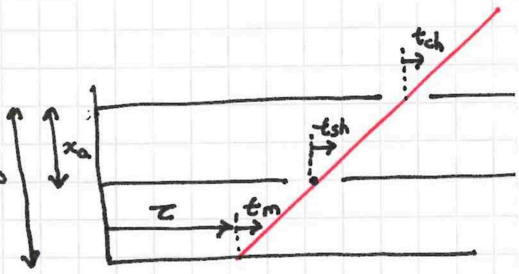
The scheme is that if one, but not both, of the contributions from the moderator and shaping chopper are set to zero, then that contribution is treated as ∞ wide and uniform.

The case when both are set to zero is a δ-function in spread at shaping and monochromating choppers, as this is interpreted as ~~both~~ having zero width at both moderator and shaping chopper.

We want to get means, and covariance of the distributions at the shaping and monochromating chopper positions. The means will in general be non-zero because the moderator pulse that is viewed by the pair of choppers maximises overall flux, and not necessarily is ~~positioned~~ phased w.r.t. choppers to centre $\langle t_{sh} \rangle$, $\langle t_{ch} \rangle$ at zero.

Specifically:

The integrand by which the flux is given is



$$m(t_m + \tau)\; s(t_{sh})\; c(t_{ch})$$

where $t_m = \left(\frac{x_0}{x_a}\right) t_{sh} - \left(\frac{x_0 - x_a}{x_a}\right) t_{ch}$

(and τ chosen to maximise flux (see earlier for quantitative equations))

mod : shape : chop :

$\underbrace{1 \quad 1 \quad 1}$

General case : 2D integral

$$\langle t_{sh}^m\, t_{ch}^n \rangle = \iint dt_{sh}\, dt_{ch}\; m(t_m+\tau)\, s(t_{sh})\, c(t_{ch})\, (t_{sh})^m (t_{ch})^n \Big/ A$$

$$A = \iint dt_{sh}\, dt_{ch}\, m(t_m+\tau)\, s(t_{sh})\, c(t_{ch})$$

$\underbrace{1 \quad 1 \quad 0}$

$c(t_{ch}) = \delta(t_{ch})$

$$\langle t_{sh}^m\, t_{ch}^n \rangle = \iint dt_{sh}\, dt_{ch}\; m(t_m+\tau)\, s(t_{sh})\, \delta(t_{ch})\; t_{sh}^m\, t_{ch}^n \Big/ A$$

if $n \neq 0$, then $\langle t_{sh}^m t_{ch}^n \rangle = 0$ because of $\delta(t_{ch})$

$$\langle t_{sh}^m \rangle = \int dt_{sh}\; m\left(\tau + \left(\tfrac{x_0}{x_a}\right) t_{sh}\right) s(t_{sh})\, t_{sh}^m \Big/ A$$

$$A = \int dt_{sh}\; m\left(\tau + \left(\tfrac{x_0}{x_a}\right) t_{sh}\right) s(t_{sh})$$

$\underbrace{1 \quad 0 \quad 1}$

$s(t_{sh}) = 1$ (ie simply not present)

$$\langle t_{sh}^m\, t_{ch}^n \rangle = \iint dt_m\, dt_{ch}\; m(t_m+\tau)\, c(t_{ch}) .\; t_{sh}^m\, t_{ch}^n$$

$$A = \iint dt_m\, dt_{ch}\; m(t_m+\tau)\, c(t_{ch})$$

where:
$t_{sh} = \alpha t_m + \beta t_{ch}$
$\alpha = x_a/x_0$
$\beta = 1 - \alpha$

$\Rightarrow \langle t_{sh} \rangle = 0 \qquad \langle t_{ch} \rangle = 0$

$$\mathrm{cov}(t_{sh}, t_{ch}) = \begin{pmatrix} \alpha^2 \sigma_m^2 + \beta^2 \sigma_{ch}^2 & \beta \sigma_{ch}^2 \\ \beta \sigma_{ch}^2 & \sigma_{ch}^2 \end{pmatrix}$$

$\underbrace{1 \quad 0 \quad 0}$

Special case of 101, with $\sigma_{ch} = 0$:

$\Rightarrow \langle t_{sh} \rangle = 0 \quad \langle t_{ch} \rangle = 0 \qquad \mathrm{cov}(t_{sh}, t_{ch}) = \begin{pmatrix} \alpha^2 \sigma_m^2 & 0 \\ 0 & 0 \end{pmatrix}$

$\underbrace{0 \quad 1 \quad 1}$

$m(t) = 1$, so simply the convolution

$$\langle t_{sh} \rangle = \langle t_{ch} \rangle = 0$$

$$\mathrm{cov}(t_{sh}, t_{ch}) = \begin{pmatrix} \sigma_{sh}^2 & 0 \\ 0 & \sigma_{ch}^2 \end{pmatrix}$$

$\underbrace{0 \quad 1 \quad 0}$

special case of above with $\sigma_{ch} = 0$:

$$\langle t_{sh} \rangle = \langle t_{ch} \rangle = 0$$

$$\mathrm{cov}(t_{sh}, t_{ch}) = \begin{pmatrix} \sigma_{sh}^2 & 0 \\ 0 & 0 \end{pmatrix}$$

$\underbrace{0 \quad 0 \quad 1}$

δ-functions all the way through (mono chopper width irrelevant)

$$\langle t_{sh} \rangle = \langle t_{ch} \rangle = 0$$

$$\mathrm{cov}(t_{sh}, t_{ch}) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

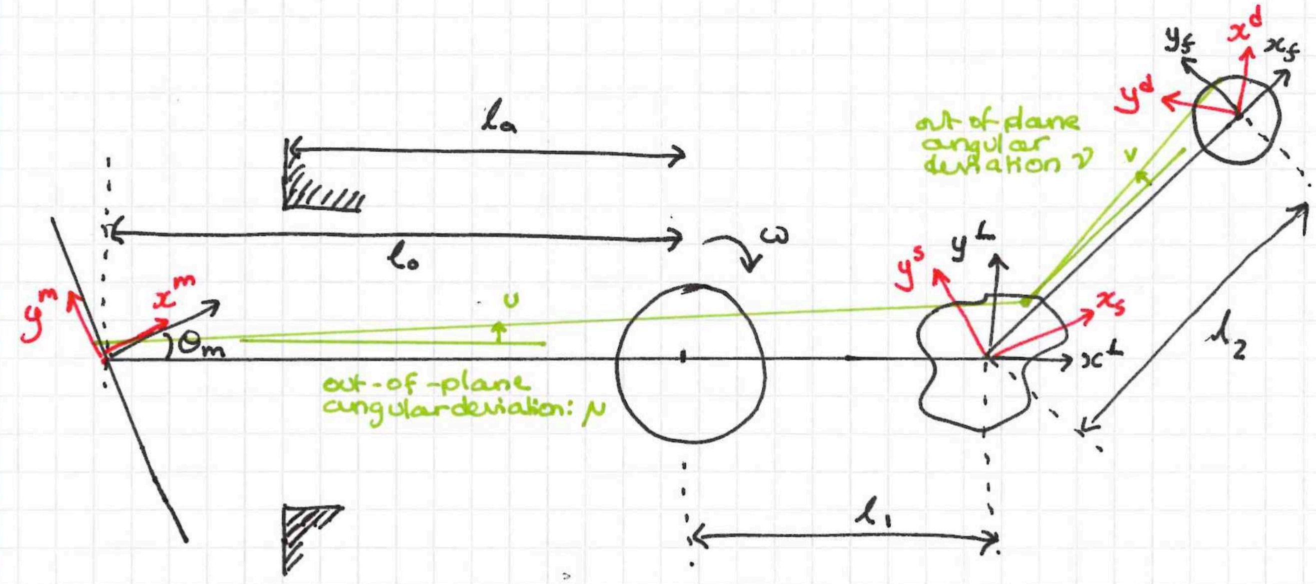
$\underbrace{0 \quad 0 \quad 0}$

same as above:

$$\langle t_{sh} \rangle = \langle t_{ch} \rangle = 0$$

$$\mathrm{cov}(t_{sh}, t_{ch}) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Tobyfit formalism for a fermi chopper spectrometer



Time of arrival at sample:

$$T_s = t_m + \left(\frac{l_0 + l_1 + \overbrace{S_{1j}\, x^s_j}^{\equiv x^L} + \overbrace{y^m \sin\theta_m}^{\text{additional term due to angled moderator face}}}{v_i} \right)$$

additional term due to angled moderator face cf. disk chopper res. func. calculation.

Time of arrival at detector: recall definition of matricies

$$X_i^{lab} = S_{ij}\, X_j^{samp}$$
$$X_i^{final} = F_{ij}\, X_j^{lab}$$
$$X_i^{final} = D_{ij}\, X_j^{det}$$

$$T_d = T_s + \left(\frac{l_2 + x_1^f - F_{1j}\, S_{jk}\, x^s_k}{v_f} \right)$$

exactly the same as disk chopper

Independent timing variables are t_m, t_{ch}, t_d; t_m & t_{ch} together define the time origin and $|\underline{k}_i|$, then t_d defines $|\underline{k}_f|$. Compared to the disk chopper instrument calculation, there are two complications. Firstly, the moderator face is angled, so there is a coupling between the transverse $\underline{k}_i$ resolution and longitudinal deviation that comes in due to the neutron path not being parallel to the beam axis. Secondly, the same angle comes into the effective open time of the chopper being u/ω earlier than the time-of-arrival at the ~~chopper axis~~ plane perpendicular to the beam axis through the chopper axis. That is, the relevant time for sampling the chopper transmission is $\tilde{t}_{ch} = t_{ch} + u/\omega$.

Time of arrival at chopper:

$$T_{ch} = t_m + \left(\frac{l_0 + y^m \sin\theta_m}{v_i} \right)$$

first order deviations approximation

$$V_i = V_I + \delta V_i \implies \frac{1}{V_i} = \frac{1}{V_I}\left(1 - \frac{\delta V_i}{V_I}\right)$$

$$V_f = V_F + \delta V_f \implies \frac{1}{V_f} = \frac{1}{V_F}\left(1 - \frac{\delta V_f}{V_F}\right)$$

Substitute into expression for T_s:

$$T_s = t_m + \frac{1}{V_I}\left(1 - \frac{\delta V_i}{V_I}\right)\left(l_0 + l_1 + S_{ij}x^s_j + y^m \sin\theta_m\right)$$

$$= t_m + \left(\frac{l_0+l_1}{V_I}\right) - \left(\frac{l_0+l_1}{V_I^2}\right)\delta V_i + \frac{S_{ij}x^s_j}{V_I} + \frac{y^m\sin\theta_m}{V_I}$$

Same approximation to T_d with the above approx. to T_s

$$T_d = T_s + \frac{1}{V_F}\left(1 - \frac{\delta V_f}{V_F}\right)\left(l_2 + x^f_i - F_{ij}S_{jk}x^s_k\right)$$

$$= \underbrace{\left(\frac{l_0+l_1}{V_I} + \frac{l_2}{V_F}\right)}_{\text{nominal time of arrival at detector}} + t_m - \left(\frac{l_0+l_1}{V_I^2}\right)\delta V_i - \frac{l_2\,\delta V_f}{V_F^2} + \frac{S_{ij}x^s_j}{V_I} - \frac{F_{ij}S_{jk}x^s_k}{V_F} + \frac{x^f_i}{V_F} + \frac{y^m\sin\theta_m}{V_I}$$

$$\implies t_d = t_m - \left(\frac{l_0+l_1}{V_I^2}\right)\delta V_i - \frac{l_2\,\delta V_f}{V_F^2} + \frac{y^m\sin\theta_m}{V_I} + \frac{S_{ij}x^s_j}{V_I} - \frac{F_{ij}S_{jk}x^s_k}{V_F} + \frac{x^f_i}{V_F}$$

We have t_m, $\tilde{t}_{ch}$, t_d, y_a, z_a, x^s_i & x^f_i (actually x^d_i) as the independent degrees of freedom, where $\tilde{t}_{ch} = t_{ch} + U/\omega$. We want to re-arrange to write δV_i & δV_f in terms of these indep. d.o.f. Actually we will write them as $\delta k_i/k_I \equiv \delta V_i/V_I$ & $\delta k_f/k_F \equiv \delta V_f/V_F$

<u>expression for $\delta V_i/V_I$:</u>

Use t_m & $\tilde{t}_{ch}$ to get this: from before

$$T_{ch} = t_m + \left(\frac{l_0 + y^m\sin\theta_m}{V_i}\right)$$

$$\implies = t_m + \frac{1}{V_I}\left(1 - \frac{\delta V_i}{V_I}\right)\left(l_0 + y^m\sin\theta_m\right)$$

nominal time of arrival at chopper

$$= \cancel{t_m}\left(\frac{l_0}{V_I}\right) + t_m - \frac{l_0\,\delta V_i}{V_I^2} + \frac{y^m\sin\theta_m}{V_I}$$

$$\therefore \tilde{t}_{ch} = t_m - \frac{l_0\,\delta V_i}{V_I^2} + \frac{y^m\sin\theta_m}{V_I} + \frac{U}{\omega}$$

Now need to replace y^m & U in terms of y_a, x^s_i

primary spectrometer:

$$U = \frac{y^L - y_a}{(l_a + l_1)}$$

$$V = \frac{z^L - z_a}{(l_a + l_1)}$$

secondary spectrometer (deviations in k_f frame)

$$u = \frac{y^s - F_{2j} S_{jk} x_k^s}{l_2}$$

$$v = \frac{z^s - F_{3j} S_{jk} x_k^s}{l_2}$$

$$y^m = \frac{y^L - (l_0 + l_1) U}{\cos\theta_m}$$

$$z^m = z^L - (l_0 + l_1) V$$

Need to eliminate y^m and U from the expression for $\tilde{t}_{ch}$, re-expressing in terms of the indep. d.o.f. y_a and $y^L \equiv S_{2j} x_j^s$

$$y^m = \left(y^L - (l_0 + l_1)\left(\frac{y^L - y_a}{l_a + l_1}\right)\right) / \cos\theta_m$$

$$= \frac{(l_0 + l_1) y_a - (l_0 - l_a) y^L}{(l_a + l_1)\cos\theta_m}$$

$$\therefore \frac{y^m \sin\theta_m}{v_I} = \frac{((l_0 + l_1) y_a - (l_0 - l_a) y^L)}{v_I (l_a + l_1)} \cdot \tan\theta_m$$

Also (putting y_a & y^L in same order):

$$\frac{U}{\omega} = \frac{-y_a + y_L}{\omega(l_a + l_1)}$$

Now substitute in the expression for $\tilde{t}_{ch}$ to get $(\delta v_i / v_I)$; we have the term

$$\frac{y^m \sin\theta_m}{v_I} + \frac{U}{\omega} = \frac{((l_0 + l_1) y_a - (l_0 - l_a) y^L)\tan\theta_m}{v_I (l_a + l_1)} + \frac{(-y_a + y_L)}{\omega(l_a + l_1)}$$

$$= \frac{1}{\omega(l_a + l_1)}\left[-\left(1 - \frac{\omega(l_0 + l_1)\tan\theta_m}{v_I}\right) y_a + \left(1 - \frac{\omega(l_0 - l_a)\tan\theta_m}{v_I}\right) y^L\right]$$

together with:
$y^L = S_{2j} x_j^s$

$$\Rightarrow \boxed{\left(\frac{l_0}{v_I}\right)\left(\frac{\delta v_i}{v_I}\right) = t_m - \tilde{t}_{ch} - \mathcal{G}_1 y_a + \mathcal{G}_2 \cdot S_{2j} x_j^s}$$

where $\mathcal{G}_1 = \frac{g_1}{\omega(l_a + l_1)}$ $\qquad g_1 = 1 - \frac{\omega(l_0 + l_1)\tan\theta_m}{v_I}$

$\mathcal{G}_2 = \frac{g_2}{\omega(l_a + l_1)}$ $\qquad g_2 = 1 - \frac{\omega(l_0 - l_a)\tan\theta_m}{v_I}$

To get the expression for $\delta v_f / v_f$, put in the small deviations approximation for t_d; along with the approx. to $\frac{y^m \sin\theta_m}{v_I}$:

$$\Rightarrow \left(\frac{l_2}{v_f}\right)\frac{\delta v_f}{v_f} = t_m - \left(\frac{l_0+l_1}{\cancel{v_I}}\right)\cdot\left(\frac{\cancel{v_I}}{l_0}\right)\left(t_m - \tilde{t}_{ch} - \mathcal{G}_1 y_a + \mathcal{G}_2 y^L\right)$$

$$+\left(\frac{(l_0+l_1)y_a - (l_0-l_a)y^L}{v_I(l_a+l_1)}\right)\tan\theta_m + \frac{S_{1j}x_j^s}{v_I} - \frac{F_{1j}S_{jk}x_k^s}{v_f}$$

$$+\frac{x_1^f}{v_f} - t_d$$

collect terms in y_a & y^L:

$$y_a: +\left(\frac{l_0+l_1}{l_0}\right)\mathcal{G}_1 + \frac{(l_0+l_1)}{v_I(l_a+l_1)}\tan\theta_m$$

$$= \frac{l_0+l_1}{l_0}\cdot\frac{g_1}{\omega(l_a+l_1)} + \frac{(l_0+l_1)}{v_I(l_a+l_1)}\tan\theta_m$$

$$= \frac{1}{\omega(l_a+l_1)}\left(g_1 + \frac{l_1}{l_0}g_1 + \overbrace{\frac{\omega(l_0+l_1)\tan\theta_m}{v_I}}^{=1-g_1}\right)$$

$$= \frac{1}{\omega(l_a+l_1)}\left(1+\frac{l_1}{l_0}g_1\right)$$

Similarly, coeff of y^L

$$y^L: -\left[\left(\frac{l_0+l_1}{l_0}\right)\mathcal{G}_2 + \frac{(l_0-l_a)}{v_I(l_a+l_1)}\tan\theta_m\right]$$

$$= -\frac{1}{\omega(l_a+l_1)}\left(g_2 + \frac{l_1}{l_0}g_2 + \overbrace{\frac{\omega(l_0-l_a)\tan\theta_m}{v_I}}^{=1-g_2}\right)$$

$$= -\frac{1}{\omega(l_a+l_1)}\left(1+\frac{l_1}{l_0}g_2\right)$$

note: $x_1^f = D_{1k}x_k^d$

$$\Rightarrow \boxed{\left(\frac{l_2}{v_f}\right)\frac{\delta v_f}{v_f} = -\left(\frac{l_1}{l_0}\right)t_m + \left(\frac{l_0+l_1}{l_0}\right)\tilde{t}_{ch} + \mathcal{F}_1 y_a + \frac{S_{1j}x_j^s}{v_I} - \mathcal{F}_2 S_{2j}x_j^s - \frac{F_{1j}S_{jk}x_k^s}{v_f} + \frac{x_1^f}{v_f} - t_d}$$

where $\mathcal{F}_1 = \frac{1}{\omega(l_a+l_1)}f_1$ $\qquad f_1 = \frac{l_0+l_1 g_1}{l_0}$

$\mathcal{F}_2 = \frac{1}{\omega(l_a+l_1)}f_2$ $\qquad f_2 = \frac{l_0+l_1 g_2}{l_0}$

Collect results. We have expressions for U, V, N, ν from earlier, and $\delta k_{iy}/k_i = U$, $\delta k_{iz}/k_i = N$ etc. Substitute $y^L = S_{2j} x_j^s$, $z^L = S_{3j} x_j^s$

We also substitute $x_i^f = D_{ik} x_k^d$ so that we deal with deviations in detector frame rather than secondary spectrometer frame.

Overall:

$$\left(\frac{l_0}{V_I}\right)\frac{\delta k_{i1}}{k_I} = t_m - \tilde{t}_{ch} - \mathcal{G}_1 y_a + \mathcal{G}_2 S_{2j} x_j^s$$

$$\left(\frac{l_2}{V_F}\right)\frac{\delta k_f}{k_f} = -\left(\frac{l_1}{l_0}\right) t_m + \left(\frac{l_0+l_1}{l_0}\right)\tilde{t}_{ch} + \mathcal{F}_1 y_a + \frac{S_{1j} x_j^s}{V_I} - \mathcal{F}_2 S_{2j} x_j^s - \frac{F_{1j} S_{jk} x_k^s}{V_F} + \frac{D_{1k} x_k^d}{V_F} - t_d$$

$$\frac{\delta k_{i2}}{k_I} = \frac{S_{2j} x_j^s - y_a}{(l_a + l_1)}$$

$$\frac{\delta k_{i3}}{k_I} = \frac{S_{3j} x_j^3 - z_a}{(l_a + l_1)}$$

$$\frac{\delta k_{f2}}{k_F} = \frac{D_{2k} x_k^d - F_{2j} S_{jk} x_k^s}{l_2}$$

$$\frac{\delta k_{f3}}{k_F} = \frac{D_{3k} x_k^d - F_{3j} S_{jk} x_k^s}{l_2}$$

recall these deviations are in the k_f frame

where
$$g_1 = 1 - \frac{\omega(l_0 + l_1)\tan\theta_m}{V_I}$$

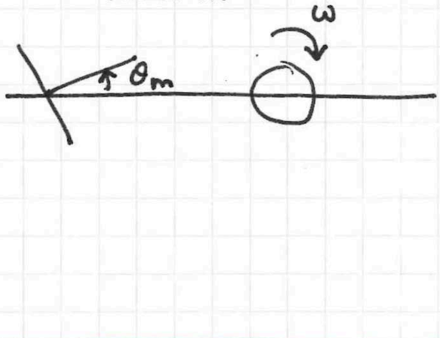
$$g_2 = 1 - \frac{\omega(l_0 - l_a)\tan\theta_m}{V_I}$$

$$f_{1,2} = \frac{l_0 + l_1 g_{1,2}}{l_0}$$

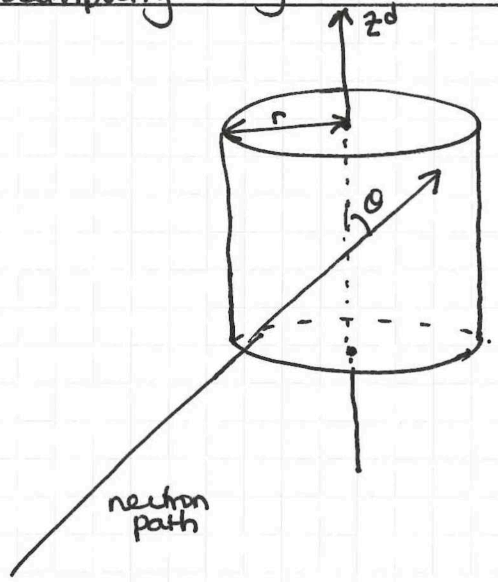
$$\mathcal{G}_{1,2} = \frac{g_{1,2}}{\omega(l_a + l_1)}$$

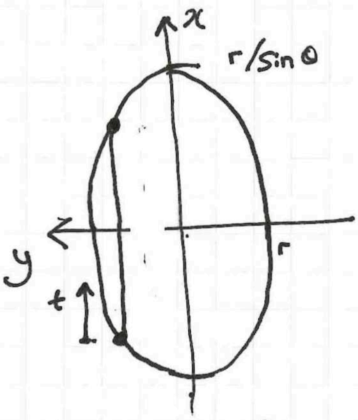
$$\mathcal{F}_{1,2} = \frac{f_{1,2}}{\omega(l_a + l_1)}$$

definition of the sense of rotation:



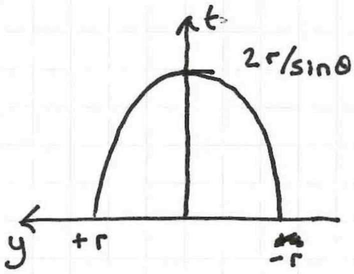
Sampling a cylindrical detector





$$\frac{x^2 \sin^2\theta}{r^2} + \frac{y^2}{r^2} = 1$$

Perform a shift on t to draw as:



$$t_{max} = 2x$$

$$\therefore t_{max}^2 = 4x^2$$

$$= 4\left(1 - \frac{y^2}{r^2}\right)\frac{r^2}{\sin^2\theta}$$

$$\text{or } t_{max} = \frac{2r}{\sin\theta}\left(1 - y^2/r^2\right)^{1/2}$$

Our scheme:

(1) Sample the truncated exponential $e^{-\Sigma t}$ over $t = [0, 2r/\sin\theta]$

(2) sample y in the range $[-r, r]$

(3) reject those points y for which $t > \frac{2r}{\sin\theta}\left(1 - y^2/r^2\right)^{1/2}$

(as these are ~~events~~ neutrons which went through the detector)

~~Note – keep the values of t and choose a set of y that are not rejected.~~

Now express this in terms of reduced coordinates:

$$\left.\begin{aligned} x' &= \Sigma t \\ y' &= y/r \\ \alpha &= (2\Sigma r) \end{aligned}\right\} \Rightarrow \begin{aligned} &\text{sample } e^{-x'} \text{ over } \left[0, \frac{\alpha}{\sin\theta}\right] \\ &\quad \text{..} \quad y' \text{ over } [-1, +1] \\ &\text{reject } \left(\frac{x'}{\alpha/\sin\theta}\right)^2 > 1 - y'^2 \end{aligned}$$

once have a set of x' & y', can then convert to x & y:

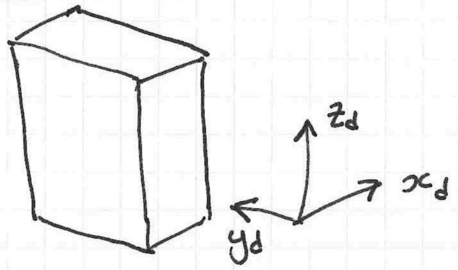
$$y = y' \cdot r$$

$$x = \left(2\frac{x'}{(\alpha/\sin\theta)} - \sqrt{1 - y'^2}\right)\left(\frac{r}{\sin\theta}\right) \quad \left(\text{as } x = t - \frac{r}{\sin\theta}\left(1 - \frac{y^2}{r^2}\right)^{1/2}\right)$$

Note: x is measured along the neutron path. We may want to get the point of absorption ⊥ tube axis, in which case we ~~measure along~~ multiply by $\sin\theta$ to get $x\sin\theta$.

Note: Actually, our algorithm rand_truncexp(α) works even when $\alpha = 0$ (which is a valid case ie limiting low efficiency detector)

Detector slab



widths W_x, W_y, W_z
attenuation length Δ

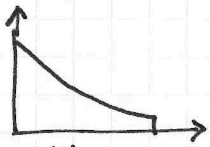
Attenuation is according to a truncated exponential

efficiency is $\varepsilon = 1 - \exp(-W_x/\Delta)$ i.e. $\boxed{\varepsilon = 1 - e^{-\alpha}}$ $(\alpha = W_x/\Delta)$

This will have numeric problems when $W_x/\Delta \to 0$

mean depth of absorbtion:

w.r.t. front face:



$$\langle x \rangle = \int_0^{W_x} dx\, x \exp(-x/\Delta) \Big/ \int_0^{W_x} dx \exp(-x/\Delta)$$

put $x' = x/\Delta$; $dx' = dx/\Delta$

$$\text{numerator} = \int_0^{W_x/\Delta} \Delta dx' \,.\, \Delta x' \exp - x'$$

$$= \Delta^2 \int_0^{\alpha} dx \,.\, x \exp - x \qquad \alpha = (W_x/\Delta)$$

$$= 1 - (1+\alpha)e^{-\alpha}$$

$$\text{denominator} = \Delta \int_0^{\alpha} dx \exp - x$$

$$= \Delta \left[-\exp - x \right]_0^{\alpha}$$

$$= \Delta (1 - \exp - \alpha)$$

$$\Rightarrow \boxed{\frac{\langle x \rangle}{\Delta} = \frac{1 - (1+\alpha)e^{-\alpha}}{1 - e^{-\alpha}} = 1 - \frac{\alpha e^{-\alpha}}{1 - e^{-\alpha}}}$$

$\alpha \to 0 : \to \alpha/2$ ✓ i.e. $\langle x \rangle \to \frac{\alpha\Delta}{2} = \frac{W_x}{2}$

$\alpha \to \infty : \to 1$ ✓ i.e. $\langle x \rangle \to \Delta$

$$\frac{\langle x^2 \rangle}{\Delta^2} = \frac{2 - (2 + \alpha(2+\alpha))e^{-\alpha}}{1 - e^{-\alpha}}$$

$$\hookrightarrow \boxed{\frac{\sigma_x^2}{\Delta^2} = \frac{1 - (2+\alpha^2)e^{-\alpha} + e^{-2\alpha}}{(1 - e^{-\alpha})^2} = 1 - \frac{\alpha^2 e^{-\alpha}}{(1 - e^{-\alpha})^2}}$$

$\alpha \to 0 : \to \frac{\alpha^2}{12}$ i.e. $\sigma_x^2 \to \frac{W_x^2}{12}$

from mathematica:

$$\varepsilon = \alpha - \frac{\alpha^2}{2!} + \frac{\alpha^3}{3!} - \frac{\alpha^4}{4!} + \ldots$$

$$\frac{\langle x \rangle}{\Delta} = \frac{\alpha}{2} - \frac{\alpha^2}{12} + \frac{\alpha^4}{720} - \frac{\alpha^6}{30240} + \frac{\alpha^8}{1209600} - \frac{\alpha^{10}}{47900160} + \frac{\alpha^{12}}{1307674368000} + \ldots$$

$$\frac{\sigma_x^2}{\Delta^2} = \frac{\alpha^2}{12} - \frac{\alpha^4}{240} + \frac{\alpha^6}{6048} - \frac{\alpha^8}{172800} + \frac{\alpha^{10}}{5322240} - \frac{691\alpha^{12}}{118879488000} + \alpha^{14}/5748019200 + \ldots$$

How many terms to keep in the Taylor series?

(1) efficiency

Typically have a function that $= 1-(1-\delta)$; if $\delta \approx 0.1$ have 16 sig fig

$\therefore$ In general we can ignore terms that are $<10^{-16}$ smaller than the first term in the series at the value of α at which $\delta \approx 0.1$

For efficiency, $\alpha = 0.1$ is where $\varepsilon = 1-e^{-\alpha}$, $e^{-\alpha} \approx 0.9$.

1st term is α

n^{th} term is $\alpha^n/n!$

$n=10$: $\alpha^{10}/10! = 3\times10^{-17}$ ie 3×10^{-16} of 1st term

$n=11$: $\alpha^{11}/11! = 2.5\times10^{-19}$ ie 2.5×10^{-18} " " "

$\Rightarrow$ keep α^{10}, but ignore α^{11} and higher powers. ~~(α^{12} is $\alpha^{12}/12! = 2\times10^{-21} = 2\times10^{-20}$ of 1st term)~~

(2) mean depth

$$\langle x\rangle/\Delta = 1 - \frac{\alpha e^{-\alpha}}{(1-e^{-\alpha})} \approx 1-\alpha/2$$

so overall lose 1 sig fig at $\alpha \approx 0.1$ in a calculation of $\langle x\rangle/\Delta$

Consider Taylor series:

1st term : $\alpha/2 = 0.05$

α^{10} : $\approx 2\times10^{-18} = 4\times10^{-17}$ of 1st term

α^{12} : $\approx 10^{-24} = 2\times10^{-23}$ " "

$\Rightarrow$ keep α^{10}, but ignore α^{12} and higher powers.

(3) variance of depth

$$\frac{\sigma_x^2}{\Delta^2} = 1 - \frac{\alpha^2 e^{-\alpha}}{(1-e^{-\alpha})^2} \approx 1 - \frac{\alpha^2}{12}$$

so lose one sig fig when $\frac{\alpha^2}{12} \approx 0.1$ ie $\alpha \approx 1$

and lose two sig fig when $\frac{\alpha^2}{12} \approx 0.01$ ie $\alpha \approx 0.35$

(or)

if $\alpha = 1$, then

1st term : ≈ 0.1

α^{12} term : $\approx 6\times10^{-9}$ $\Rightarrow$ have only 8 sig fig

α^{14} " :

If $\alpha = 0.35$

1st term: ≈ 0.010

α^{12} term: $\approx 2\times10^{-14}$ $\Rightarrow$ have ≈ 12 sig fig; drop 14 sig fig

α^{14} term : $\approx 6\times10^{-16}$ $\Rightarrow$ " ≈ 14 " "

So going to α^{14} for $\alpha < 0.35$ $\Rightarrow$ approx 15–16 sig fig overall.

For algorithms, let us calculate mean depth w.r.t. middle of the detector – this is for three reasons

- consistent with 3He tube
- at high energy, this is the limiting case ($\alpha \to 0$)
- numerically stable, as takes the first term $\alpha/2$ in $\langle x \rangle/\Delta$ out of the calculation. In the limit of $\alpha \to 0$ this is because $\Delta \to \infty$ (W_x will always be sensible). We otherwise have

We also

In summary:

If $\alpha = W_x/\Delta$ $\quad$ W_x = full depth

Δ = attenuation length

$$\varepsilon = 1 - e^{-\alpha} \qquad (\alpha \geq 0.1)$$

$$= \alpha\left(1 - \frac{\alpha}{2!} + \frac{\alpha^2}{3!} - \frac{\alpha^4}{4!} \ldots\ldots \frac{\alpha^9}{10!}\right) \qquad (\alpha < 0.1)$$

now w.r.t. centre of detector

$$\frac{\langle x \rangle}{W_x} = -\frac{1}{2} + \frac{1}{\alpha} - \frac{e^{-\alpha}}{1-e^{-\alpha}} \qquad (\alpha \geq 0.1)$$

$$= \alpha\left(-\frac{1}{12} + \frac{\alpha^2}{720} - \frac{\alpha^4}{30240} + \frac{\alpha^6}{1209600} - \frac{\alpha^8}{47900160}\right) \qquad (\alpha < 0.1)$$

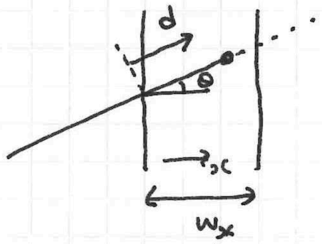
$$\frac{\sigma_x^2}{W_x^2} = \frac{1}{\alpha^2} - \frac{e^{-\alpha}}{(1-e^{-\alpha})^2} \qquad (\alpha \geq 0.35)$$

$$= \left(\frac{1}{12} - \frac{\alpha^2}{240} + \frac{\alpha^4}{6048} - \frac{\alpha^6}{172800} + \frac{\alpha^8}{5322240} - \frac{\alpha^{10}.691}{118.879.488.000} + \alpha^{12}/5\,748\,019\,200\right)$$

$$(\alpha < 0.35)$$

Note: these equations work for any value of $0 \leq \Delta \leq \infty$ for finite W_x

Path of neutron not $\parallel$ to x_d :



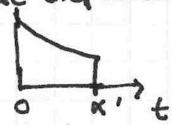
All calculations proceed with $w_x \to (w_x/\cos\theta)$; $x \to d$ (distance along neutron path)

so $\alpha \to \alpha' = (w_x/\cos\theta)/\Delta$

$$\varepsilon = 1 - e^{-\alpha'}$$

$$\frac{\langle d \rangle}{(w_x/\cos\theta)} = -\frac{1}{2} + \frac{1}{\alpha'} - \frac{e^{-\alpha'}}{1-e^{-\alpha'}}$$

ie $\langle d \rangle = \left(\frac{w_x}{\cos\theta}\right)\left(-\frac{1}{2} + \frac{1}{\alpha'} - \frac{e^{-\alpha'}}{1-e^{-\alpha'}}\right)$ $\Leftarrow$ To get Monte Carlo random points: sampled from truncated exponential e^{-t}



& $\langle \sigma_d^2 \rangle = \left(\frac{w_x}{\cos\theta}\right)^2 \left(\frac{1}{\alpha'^2} - \frac{e^{-\alpha'}}{(1-e^{-\alpha'})^2}\right)$

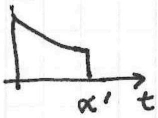
then scale by $\frac{(w_x/\cos\theta)}{\alpha'} = \Delta$

Projection along x axis: $x = d\cos\theta$, so

$$\langle x \rangle = w_x \left(-\frac{1}{2} + \frac{1}{\alpha'} - \frac{e^{-\alpha'}}{1-e^{-\alpha'}}\right)$$

$\Leftarrow$ Random points: projection of above by $\cos\theta$, so sample from e^{-t}

$$\sigma_x^2 = w_x^2 \left(\frac{1}{\alpha'^2} - \frac{e^{-\alpha'}}{(1-e^{-\alpha'})^2}\right)$$

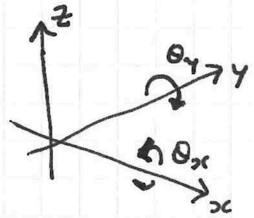


then scale by $\Delta\cos\theta$

Mosaic Spread

23/7/19 mosaic-

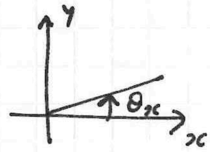
Consider successive rotations around the x-axis, y-axis, z-axis is
Active rotations



x-axis:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & C_x & -S_x \\ \cdot & S_x & C_x \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

where $C_x = \cos(\theta_x)$
$S_x = \sin(\theta_x)$



y-axis:

$$\begin{pmatrix} x' \\ y \\ z' \end{pmatrix} = \begin{pmatrix} C_y & \cdot & S_y \\ - & 1 & \cdot \\ -S_y & \cdot & C_y \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

z-axis:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} C_z & -S_z & \cdot \\ S_z & C_z & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Rotate about x, then y, then z: overall matrix is

$$\begin{pmatrix} C_z & -S_z & \cdot \\ S_z & C_z & \cdot \\ \cdot & \cdot & 1 \end{pmatrix} \begin{pmatrix} C_y & \cdot & S_y \\ - & 1 & \cdot \\ -S_y & \cdot & C_y \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & C_x & -S_x \\ \cdot & S_x & C_x \end{pmatrix}$$

$$= \begin{pmatrix} C_y C_z & S_x S_y C_z - C_x S_z & C_x S_y C_z + S_x S_z \\ C_y S_z & S_x S_y S_z + C_x C_z & C_x S_y S_z - S_x C_z \\ -S_y & S_x C_y & C_x S_y \end{pmatrix}$$

small angle approx: $c_i \to 1$, $S_i \to \theta_i$ but keep only single S_i
(ie 1st-order)

$$R = \begin{pmatrix} 1 & -\theta_3 & \theta_2 \\ \theta_3 & 1 & -\theta_1 \\ -\theta_2 & \theta_1 & 1 \end{pmatrix}$$

The change in a vector is given by subtracting the diagonal, as

$$\delta \underline{Q} = \underline{\underline{R}}\,\underline{Q} - \underline{Q}$$

ie $\delta Q_i = R_{ij} Q_j - \delta_{ij} Q_j$

ie $\delta Q_i = M_{ij} Q_j$

proof: simply enumerate

$$M = \begin{pmatrix} 0 & -\theta_3 & \theta_2 \\ \theta_3 & 0 & -\theta_1 \\ -\theta_2 & \theta_1 & 0 \end{pmatrix} \equiv M_{ij} = -\varepsilon_{ijk}\theta_k$$

This gives a way of expressing the function along any direction in $\underline{Q}$-space

consider a unit vector $\underline{n} \perp \underline{Q}_0$, what is the mean & variance of the mosaic spread in that direction? (here $\underline{Q}_0$ is our $\underline{Q}$ vector)
We have a p.d.f. for the mosaic, $p(\theta_x, \theta_y, \theta_z)$

Distance along $\underline{n}$ is given by

$$q = \underline{n} \cdot \delta \underline{Q}$$
$$= n_i \, \delta Q_i$$
$$= n_i \, M_{ij} \, Q_{oj}$$
$$\therefore \; q = -\varepsilon_{ijk} \, n_i Q_{oj} \, \theta_k$$

mean:

$$\langle q \rangle = -\varepsilon_{ijk} \, n_i Q_{oj} \langle \theta_k \rangle$$
$$= 0 \quad \text{if all } \langle \theta_k \rangle = 0$$

variance:

$$\langle q^2 \rangle = \underbrace{\varepsilon_{ijk} \, \varepsilon_{lmn}} \, n_i n_l \, Q_{oj} Q_{om} \langle \theta_k \theta_n \rangle$$

See Riley, Hobson & Bence 3rd ed. p944 for the general expression of this as a 3x3 determinant of Kronecker δ-~~functio~~ symbols

If $\langle \theta_{kn}^2 \rangle = \langle \theta^2 \rangle \delta_{kn}$ ie $\langle \theta^2 \rangle$ along all 3 ⊥ directions, then simplifies as $k \equiv n$:

$$\Rightarrow \quad \varepsilon_{ijk} \, \varepsilon_{lmk} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}$$

$$\therefore \langle q^2 \rangle = \langle \theta^2 \rangle \left(n_i n_i \, Q_{oj} Q_{oj} - n_i Q_{oi} \, n_j Q_{oj} \right)$$
$$= \langle \theta^2 \rangle \left((\underline{n} \cdot \underline{n})(\underline{Q}_o \cdot \underline{Q}_o) - (\underline{n} \cdot \underline{Q}_o)^2 \right)$$

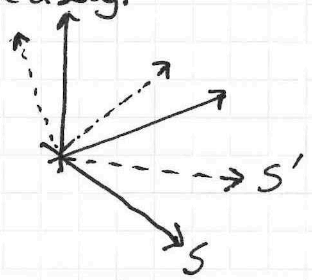
We have $|\underline{n}|^2 = 1$ by supposition
in the case of $\underline{n} \perp \underline{Q}_0$ (which is what we usually consider)

$$\Rightarrow \langle q^2 \rangle = \langle \theta^2 \rangle |\underline{Q}_o|^2$$

Implementing mosaicspread

Suppose we have a rotation vector $\underline{\Theta}$ that defines the rotation of a crystallite w.r.t. nominal crystal orientation. We need the matrix to ~~take a vector~~ get (h, k, l) for the crystallite given $(h k l)$ in the nominal crystal.

More precisely:



S is an orthonormal frame fixed in the nominal crystal.

S' is an orthormal frame obtained by rotating S by $\underline{\Theta}$

What we want is the matrix that converts the components of a vector $\underline{Q}$ expressed in rlu} in frame S into the components in rlu in frame S'.

UB matrix, U, relates components in rlu to components in an orthonormal frame:

$$\underline{Q}^{orth} = U \underline{Q}^{rlu}$$

The rotation matrix, $R(\underline{\Theta})$, actively rotates a vector in a fixed frame so that its components in that orthonormal frame are changed:

$$\underline{V}^{new} = R(\underline{\Theta}) \underline{V}^{old}$$

If the coordinate frame is rotated, but the vector is fixed, we can use the same matrix generator to get the components of the vector in S' given those in S:

$$\underline{V}^{S'} = R(-\underline{\Theta}) \underline{V}^{S}$$

– rotating S by $\underline{\Theta}$ is like rotating the vector by $-\underline{\Theta}$

Putting together:

$$\underline{Q}^{S} = U \underline{Q}^{rlu}$$

$$\underline{Q}^{S'} = R(-\underline{\Theta}) \underline{Q}^{S}$$

$$= R(-\underline{\Theta}) U \underline{Q}^{rlu}$$

$$\therefore \boxed{\underline{Q}^{rlu, mos} = U^{-1} R(-\underline{\Theta}) U \underline{Q}^{rlu}}$$

note: $U^{-1} \neq U^{T}$ as not orthogonal matrix in general.

note $R(-\Theta) = R^{T}(\Theta)$ as R is orthogonal, so its inverse is its transpose

mosaic distribution

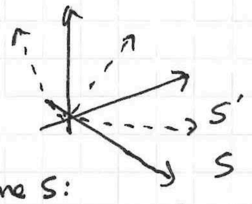
Suppose we have a function that gives the probability distribution of mosaic spread, $P(\underline{\theta})$: $\int P(\underline{\theta})\, d\underline{\theta} = 1$

We will have to randomly sample this and use the transformation matrix $U^T R(-\underline{\theta}) U$ (see earlier) to transform a nominal $\underline{Q}^{rlu}$ to $\underline{Q}^{rlu,mos}$.

Special case of Gaussian form

$$P(\underline{\theta}) \propto \exp -\tfrac{1}{2}\left(\underline{\theta}^T C^{-1} \underline{\theta}\right) \qquad C = \text{covariance matrix}. \quad = M^{-1}$$

(i) It turns out that rotation vectors transform like the components of any other vector when you change coordinate frame.



in frame S:

$$\bar{\underline{V}}^{s} = R(\underline{\theta}^{s})\, \underline{V}^{s} \quad \ldots (1) \qquad R(\underline{\theta}) \text{ is a } 3\times3 \text{ matrix created from the components } \theta_1, \theta_2, \theta_3$$

in frame S':

$$\bar{\underline{V}}^{s'} = R(\underline{\theta}^{s'})\, \underline{V}^{s'} \quad \ldots (2)$$

We have $\bar{\underline{V}}^{s'} = O\,\bar{\underline{V}}^{s}$ and $\underline{V}^{s'} = O\,\underline{V}^{s}$, where O is an orthogonal matrix.
Use these in (1) to get

$$\bar{\underline{V}}^{s'} = O\underline{V}^{s} = O R(\underline{\theta}^{s}) O^{-1} \underline{V}^{s'}$$

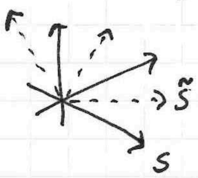
$$\Rightarrow R(\underline{\theta}^{s'}) = O R(\underline{\theta}^{s}) O^{-1}$$ This is a required identity.

If $\underline{\theta}$ transforms like any other vector, then we will find that

$$\underline{\theta}^{s'} = O\,\underline{\theta}^{s}$$

I've not tried to prove it, but proof-by-random-examples suggests it is true.

(ii) This gives the lead-in to randomly sampling $P(\underline{\theta})$ – we do the standard trick of getting eigenvectors and eigenvalues:



transform to another orthonormal frame $\tilde{S}$ where we have

$$\underline{\theta}^{\tilde{s}} = V^T \underline{\theta}^{s} \qquad (V^T = V^{-1} \text{ as orthogonal matrix, due to being a rotation})$$

$$f = \underline{\theta}^{s,T} M \underline{\theta}^{s}$$

$$= \underline{\theta}^{\tilde{s},T} (V^T M V)\, \underline{\theta}^{\tilde{s}} \qquad D \text{ diagonal}$$

therefore

$$D = V^T M V$$

or $$MV = VD$$

V transforms from diagonal frame to the initial frame

This is the standard diagonalisation equation (eg) solved by linear algebra function 'eig' in Matlab

Matlab function eig: $[V, D] = eig(A)$

D = diagonal matrix of eigenvalues

V = matrix of eigenvectors s.t. $AV = VD$

ie $D = \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{pmatrix}$ $\quad V = \begin{pmatrix} e_1 & e_2 & \cdots \\ \downarrow & \downarrow & \end{pmatrix}$

If A is real and symmetric, then λ_i are real & the columns of V are orthogonal – as indeed are the rows. V is an orthogonal matrix

(III) we can work [redacted] with C rather than M

$$MV = VD$$

invert: $V^T C = D^{-1} V^T$ $\quad (V^{-1} = V^T ; C = M^{-1}$ by definition$)$

pre-multiply by V & post-multiply by V:

$$CV = VD^{-1}$$

<u>Summary</u>

$$P(\underline{\theta}) = \exp -\frac{1}{2} \underline{\theta}^T C \underline{\theta}$$

solve

$$CV = VD^{-1}$$

sample the Gaussian form in $\underline{\tilde{\theta}}$ defined by D^{-1}

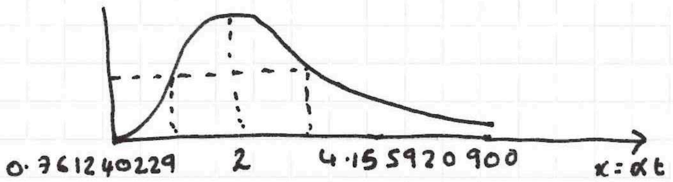
Get $\quad \underline{\theta} = V \underline{\tilde{\theta}}$

Moderator width   19/8/19

$$M(t) = \frac{\alpha^3 t^2}{2} e^{-\alpha t} \quad (t>0) \quad \text{(normalised)}$$

$\alpha = \Sigma v$ ← neutron velocity

Σ ← macroscopic scattering crossection.



$\langle x \rangle = 3$

$\sigma_x^2 = 3$

peak $= 2$

$\frac{\text{fwhh}}{\sigma} = 1.959919799$

fwhh $= 3.394680671$

centre-fwhh $= 2.45858057$

Value of α

Have always used $\Sigma = 0.125\ \text{mm}^{-1}$ $\Rightarrow$ $1/\Sigma = 8\text{mm}$

Time constant $\tau = 1/\alpha = (1/\Sigma)/v$ ie 8 mm is distance neutron travels in time τ

so FWHH $= (3.3947/\Sigma)/v$ ie 27mm is distance neutron travels in FWHH

Where does this figure come from?, of $1/\Sigma = 8\text{mm}$?

H_2O density: 1g/cm³

mass per mol: 18g

$\Rightarrow 6.022 \times 10^{23}/18 = 3.346 \times 10^{18}$ molecules/cm³

Cross-section of hydrogen: 1 barn $= 10^{-24}$ cm²

bound cross-section $= 82.02$ barn

free cross-section $= 20$ barn ← 10meV → 10keV free atom $19.2 < \sigma < 20.$

1eV → 10keV water $19.2 < \sigma < 21.6$

[A. Horsley, AWRE, 1966?]

[The "bound" cross-section is reached in water only by an energy of between 1 meV & 10meV according to Horsley.]

Thus cross-section per cm³ for bound H $= 82.02 \times 10^{-24} \times 2 \times 3.346 \times 10^{22}$

$= 5.49\ \text{cm}^{-1}$

$= 0.549\ \text{mm}^{-1}$

So for bound hydrogen $\therefore 1/\Sigma_{\text{bound}} = 1.82\text{mm}$

And for free hydrogen: $1/\Sigma_{\text{free}} = 7.47\text{mm}$ ⇐ This is the origin of the "8mm" I've always been using

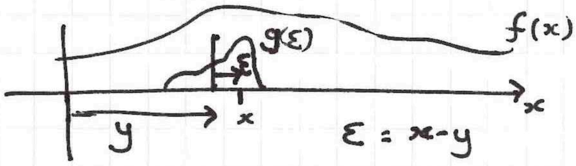
And '8 = 28mm' is the distance travelled in FWHH $= 3.3947\,(1/\Sigma) = 25.4\text{mm}$ ✓

Using $v_{m/s} = 437.39\sqrt{E_{meV}}$ results in FWHH μs: $7.761\,(1/\Sigma)\text{mm}/\sqrt{E_{meV}}$ & $\tau_{\mu s} = 2.286\,(1/\Sigma)\text{mm}/\sqrt{E_{meV}}$

$\Rightarrow$ $\text{FWHH}_{\text{bound}} = 14.1/\sqrt{E_{meV}}$ $\tau_{\text{bound}} = 4.16/\sqrt{E_{meV}}$

$\text{FWHH}_{\text{free}} = 58.0/\sqrt{E_{meV}}$ $\tau_{\text{free}} = 17.1/\sqrt{E_{meV}}$

Convolution of sums of functions



$$h(y) = \int f(x)\, g(x-y)\, dx$$
$$= \int f(x+y)\, g(x)\, dx$$

If $f(x) = \sum_{i=1}^{n_f} f_i(x)$

$g(x) = \sum_{i=1}^{n_g} g_i(x)$

$$\Rightarrow h(y) = \sum_{i=1}^{n_f} \sum_{j=1}^{n_g} \int f_i(x)\, g_j(x-y)\, dx$$

Case of distinct regions

Assume $f_i(x) = 0$ unless $x_i^f \leq x \leq x_{i+1}^f$

and similary $g_i(x) = 0$ " $x_i^g \leq x \leq x_{i+1}^g$

We will have functional forms for $f_i(x)$ & $g_i(x)$, but we need to find the limits for the integration.

Let us consider two specific functions $f_i(x)$ & $g_j(x)$

Then contribution to the integral is:

$$I = \int f_i(x)\, g_j(x-y)\, dx$$

$-f_i$ restricts range to $[x_i^f, x_{i+1}^f]$

$-g_j$ " " " $[x_j^g + y, x_{j+1}^g + y]$

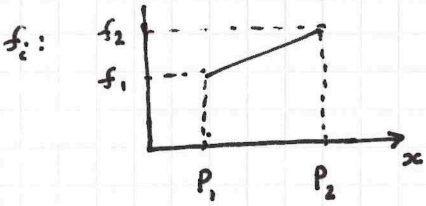
$$\Rightarrow \boxed{\text{Range is } [\max(x_i^f, x_j^g + y), \min(x_{i+1}^f, x_{j+1}^g + y)] = [x_{lo}, x_{hi}] \\ \& \ I = 0 \text{ if } x_{lo} \geq x_{hi}}$$

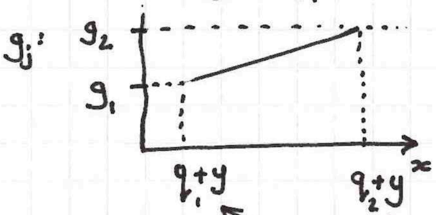
This result applies whatever the functional form of $f_i(x), g_j(x)$.

case of linear sections

$f_i(x)$ & $g_j(x)$ are linear functions (eg) piecewise approximations to true functio[n]

for the sake of notational simplicity, suppose





define $f' = \dfrac{f_2 - f_1}{p_2 - p_1}$

define $g' = \dfrac{g_2 - g_1}{q_2 - q_1}$

because $\int f_i(x)\, g_j(x-y)$ so in the integral must offset the x values.

$$I = \int_{x_{lo}}^{x_{hi}} dx \; f_i(x)\, g_j(x-y) \qquad \text{where: } \begin{cases} x_{lo} = \max(p_1,\, q_1+y) \\ x_{hi} = \min(p_2,\, q_2+y) \end{cases}$$

$$= \int_{x_{lo}}^{x_{hi}} dx \; \big(f_1 + (x-p_1) f'\big)\big(g_1 + (x - q_1 - y) g'\big)$$

$$= \int_{x_{lo}}^{x_{hi}} dx \; \big((f_1 - p_1 f') + x f'\big)\big((g_1 - (q_1+y) g') + x g'\big)$$

Transform $\theta = x - x_{av}$ where $x_{av} = 1/2\,(x_{lo} + x_{hi})$; put $\Delta x = (x_{hi} - x_{lo}$

$$I = \int_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}} d\theta \Big(\big(f_1 + f'(x_{av} - p_1)\big) + \theta f'\Big)\Big(\big(g_1 + g'(\underbrace{(x_{av} - y)}_{} - q_1)\big) + \theta g'\Big)$$

this will be comparable to the integration range, so no numeric problem.

$$= \int_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}} d\theta \; (f_{av} + \theta f')(g_{av} + \theta g')$$

$$= f_{av} g_{av}\, \theta + (f' g_{av} + f_{av} g')\frac{\theta^2}{2} + \frac{\theta^3}{3} f' g' \Bigg|_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}}$$

$$= f_{av} g_{av} \Delta + f' g' \frac{\Delta^3}{12}$$

$$= \Delta \Big(f_{av} g_{av} + f' g' \frac{\Delta^2}{12}\Big)$$

width x 'average' height

correction for non-zero width

$f_{av} = f(x_{av})$

$g_{av} = g(x_{av} - y)$

By definition this point will lie in the integration range – the range is defined by non-zero range of both f_i and g_j

Piece wise Linear function: get λ, σ^2

How to get λ, σ^2 from breakdown into trapezoids – actually any funcs.

(1) $A = \int \sum_i f_i(x)\,dx = \sum_i \int f_i(x)\,dx$

$\Rightarrow \boxed{A = \sum_i A_i}$

(2) $A\lambda = \int x \sum_i f_i(x)\,dx = \sum_i \int x f_i(x)\,dx$

$\Rightarrow \boxed{A\lambda = \sum_i A_i \lambda_i}$

(3) $A\sigma^2 = \int (x-\lambda)^2 \sum_i f_i(x)\,dx$

$$= \sum_i \int \left((x-\lambda_i) - (\lambda-\lambda_i)\right)^2 f_i(x)\,dx$$

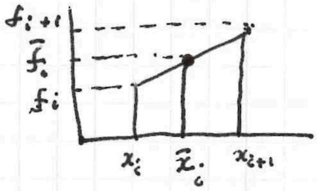
$$= \sum_i \left(\int (x-\lambda_i)^2 f_i(x)\,dx - 2(\lambda-\lambda_i) \underbrace{\int (x-\lambda_i) f_i(x)\,dx}_{0} + (\lambda-\lambda_i)^2 \int f_i(x)\,dx \right)$$

$$= \sum_i \left(A_i\sigma_i^2 - 2(\lambda-\lambda_i)\times 0 + (\lambda-\lambda_i)^2 A_i \right)$$

$\Rightarrow \boxed{A\sigma^2 = \sum_i A_i \left(\sigma_i^2 + (\lambda-\lambda_i)^2\right)}$ ← $A_i\sigma_i^2$ from the function
$A_i(\lambda-\lambda_i)^2$ from the offset of the mean w.r.t the overall mean

Case of piecewise linear sections

Now compute λ_i, σ_i^2 for trapezoid



$m_i = \frac{f_{i+1} - f_i}{\Delta_i}$ $\qquad \Delta_i = x_{i+1} - x_i$

We assume
want to handle special cases in a robust fashion
- $\Delta_i = 0$ (ie a step function)
- $f_{i+1} = f_i = 0$ (ie nothing present)

Drop subscripts for convenience.

Area

$\boxed{A = \bar{f}\Delta}$ no problems with numerics: $\bar{f} = 0$ or $\Delta = 0$ both ok

Mean

$$A\lambda = \int_{x_{lo}}^{x_{hi}} x\left(\bar{f} + m(x-\bar{x})\right)dx$$

Put $\varepsilon = x - \bar{x}$

$$= \int_{-\Delta/2}^{+\Delta/2} (\varepsilon + \bar{x})(\bar{f} + m\varepsilon)\,d\varepsilon$$

$$= \bar{x}\underbrace{\int_{-\Delta/2}^{\Delta/2} (\bar{f} + m\varepsilon)\,d\varepsilon}_{} + \underbrace{\int_{-\Delta/2}^{+\Delta/2} (\varepsilon\bar{f} + m\varepsilon^2)\,d\varepsilon}_{}$$

$= \left(\bar{f}\varepsilon + \frac{1}{2}m\varepsilon^2\right)\Big|_{-\Delta/2}^{+\Delta/2}$ $\qquad$ $\left(\frac{1}{2}\bar{f}\varepsilon^2 + \frac{1}{3}m\varepsilon^3\right)\Big|_{-\Delta/2}^{\Delta/2}$

$= \bar{f}\Delta$

$= A$ $\qquad$ $= \frac{m\Delta^3}{12}$

$\boxed{\therefore A\lambda = A\bar{x} + \frac{m\Delta^3}{12} \quad \text{or} \quad A\theta = \frac{m\Delta^3}{12}}$ where $\theta = \lambda - \bar{x}$

$=$ for stability: $m = \infty$ for a step, so write $m\Delta = \delta f$ where $\delta f = f_{x_{hi}} - f_{x_{lo}}$ $\Rightarrow$ $\boxed{A\lambda = A\bar{x} + \frac{\Delta^2}{12}\delta f \quad A\theta = \frac{\Delta^2}{12}\delta f}$

variance

$$A\sigma^2 = \int_{x_{lo}}^{x_{hi}} (x-\lambda)^2 (\bar{f} + m(x-\bar{x}))\,dx$$

$$= \int_{x_{lo}}^{x_{hi}} (x-\bar{x} - (\lambda - \bar{x}))^2 (\bar{f} + m(x-\bar{x}))\,dx$$

$\varepsilon = x - \bar{x}$ as before ; call $\lambda - \bar{x} = \theta$

$$A\sigma^2 = \int_{-\Delta/2}^{+\Delta/2} (\varepsilon - \theta)^2 (\bar{f} + m\varepsilon)\,d\varepsilon$$

$$= \int_{-\Delta/2}^{\Delta/2} (\varepsilon^2 - 2\theta\varepsilon + \theta^2)(\bar{f} + m\varepsilon)\,d\varepsilon$$

odd powers of ε $\Rightarrow$ even powers when integrated $\Rightarrow$ zero contribution

$$\therefore \quad = \bar{f}\int_{-\Delta/2}^{\Delta/2} (\varepsilon^2 + \theta^2)\,d\varepsilon - 2\theta m\int_{-\Delta/2}^{\Delta/2} \varepsilon^2\,d\varepsilon$$

$$= \bar{f}\left(\frac{\varepsilon^3}{3} + \varepsilon\theta^2\right)\Big|_{-\Delta/2}^{+\Delta/2} - 2\theta m\left(\frac{\varepsilon^3}{3}\right)_{-\Delta/2}^{\Delta/2}$$

$$= \underbrace{\bar{f}\frac{\Delta^3}{12}}_{=\bar{f}\Delta\cdot\frac{\Delta^2}{12}} + \underbrace{\bar{f}\Delta\theta^2}_{=A\theta^2} - \underbrace{\frac{\theta m\Delta^3}{6}}_{=\theta\cdot 2A\theta} \qquad \left(\text{as } A\theta = \frac{m\Delta^3}{12}\text{, previous page}\right)$$

$$= A\cdot\frac{\Delta^2}{12}$$

$$\therefore \boxed{A\sigma^2 = A\left(\frac{\Delta^2}{12} - \theta^2\right)}$$

if $A = 0$ this has a numeric problem, as expressed, because θ is undefined.

combine results for the sum of trapezoids

~~Now use subscript i again, and reserve unsubscripted~~ quantities for the whole function

$$A = \sum_i A_i$$

$$\lambda = \left(\sum_i A_i\lambda_i\right)/A$$

$$\sigma^2 = \sum_i A_i(\sigma_i^2 + (\lambda_i - \lambda)^2)/A$$

so for trapezoids:

$$\boxed{A = \sum_i \bar{f}_i\Delta_i}$$

$$\boxed{\lambda = \sum_i \left(A_i\bar{x}_i + \frac{\Delta^2 \delta f_i}{12}\right)/A} \qquad \text{where } A_i = \bar{f}_i\Delta_i$$

$$\sigma^2 = \sum_i A_i\left(\left(\frac{\Delta_i^2}{12} - \theta_i^2\right) + (\lambda_i - \lambda)^2\right)/A$$

There is a numerical problem with the expression for σ^2 because one or more θ_i could be undefined, even if the overall function is ok (eg) if a step or $A_i = 0$. However, assuming the overall function is ok ie $A \neq 0$, then can do a trick

$$\sigma^2 = \sum_i A_i\left(\left(\frac{\Delta_i^2}{12} - \theta_i^2\right) + (\bar{x}_i + \theta_i - \lambda)^2\right)/A \qquad \text{as } \theta_i = \lambda_i - \bar{x}_i$$

$$= \sum_i A_i\left(\frac{\Delta_i^2}{12} + (\bar{x}_i - \lambda)(\bar{x}_i - \lambda + 2\theta_i)\right)/A$$

Now only single power of θ_i, and we can replace $A_i\theta_i = \frac{\Delta_i^2}{12}\delta f_i$

$$\boxed{\sigma^2 = \sum_i \left(\frac{A_i\Delta_i^2}{12} + (\bar{x}_i - \lambda)\left(A_i(\bar{x}_i - \lambda) + \frac{\Delta_i^2\delta f_i}{6}\right)\right)/A} \qquad \text{where } A_i = \bar{f}_i\Delta_i$$

The boxed expressions are all numerically stable.

Bounds implementation in optimisation

$P_{min} \le P \le P_{max}$

$$P_{int} = \sin^{-1}\left(\frac{2(P - P_{min})}{(P_{max} - P_{min})} - 1\right)$$

$-\infty \le P_{int} \le \infty$

[Period: $-\frac{\pi}{2} \le P_{int} \le \pi/2$]

$$P = P_{min} + (\sin(P_{int}) + 1)\left(\frac{P_{max} - P_{min}}{2}\right)$$

$P_{min} \le P \le P_{max}$

$P_{min} \le P$

$$P_{int} = \sqrt{(P - P_{min} + 1)^2 - 1}$$

$$P = P_{min} - 1 + \sqrt{P_{int}^2 + 1}$$

$-\infty \le P_{int} \le \infty$

[$P_{int} = 0 \Rightarrow P = P_{min}$]

$P_{min} \le P$

$P \le P_{max}$

$$P_{int} = \sqrt{(P_{max} - P + 1)^2 - 1}$$

$$P = P_{max} + 1 - \sqrt{P_{int}^2 + 1}$$

$-\infty \le P_{int} \le \infty$

[$P_{int} = 0 \Rightarrow P = P_{max}$]

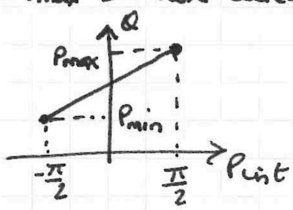
$P \le P_{max}$

These equations do not have an intuitive mapping between P & P_{int}.
Can make linear transforms so that the limits match those of P_i in the case of the semi intervals $P \approx P_{int}$ when $P \gg P_{min}$, $P \ll P_{max}$ so these already are intuitive

$P_{min} \le P \le P_{max}$

want $\theta = P_{min} \Rightarrow P_{min}$, $\theta = P_{max} \Rightarrow P_{max}$

$$P_{int} = -\frac{\pi}{2} + \pi\left(\frac{\theta - P_{min}}{P_{max} - P_{min}}\right)$$



$$\therefore \sin(P_{int}) = \sin\left(-\frac{\pi}{2} + \alpha\right) = -\cos\alpha \qquad \left(\alpha = \pi\left(\frac{\theta - P_{min}}{P_{max} - P_{min}}\right)\right)$$

$$\therefore 1 + \sin(P_{int}) = 1 - \cos\alpha = 2\sin^2\left(\frac{\alpha}{2}\right)$$

$-\infty \le \theta \le \infty$

period: $P_{min} \le \theta \le P_{max}$

$$\Rightarrow P = P_{min} + (P_{max} - P_{min})\sin^2\left(\frac{\pi}{2}\left(\frac{\theta - P_{min}}{P_{max} - P_{min}}\right)\right)$$

$$\theta = P_{min} + \frac{2(P_{max} - P_{min})}{\pi}\sin^{-1}\sqrt{\frac{P - P_{min}}{P_{max} - P_{min}}}$$

$P \ge P_{min}$

$P_{int} = \theta - P_{min}$

$$P = (P_{min} - 1) + \sqrt{(\theta - P_{min})^2 + 1}$$

$$\theta = P_{min} + \sqrt{(P - P_{min} + 1)^2 - 1}$$

$-\infty \le \theta \le \infty$

$\theta = P_{min} \Rightarrow P = P_{min}$

$P \le P_{max}$

$P_{int} = \theta - P_{max}$

$$P = (P_{max} + 1) - \sqrt{(\theta - P_{max})^2 + 1}$$

$$\theta = P_{max} + \sqrt{(P_{max} - P + 1)^2 - 1}$$

coordinate transformations

Have frame S $\quad \underline{x} = x_i \underline{e}_i$

" " S' $\quad \underline{x} = x_i' \underline{e}_i'$

Relation:

$$\underline{x} \equiv x_i \underline{e}_i = x_i' \underline{e}_i'$$

$$\underline{e}_j \cdot \underline{x} \equiv x_i \underbrace{\underline{e}_i \cdot \underline{e}_j}_{\delta_{ij}} = (\underline{e}_i' \cdot \underline{e}_j) x_i'$$

$$\therefore \quad x_j = (\underline{e}_j \cdot \underline{e}_i') x_i'$$

Renaming labels:

$$x_i = (\underline{e}_i \cdot \underline{e}_j') x_j'$$

Similarly,

$$x_i' = (\underline{e}_i' \cdot \underline{e}_j) x_j$$

Here we have used the explicitly orthonormal definition of $\underline{e}_i$ & $\underline{e}_i'$ to show that the transformations are the transpose of the other. We could have used the constraint that $\underline{x} \cdot \underline{x}$ is invariant to demonstrate this without reference to basis vectors:

$$x_i' = O_{ij} x_j \Rightarrow x_i' x_i' = O_{ij} O_{ik} x_j x_k = \delta_{jk} x_j x_k$$

$$\Rightarrow O_{ij} O_{ik} = \delta_{jk} \quad \text{ie} \quad \underline{\underline{O}}\,\underline{\underline{O}}^T = \underline{\underline{I}}$$

However, it is very convenient to refer explicitly to basis vectors as this is what we do in code: we always know which basis we are working in.

$$x_i' = O_{ij} x_j$$

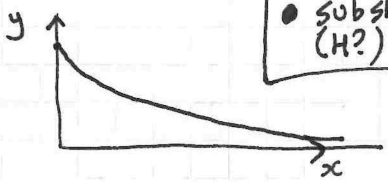
$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} [\underline{e}_1' \text{ in } \underline{e} \rightarrow] \\ [\underline{e}_2' \text{ in } \underline{e} \rightarrow] \\ [\underline{e}_3' \text{ in } \underline{e} \rightarrow] \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$= \left(\begin{bmatrix} \underline{e}_1 \\ \text{in} \\ \underline{e}' \\ \downarrow \end{bmatrix} \begin{bmatrix} \underline{e}_2 \\ \text{in} \\ \underline{e}' \\ \downarrow \end{bmatrix} \begin{bmatrix} \underline{e}_3 \\ \text{in} \\ \underline{e}' \\ \downarrow \end{bmatrix} \right) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

Sampling 23/7/19

- post-doc
- Xtra 15K
- substantive G (H?)

One dimension



$$f(y)\delta y = g(x)\delta x$$

$$\therefore f(y) = g(x)\left|\frac{dx}{dy}\right| \iff g(x) = f(y)\left|\frac{dy}{dx}\right|$$

If have $g(x)$ sample-able, and can write

$y = e^{-x}$ $\Rightarrow$

$\ln y = -x$

$y = [0,1] \Rightarrow x = [\infty, 0]$

$x = -\ln y$

$\frac{dx}{dy} = -\frac{1}{y}$ ✓

$\frac{dy}{dx} = -e^{-x} = -y$

$$\therefore \quad g(x) = f(y)\, e^{-x}$$
$$= f(y)\,.\,y$$

$f(y)$ uniform $\Rightarrow$ $g(x) = e^{-x}$

Sample ~~x~~ y ~~unif~~ $\Rightarrow g(x) = -\ln y$

We want to sample a function ~~g~~ ~~f(x)~~. $g(x)$

~~Suppose we can sample a~~

If $y = y(x)$, then $f(y)$ is ~~defined~~ given by $g(x) = f(y)\left(\frac{dy}{dx}\right)$

if can write ~~f(x)~~ x' as $x'(y)$ then or $g(x) = f(y) \Big/ \left(\frac{dx}{dy}\right)$

$y = e^{-x} \Rightarrow x = -\ln y \Rightarrow x' = -\frac{1}{y}$ $\therefore g(x) = f(y)\,.\,y$

$y = \frac{x^2}{2}$ $y' = x$ $g(x) = f(y)\,.\,x$

$g(x) = \sqrt{2y}$

Sample e^{-y}, then with $y = \frac{x^2}{2}$ $g(x) = x\, e^{-x^2/2}$

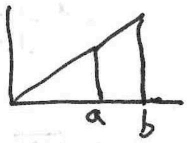
$g(x) = e^{-y}.\sqrt{2y}$

In 2D

[redacted] $f(y_1, y_2)\, \delta y_1 \delta y_2 = g(x_1, x_2)\, \delta x_1 \delta x_2$

$$f(y_1, y_2)\left|\frac{\partial(y_1, y_2)}{\partial(x_1, x_2)}\right| = g(x_1, x_2)$$

annulus



sample btwn a & b

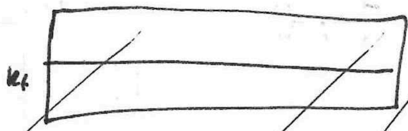
sphere

sample x^2

sample $\sin\theta$

$A(\theta) = \int_0^\theta \sin\xi \, d\xi = (1-\cos\theta)$

1	t_m
2 → 3	y_0, z_0
4	t_{ch}
5 → 7	S
8 → 10	D
11	t_d



object > object if name>

$\phi(v,t)$

A

4	$k_{f\parallel}$
5	k_{fy}
6	k_{fz}

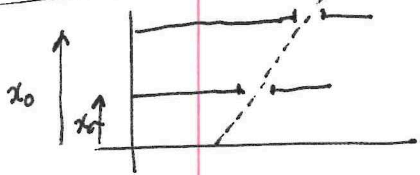
When is a ~~bank~~ det bank > or >, another?

- $n\det_1 > n\det_2$

~~array~~ $a_1 > a_2$

$c_1 > c_2$

8:45 on stand



$$S(n) = \sum_{i=1}^{n-1} \left(\frac{y_i - y_n}{e_i}\right)^2$$

$$S(n+1) = \sum_{i=1}^{n} \left(\frac{y_i - y_{n+1}}{e_i}\right)^2$$

$$= \sum_{i=1}^{n-1} \left(\frac{(y_i - y_n) + (y_n - y_{n+1})}{e_i}\right)^2 + \left(\frac{y_n - y_{n+1}}{e_n}\right)^2$$

$$= \sum_{i=1}^{n-1} \left(\frac{y_i - y_n}{e_i}\right)^2 + 2(y_n - y_{n+1}) \sum_{i=1}^{n-1} \left(\frac{y_i - y_n}{e_i^2}\right) + (y_n - y_{n+1})^2 \sum_{i=1}^{n-1} \frac{1}{e_i^2} + \frac{(y_n - y_{n+1})^2}{e_n^2}$$

$$= \sum_{i=1}^{n-1} \left(\frac{y_i - y_n}{e_i}\right)^2 + 2(y_n - y_{n+1}) \sum_{i=1}^{n-1} \left(\frac{y_i - y_n}{e_i^2}\right)^2$$

$$+ (y_n - y_{n+1})^2 \sum_{i=1}^{n} (1/e_i^2)$$

$$S(n+1) = S(n) + 2\underbrace{(y_n - y_{n+1})}_{-ve} \sum_{i=1}^{n-1} \underbrace{\left(\frac{y_i - y_n}{e_i^2}\right)}_{-ve} + (y_n - y_{n+1})^2 \sum_{i=1}^{n} \left(\frac{1}{e_i^2}\right)$$

So no funny cancellations if iterate $S(n)$

Define $E(n) = \sum_{i=1}^{n} 1/e_i^2$

$$T(n) = \sum_{i=1}^{n-1} \left(\frac{y_n - y_i}{e_i^2}\right) \quad n \geq 2 \quad \text{(note sign change w.r.t sum above)}$$

$$= 0 \quad n = 1$$

$$\Rightarrow \quad S(n) = S(n-1) + 2(y_n - y_{n-1})\, T(n-1) + (y_n - y_{n-1})^2\, E(n-1) \quad (n \geq 2)$$

$$= 0 \quad (n = 1)$$

Can re-express $T(n)$ as a difference:

$$T(n) = \sum_{i=1}^{n-1} \left(\frac{(y_n - y_{n-1}) + (y_{n-1} - y_i)}{e_i^2}\right)$$

$$= \sum_{i=1}^{n-1} \left(\frac{y_{n-1} - y_i}{e_i^2}\right) + \sum_{i=1}^{n-1} \left(\frac{y_n - y_{n-1}}{e_i^2}\right)$$

$$= \sum_{i=1}^{n-2} \left(\frac{y_{n-1} - y_i}{e_i}\right) + (y_n - y_{n-1}) \sum_{i=1}^{n-1} \frac{1}{e_i^2}$$

$$T(n) = T(n-1) + (y_n - y_{n-1})\, E(n-1) \quad (n \geq 2)$$

$$= 0 \quad (n = 1)$$

To summarise:

$$\Delta E(n) = E(n) - E(n-1) = \frac{1}{e_n^2} \quad (n \geq 2)$$

$$E(1) = 1/e_1^2$$

$$\Delta T(n) = T(n) - T(n-1) = (y_n - y_{n-1})\, E(n-1) \quad (n \geq 2)$$

$$T(1) = 0$$

$$\Delta S(n) = S(n) - S(n-1) = 2(y_n - y_{n-1})\, T(n-1) + (y_n - y_{n-1})^2 E(n-1) \quad (n \geq 2)$$

$$S(1) = 0$$