Scherm

ANOTHER TIME OF FLIGHT SPECTROMETER?

or

IN5 bis

A PROPOSAL by

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ANOTHER TIME OF FLIGHT SPECTROMETER

Introduction

1. The high resolution time of flight spectrometer, IN5, is unique amongst I.L.L. instruments, and proposals to the Scientific Council for its use have consistently exceeded time available by a factor of between two and three since the machine began regular operation at the end of 1974. Table I shows the strength of this demand and its distribution according to the Scientific Subcommittees of the I.L.L.

TABLE 1: Requested days on IN5 in the sceduling periods

Subcommittee	March 1975	October 1975	March 1976	October 1976
4 (Excitations)	14	14	14	10
5 (Crystallography)	0	0	0	0
6 (Liquids)	72	96	97	144
7 (Imperfections)	7	36	59	41
8 (Biology)	10	9	32.5	20.5
9 (Physical Chemistry)	194	97	74	71
TOTAL REQUIRED	235	252	276.5	286.5
TOTAL AVAILABLE	139†	71	88	105

† allowed spill over into next period

2. Table 1 illustrates the wide and growing demand for IN5. The demand has continued to increase despite heavy cuts in requested allocations, but it is noticeable that the low availability of time has slackened proposals in some areas. The machine's use can be roughly divided into two categories; that which uses the excellent quasi-elastic energy resolution of ca. 30 μeV when operating at wavelengths between 8 Å and 12 Å, and that which exploits the high intensities available in the peak flux band of wavelengths 4.5 Å to 6 Å whilst tolerating the deteriorated energy resolution ca. 200 μeV.

3. In March 1976 a working group comprising C. Carlile, J. Dianoux, F. Douchin, J. Faudou, R. Lechner, A. Murani, R. Scherm, J. Suck and J. White was set up to examine ways of relieving the overload on IN5. The improvement of IN7 was examined and seen to be desirable in the range of shorter wavelength, but not sufficient in the cold neutron range. Further the possibility of lètting the chopped IN5 beam impinge on a second sample was discussed. This method suffers however from poor performances of the "waste" spectrometer and from the mutual interdependence of the two instruments. It was soon apparent that the best option was to study a new spectrometer for the 4 - 6 Å band with improved resolution compared to IN5 i.e. about 100 μeV and hopefully comparable intensity.

4. To build a replica of IN5 is impossible, first for financial reasons and second because a multichopper requires an end position of a cold guide, which is not available. Therefore only a crystal, static or rotating, can be used to reflect the beam out of an existing neutron guide. In the wavelength band of interest this automatically gives

an energy resolution better than IN5. The problem therefore is to recover as much intensity as possible to match that of IN5.

5. Usually problems tackled on TOF spectrometers allow relaxed resolution in Q and for this, large solid angles are used on the detector side. Unfortunately a neutron guide offers only a small solid angle on the primary side. In our scheme a doubly bent monochromator focusses a large beam area on to a small sample thereby increasing the solid angle to about $3° \times 3°$. This transformation conserves the product of area x solid angle. Since the guide is tall (20 cm) this can be easily achieved in a vertical direction. However, as its width is only 3 cm, we envisage a series of monochromators one behind another projecting adjacent wavelength bands upon the sample./1/ Unfortunately the advantage of the increase in intensity is paid for by worsening of the energy resolution. In order to recover this resolution, it is proposed to use a technique of time focussing.

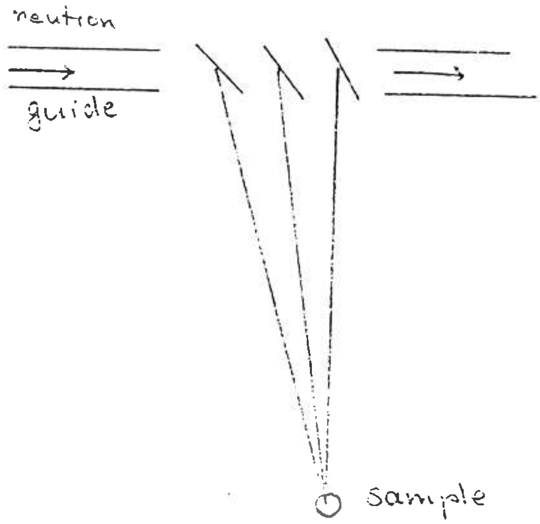

Figure 1: focussing monochromator assembly

6. Principles of Time Focussing

In the method of time focussing, one allows the fast neutrons to start after the slow ones, which are then overtaken by the faster neutrons, at some distance, the "focussing distance" f_{EL}. If the detector is placed at this crossover point, where the neutron burst

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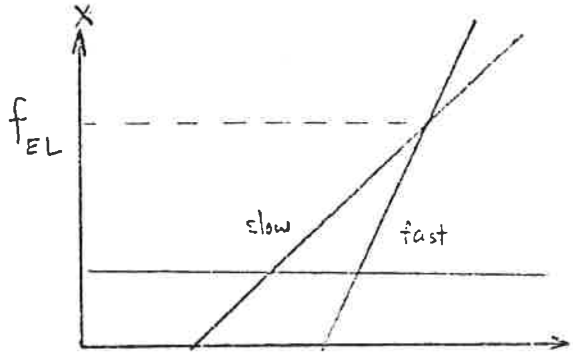
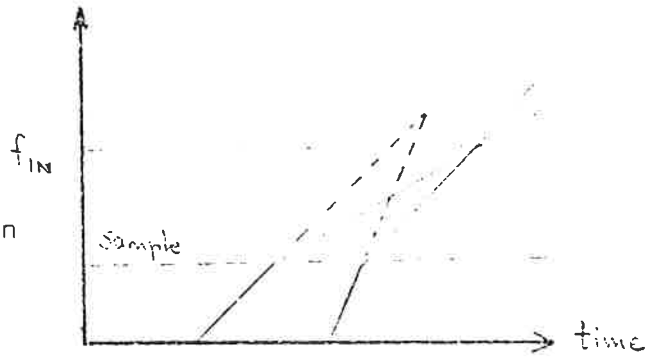
/1/ Maier-Leibnitz: Annales Academiae Scientiarum Fennicae, Series A V1 Physics 267 (1967).

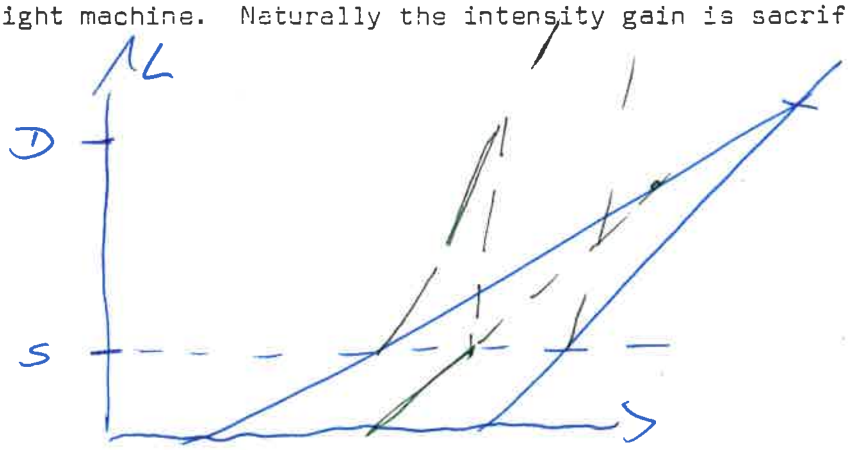
is narrowest, the resolution in energy transfer $\Delta\hbar\omega$ is better than for the in-ident beam. The principle is illustrated in Fig. 2a.



7. The principle can be generalized to inelastic scattering (Fig. 2b). How- ever the time focus is exact for only one chosen energy transfer, but the following analysis will show that this technique gives good resolution for an interesting range of energy transfers in both up and down scattering.



8. The price that must be paid for the intensity increase is that the resolution function becomes complicated. This question is studied in § 16 but as will be seen from the reference design, provision has been made to reduce, by simple means, the instrument to a classical time of flight machine. Naturally the intensity gain is sacrificed by this.



PRINCIPLES OF THE INSTRUMENT

9. Fig. 3 shows schematically the proposed instrument.

distances:

L_{12}	monochr. - chopper
L_{23}	chopper - sample
L_{34}	sample - detector
W	beam width
d_3	sample thickness
d_4	detector thickness
2θ	monochr. take off angle
Φ	scattering angle
ψ	sample orientation
$2\pi\nu$	chopper speed

divergences:

α_1	neutron guide
η	monochromator mosaic
β	chopper collimation
α_2	acceptance angle at sample
λ_I, λ_F	incident, final wavelength
E_I, E_F	incident, final energy
$\hbar\omega = E_I - E_F$	energy transfer

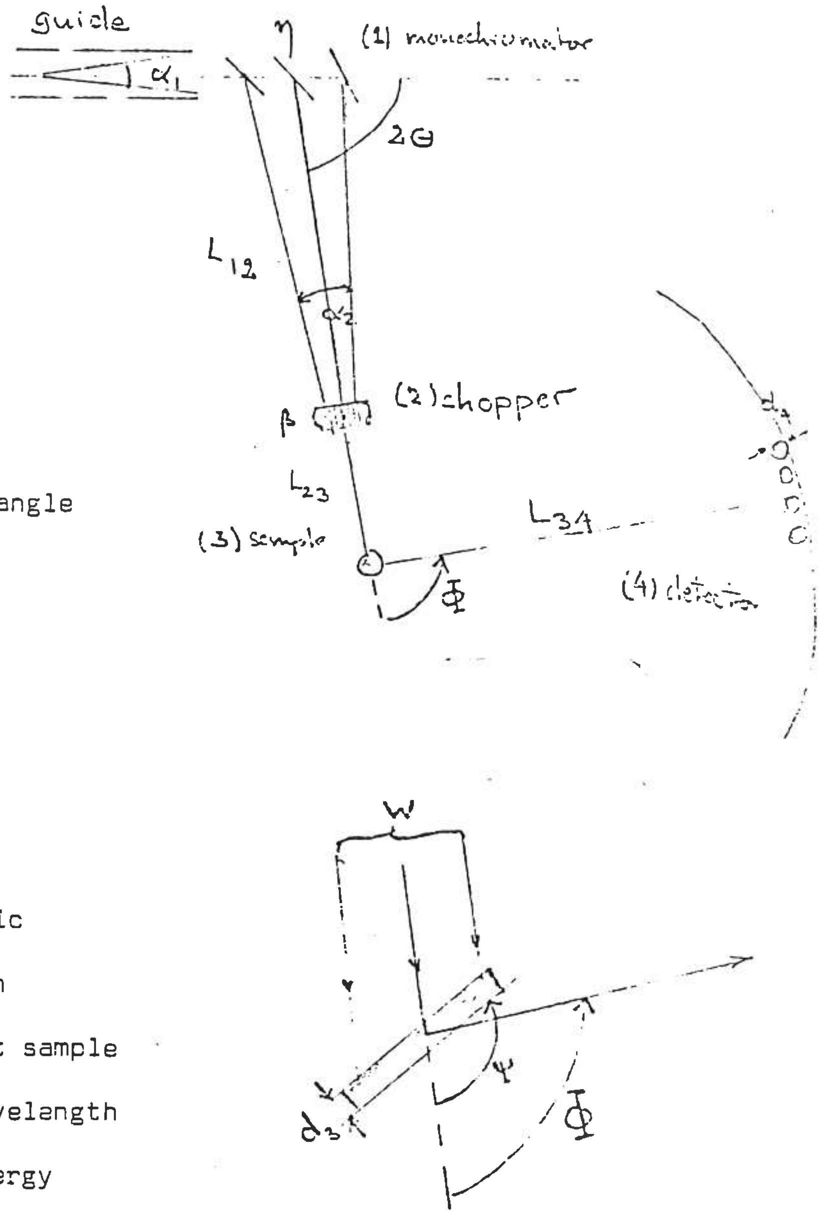


Fig.3 Schematic sketch of the instrument.

10. Elastic Time Focussing

Time focussing techniques are well known from rotating crystal spectrometers /2-5/ . Here both the time dependence of the Bragg angle and the Dopplershift of the neutrons are used to achieve the desired effect. In the method proposed in this paper an analogy to the first effect is used.

The highly collimated beam from a neutron guide is focussed by a crystal system on to the sample (fig. 4). The neutrons in the rays A, B have different directions $2\theta_A$ .. $2\theta_B$ and according to Bragg's Law

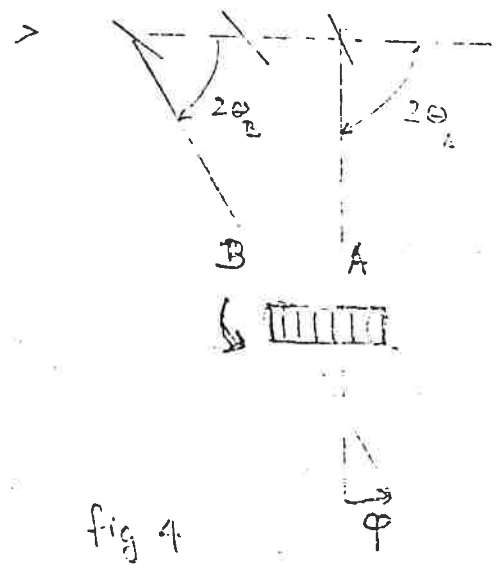


fig 4

$$\lambda = 2\,d \sin\Theta \tag{1}$$

different wavelengths. Let ϕ be the angular difference between rays A and B

$$\varphi = \Delta(2\Theta) = 2\,\Theta_A - 2\,\Theta_B \tag{2}$$

Then the wavelength difference is

$$\Delta\lambda = 2d \cos\Theta \cdot \varphi/2 \tag{3}$$

The flight time for a general distance L is

$$T = C \cdot L \cdot \lambda \tag{4}$$

with the constant C = 252.77 (μsec/meter Å).

/2/ Brockhouse, Inelastic Scattering of Neutrons in Solids and Liquids pp. 113 Vienna:IAEA (1361).
/3/ Carvallio, Ehret, Gläser; Nuclear Instr. and Methods 49, 197 (1967).
/4/ Meister, Weckermann; Neutron Inelastic Scattering, Grenoble IAEA 1972 pp. 713.
/5/ Carlile, Ross J. Appl. Cryst. 8, 292 (1975).

The neutrons "A" are slower than "B". The difference in flight time between them is given by combining (4) and (3)

$$\Delta\tau = C \cdot L \cdot 2d \cos\Theta \cdot \varphi/2 \qquad (5)$$

On the other hand the chopper, rotating with frequency ν lets the "A" beam pass Δt seconds earlier than "B".

$$\Delta\tau = \Delta t$$

$$\Delta t = \varphi/2\pi\nu \qquad (6)$$

$$L\cos\Theta \cdot \cancel{\varphi/2} \sim \frac{\varphi}{2\pi} \cdot \frac{1}{\nu}$$

We define as <u>elastic focussing distance f_{eL}</u> the distance L from the chopper where the faster "B" neutrons overtake the "A"'s, or where the handicap Δt in starting time is just compensated by the difference in flight time $\Delta\tau$. Equating (5) and (6) we obtain;

$$f_{eL} = (2\pi\nu \cdot C \cdot d \cos\Theta)^{-1} \qquad (7)$$

The flight time from the chopper to the crossover point is

$$T_{f_{EL}} = \frac{2 \operatorname{tg}\Theta}{2\pi\nu} \qquad (8)$$

In practice the detector is placed at a fixed distance from the chopper $L_{24} = L_{23} + L_{34}$. To obtain focussing (7) one has to adjust the chopperspeed:

$$\boxed{2\pi\nu = (L_{24} \cdot C \cdot d \cos\Theta)^{-1}} \qquad (9)$$

To get an order of magnitude we take typical values:

$\lambda = 4.5$ Å $\quad E_I = 4$ meV

Graphite 002 $\quad d = 3.355$ Å $\quad \theta = 42.12°$

$L_{24} = 2.6$ metres and so $\nu = 5829$ RPM.

which is technologically quite reasonable.

Time Focussing for Inelastic Scattering

11 We derive now the focussing condition for the general case of inelastic scattering. The energy E of a neutron is related to its wavelength λ by

$$E = \frac{\hbar^2}{2m} \left(\frac{2\pi}{\lambda}\right)^2 \tag{10}$$

For an energy transfer

$$\hbar\omega = E_I - E_F \qquad E_F = E_i - \hbar\omega \tag{11}$$

the wavelength of the scattered neutrons λ_F is $\frac{E_F}{E_i} = \left(1 - \frac{\hbar\omega}{E_i}\right)$

$$\lambda_F = \lambda_I \cdot \left(1 - \frac{\hbar\omega}{E_I}\right)^{-1/2} \quad \left(1 - \frac{\lambda_i}{\lambda_i - \lambda_F}\right) \tag{12}$$

$\frac{\lambda_i}{\left(1 - \frac{\hbar\omega}{E_i}\right)^{2}}$ $\left(1 - \frac{\lambda_i}{\lambda_i^2 - \lambda_F^2}\right)$

The flight time T_{24} from the chopper to the detector is composed of the flight time T_{23} = chopper - sample and T_{34} = sample - detector

$$T_{24} = T_{23} + T_{34}$$

$$= C\left\{L_{23}\lambda_I + L_{34}\lambda_F\right\} \tag{13}$$

inserting (12) leads to

$$T_{24} = \lambda_I \cdot C \left\{ L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-1/2} \right\} \quad ? \tag{14}$$

Differentiating $\frac{\delta T_{24}}{\delta \lambda_I}$ at constant ω ($E_I \sim \frac{1}{\lambda_I^2}$) yields

$$\frac{\partial T_{24}}{\partial \lambda_I} = C \left\{ L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2} \right\} \tag{15}$$

Following the same argument as §10 we combine eqns.(3) and (15) with (6)

$$\Delta\tau = C\left\{L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2}\right\} \cdot 2d\cos\Theta \cdot \varphi/2 = \Delta t = \frac{\varphi}{2\pi\nu} \tag{16}$$

So the focussing condition for inelastic scattering is

$$\left\{L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2}\right\} = \left(2\pi\nu\, C \cdot d \cos\Theta\right)^{-1} \equiv f_{EL} \qquad (17)$$

For $\hbar\omega = 0$ eqn.(17) reduces of course to (9).

To adjust the focussing to the desired energy transfer $\hbar\omega_f$ one can either vary the distances or, which seems more practical, one changes the chopper speed ν at fixed distances L_{23} and L_{24}.

$$2\pi\nu_{foc} = \left[C\, d \cos\Theta \left\{L_{23} + L_{34}\left(1 - \frac{\hbar\omega_f}{E_I}\right)^{-3/2}\right\}\right]^{-1} \qquad (18)$$

Fig.(5) shows the focussing chopper speed ν_{foc} for the "reference design" as function of $\hbar\omega$.

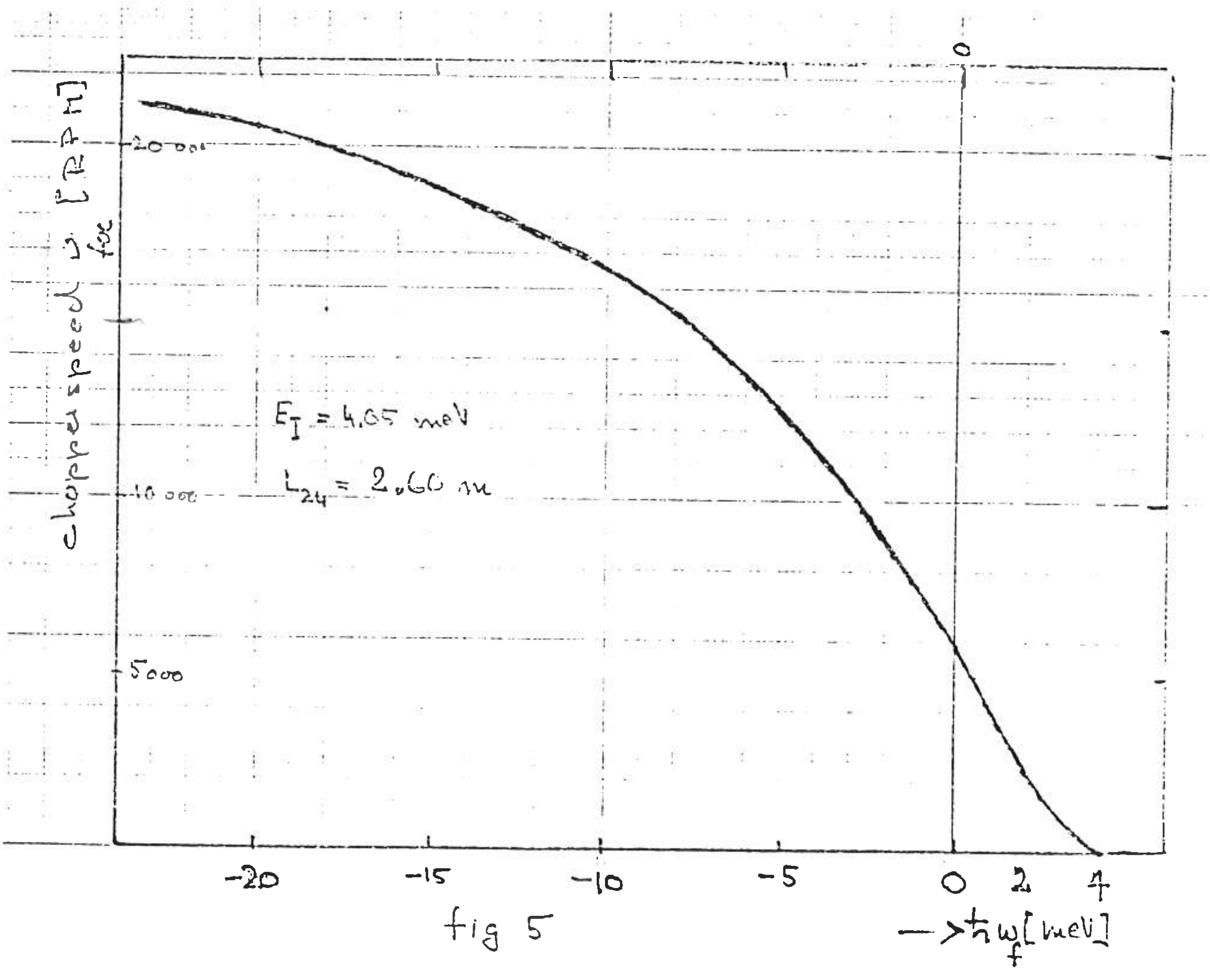


fig 5

RESOLUTION

12 We summarize here the main contributions to the energy resolution of the proposed arrangement. A detailed derivation is given in Appendix I. We label the contributions typical for a classical Fermi chopper instrument (i.e. $\alpha_2 \lesssim \beta$) by using the lower case delta δ, whereas the contribution coming from the extended array of monochromator crystals is indicated by Δ. The classical contributions are:

a) wavelength spread

$$\delta\tau_1 = \sqrt{\alpha_1^2+\beta^2}\cdot C\,\frac{\lambda_I}{2}\,\mathrm{ctg}\,\Theta\left\{L_{23}+L_{34}\left(1-\frac{\hbar\omega}{E_I}\right)^{-3/2}\right\} \quad (19)$$

b) beam width w, sample orientation ψ

$$\delta\tau_{31} = \frac{w}{2\sin\psi}\cdot C\left[\lambda_I\cos\psi - \lambda_F\cos(\psi-\phi)\right] \quad (20)$$

c) sample thickness d_3

$$\delta\tau_{32} = 0.68\,\frac{d_3}{\sin\psi}\,C\left[\lambda_I - \lambda_F\cos\Phi\right] \quad (21)$$

d) detector thickness d_4

$$\delta\tau_4 = C\,\lambda_F\cdot d_4 \quad (22)$$

13 The "nonclassical" contribution from the incident beam spread α_2 is:

$$\Delta\tau_2 = \alpha_2\left[C\,\frac{\lambda_I}{2}\,\mathrm{ctg}\,\Theta\left\{L_{23}+L_{34}\left(1-\frac{\hbar\omega}{E_I}\right)^{-3/2}\right\} - \frac{1}{2\pi\nu}\right] \quad (23)$$

The condition of time focussing eqn.(18) arises when this term is zero and so the resolution of the machine is that of a classical monochromator.

14 For a given λ_I and $\hbar\omega$ and chopper speed ν the resolution is a function of the following instrument parameters:

α_1	guide collimation: $\alpha_1 = 0.13° \times \lambda$ [Å]
β	chopper collimation
w	beam width which depends on the "quality" of the spot focussed on the sample (Appendix II)
d_3	the sample thickness for a plate geometry
d_4	the effective detector thickness
and α_2	the angle subtended by the monochromator at the sample.

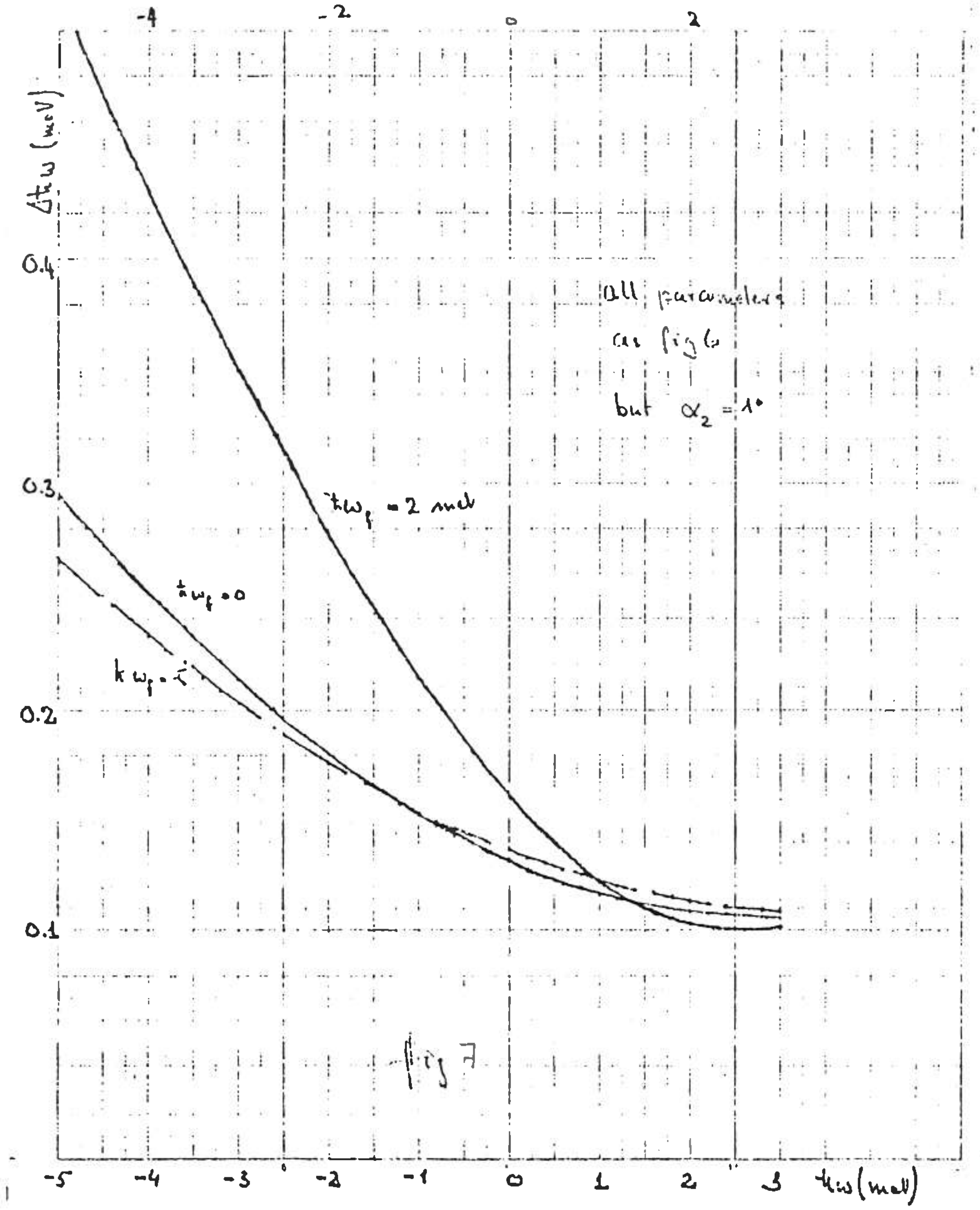
REFERENCE DESIGN

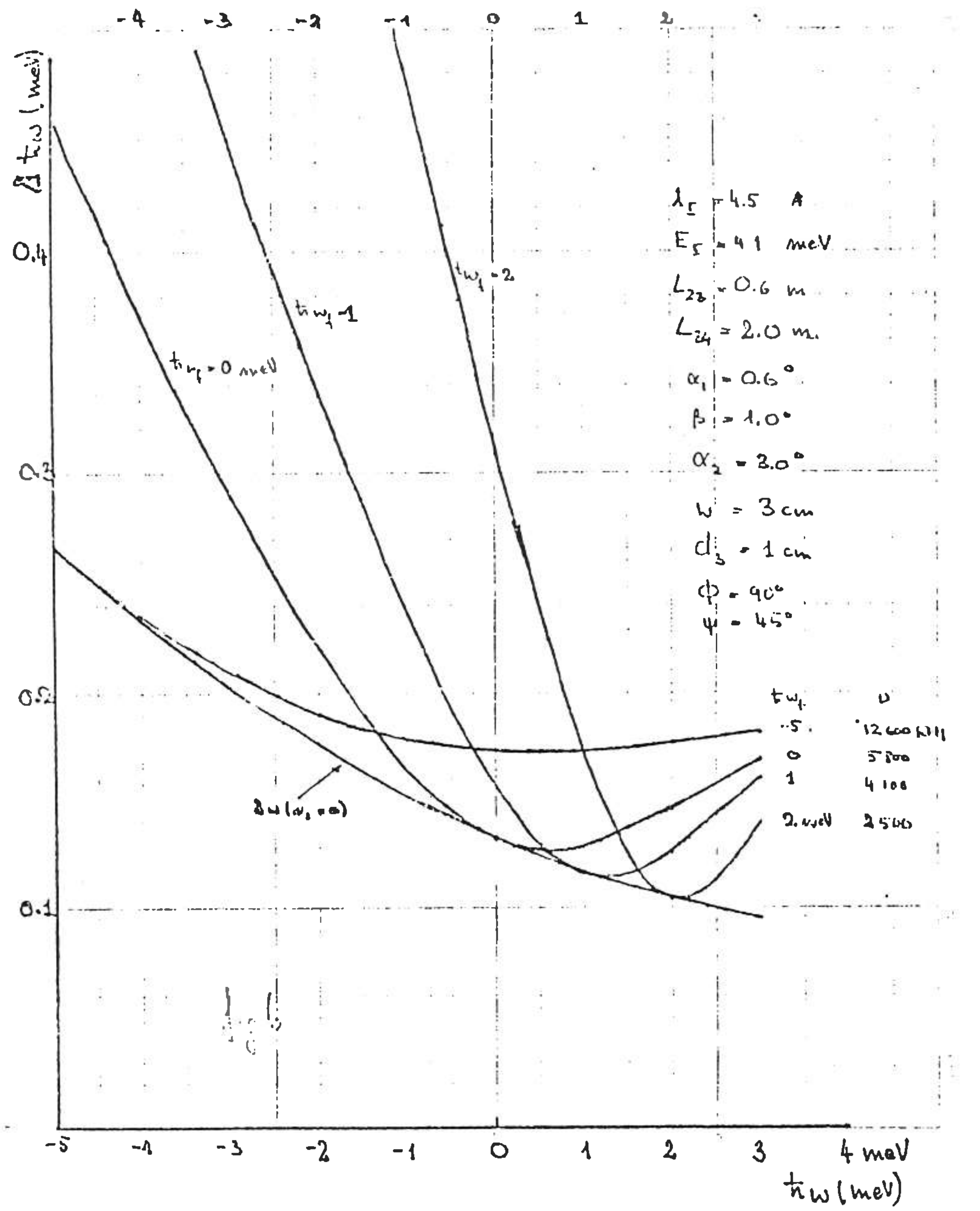
15 In order to make some comparisons with other instruments and to find the sensitivity to the above parameters, we choose a reference set of dimensions and parameters (Table II). They represent a first order approximation to a realistic choice of the spectrometer design. A final layout however necessitates still a more careful optimization.

16 Fig. 6 shows the energy resolution as a function of energy transfer for down and up scattering. The spectrometer parameters are those of Table II with $\alpha_2 = 3°$. The differences correspond to various chopper speeds corresponding to focussing on different energy transfers $\hbar\omega_f$. $\delta\hbar\omega$ denotes the lower limit

TABLE II REFERENCE DESIGN

λ_I	=	4.5 Å	E_I = 4.05 meV
θ	=	42.1°	Bragg angle
ϕ	$\leqslant$	130°	scattering angle
L_{13}	=	1.80 m	distance monochr, - sample
L_{23}	=	0.60 m	distance chopper - sample
L_{34}	=	2.00 m	distance sample - detector
w	=	3 cm	beam width
d_3	=	1 cm	sample thickness
d_4	=	1 cm	detector thickness
α_1	=	0.5°	guide divergence
β	=	1.0°	chopper collimation
α_2	=	3.0°	acceptance angle
$\Delta h\omega$	=	0.132 meV	elastic energy resolution


Δħω (meV)
0.4
0.3
0.2
0.1
-4
-2
0
2
-5
-4
-3
-2
-1
0
1
2
3
ħω (meV)
All parameters
as fig 6
but $\alpha_2 = 1°$
$\hbar\omega_f = 2$ meV
$\hbar\omega_f = 0$
fig 7


Δħω (meV)
0.4
0.3
0.2
0.1
-4
-3
-2
-1
0
1
2
-5
-4
-3
-2
-1
0
1
2
3
4 meV
ħω (meV)
$\lambda_5 = 4.5$ Å
$E_5 = 4.1$ meV
$L_{23} = 0.6$ m
$L_{24} = 2.0$ m.
$\alpha_1 = 0.6°$
$\beta_1 = 1.0°$
$\alpha_2 = 3.0°$
$w = 3$ cm
$d_3 = 1$ cm
$\phi = 90°$
$\psi = 45°$
$\hbar\omega_f = 0$ meV
$\hbar\omega_f = 1$
$\hbar\omega_f = 2$
$\delta\omega(\alpha_1 = 0)$
$\hbar\omega_f$
-.5
0
1
2. meV
12600 RPM
5800
4100
2500
fig 6

with $\alpha_2 = 0$ i.e. the "classical" part. Running the chopper at high speed, i.e. focussing at -5 meV upscattering, gives a rather flat dependence of $\Delta\hbar\omega$ on $\hbar\omega$. In this case the spectrometer works practically as a classical machine with short pulses.

17 In Fig. 7 the effect of reducing the acceptance angle to $\alpha_2 = 1°$ is shown and since the intensity is proportional to α_2 a compromise, adapted to particular experimental needs, can be found which maximises resolution over a given range of energy transfers.

18 Fig. 8 shows the dependence of the quasielastic resolution on incoming wavelength and Fig. 9 shows the same thing as

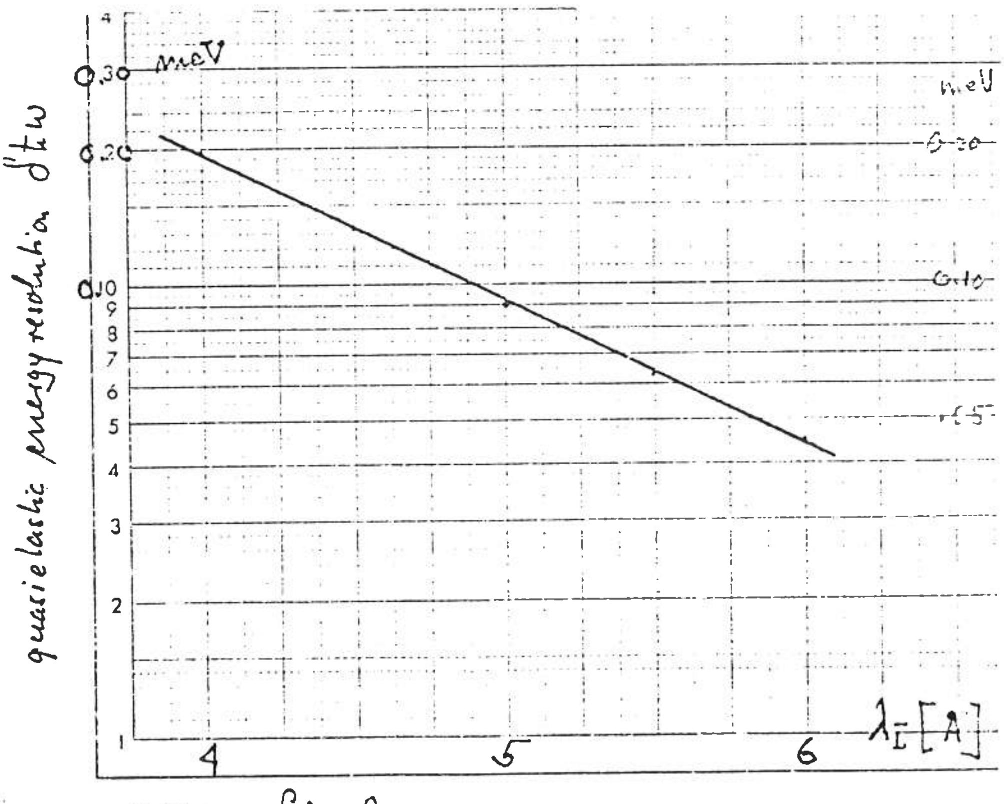


fig 8

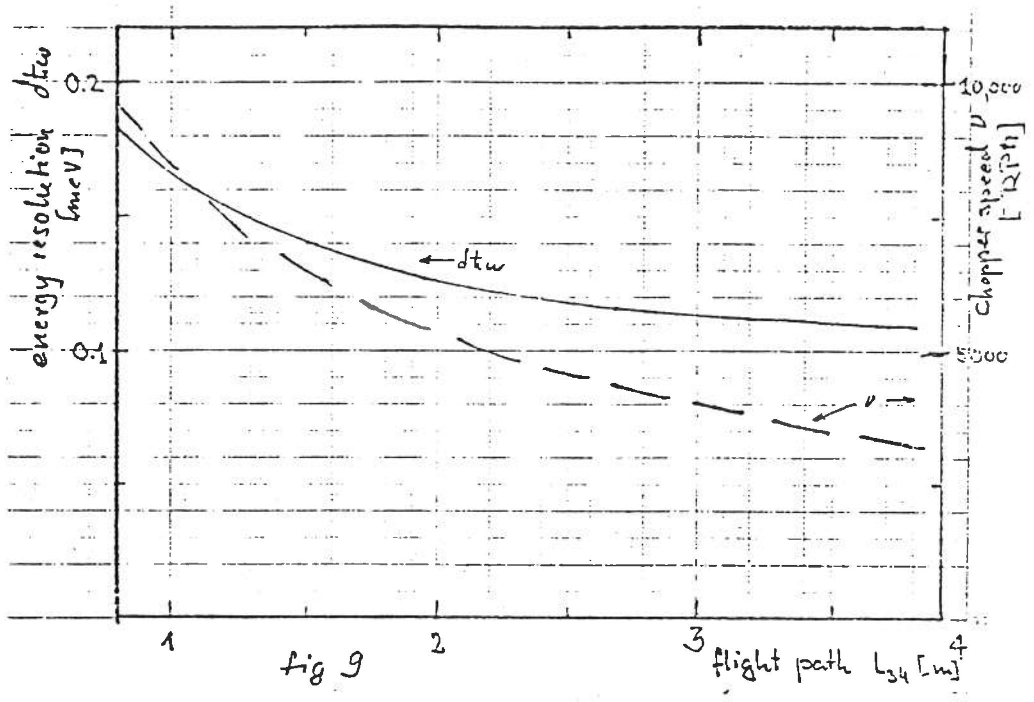


fig 9

a function of detector distance. The slow dependence of resolution of detector distance is due to the correlation (eqn.(9)) between detector distance and chopper speed necessary to fulfil the focussing condition. Thus the scaling of the instrument is determined. Obviously one wishes to go to shortest possible distances but this reduction in size is limited by the maximum speed to which choppers can be run and by characteristic distances such as the detector thickness d_4 and the sample size. This led to the choice of $L_{34} = 2$ m in the reference design. For certain applications chopperspeeds may be low enough to allow short distances to be used and a variable sample-detector distance might be of value.

INTENSITY

19 Intensity calculations have been made in Appendix II leading to estimated counting rates for this spectrometer with $\alpha_2 = 3°$, compared with the "classical" Fermi chopper with $\alpha_2 = 0.6°$, a rotating crystal spectrometer and IN5. The machine parameters corresponding to the reference design) as well as the fluxes at the samples and expected countrates are listed in Table III.

TABLE III

		Foc. Chopper	Fermi Chopper	Rot. Cryst.	IN5	
vertical collimation	α_1	3	3	0.6	0.6	(°)
acceptance angle	α_2	3	0.6	0.6	0.6	(°)
incom. solid angle	$\Delta\Omega_o$	2.7	0.54	0.11	0.11	$\times 10^{-3}$ (sterad)
incident ware uncertainty	$\delta\lambda_o$	5.1	5.1	8.9	11.3	$\times 10^{-2}$ (Å)
loss factor	f_o	0.62	0.74	0.87	1.0	
duty cycle	f_t	6.5	6.5	5.5	15.0	$\times 10^{-3}$
flux on the sample	$\frac{I_o}{F}$	7.5	1.8	0.6	2.5	$\times 10^5$ (1/ cm^{2}sec)
beam area	F	9	9	30	10	(cm)
intensity on the sample	I_o	6.7	1.6	1.9	2.5	$\times 10^6$ $(\frac{1}{sec})$
distance sample-detector	L_{34}	2	2	2	4	(m)
intensity of the detector	$I_D(\Delta E)$ $(\hbar\omega=0)$	994	237	221	203	$(\frac{1}{sec})$
resolution	$\Delta\hbar\omega$ $(\hbar\omega=0)$	0.132	0.132	0.123	0.292	(meV)
chopper speed	ν	5828	5828	9076	10000	(RPM)

One expects the highest intensity at the best resolution from the focussing chopper, provided one restricts oneself to the energy on which the instrument is focussed. The intensity gain comes from the large acceptance angle of $3 \times 3^\circ$ possible with doubly bent monochromators.

20 In order to be able to compare easily the different instruments we adopted most parameters from the "reference design" also for the rotating crystal instrument. Optimising the latter design independently might make its performance somewhat better, but not yet superior to the focussing scheme.

PRACTICAL CONSIDERATIONS

21 Chopper Characteristics

The chopper is assumed to be 120 cms from the monochromating crystals and 60 cms from the sample position. The size of the chopper aperture must therefore be $\sim 4.8 \times 4.8$ cm.

It should be noted that because of the focussing nature of the spectrometer, the chopper must be capable of spinning at several speeds and yet have a high transmission of the incident wavelength neutrons.

Disc choppers must be discounted because they scan through the position of the incident beam rather than its direction and thus would not fulfil the basic principle of the spectrometer if some slight misalignment of the monochromating system existed.

22 Fermi choppers must therefore be considered for the solution. One can consider curved or stright slot choppers. The former suffer the disadvantage that they have a transmission function which is optimised for a given rotational speed, ν at any selected

wavelength λ_T and would be very narrow if one utilises a chopper radius large eneough to avaoid a line of sight through the chopper. Thus one could use a series of choppers each optimised for a given ν and λ_T or one could reduce the radius of the chopper in order to widen the transmission function but thereby risking the possibility of having two pulses - one strong and one weak - per revolution. Neither solution is satisfactory.

The remaining solution is that of a staight slit chopper which is short in the direction of neutron transmission. The transmission of a straight slot chopper is given by Stone and Slovacek [KAPL 1499 (1956)] as:

$$T(\Omega) = 1 - \frac{8}{3}\Omega^2 \qquad 0 \le \Omega \le 1/4$$

$$T(\Omega) = \frac{16}{3}\Omega^{1/2} - 8\Omega + \frac{8}{3}\Omega^2 \qquad 1/4 \le \Omega \le 1$$

$$T(\Omega) = 0 \qquad \Omega > 1$$

where

$$\Omega = \frac{l\,[cm]\ \nu\,[RPM]\ \tau\,(\mu sec/m]}{\beta\,[degrees}$$

with $k = 1.5 \times 10^{-8}$

l = slot length

ν = chopper speed

τ = reciprocal neutron velocity

β = collimation of slot system

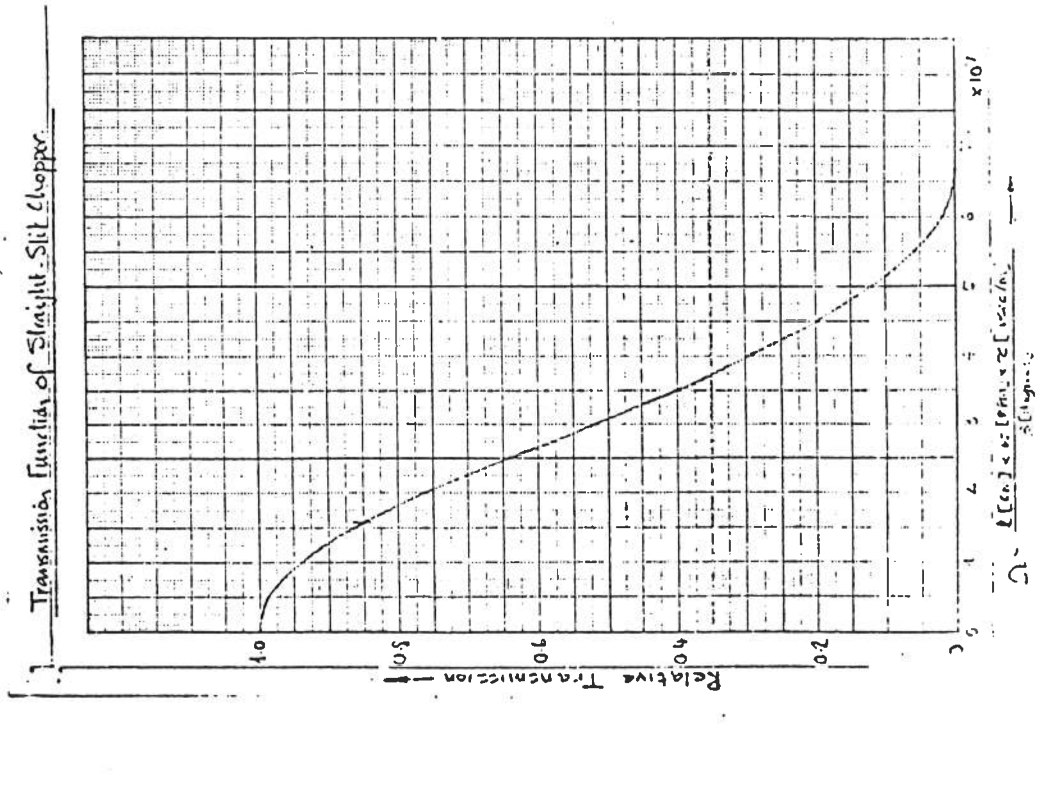
23 A universal transmission function [i.e. $T\nu^{l w \tau}/\beta$] for a straightslit chopper is shown in Fig. 10.

Utilising the values of ν and τ for $\lambda = 4.5$ Å with $\beta = 1°$ and $l = 1$ cm, one obtains from the curve the following values of the transmission of the rotor:

TABLE IV

focussing energy w_t	chopper frequency	"geometrical" transmission	transmission
+ 2 meV	2 471 RPM	0.995	0.76
0	5 829	0.974	0.74
- 2	8 932	0.938	0.70
- 4	11 525	0.896	0.69
- 8	15 299	0.820	0.63

Above approximately - 5 meV the curves for resolution tend to converge at higher energy transfers. There is no point therefore in designing a chopper to focus beyond this value. To realise this chopper it is envisaged building the slot system from pure aluminium of thickness 0.17 mms with gadolmium spaces of thickness 0.025 mms. The transmission at 4.5 Å of 1 cm of aluminium is 0.082 and the ratio of open to total area on the chopper face is 0.872. This loss factor is included in the last column of Table IV.



GUIDE LOSSES

24 In order to reflect a beam out of an existing guide, the guide would have to be interrupted for about 15 cm. The corresponding losses as well as the transmission of graphite crystals in off-reflection are listed below:

transmission due to	λ = 4.5 Å	λ = 10 Å
gap in guide	0.96	0.91
2Al windows	0.98	0.98
Graphite crystals 7 mm) measured	0.98	0.98
total	0.92	0.87

IMPLEMENTATION

25 It is proposed that the spectrometer be built on the H15 guide, before D7, IN10 and D11. The losses to these three instruments being less than 13% can be considered tolerable when one considers the gain of another spectrometer with rather unique characteristics.

The chopper which is a region for development, could be built in-house by Gobert who has already built several high-speed Fermi choppers for Karlsruhe. One could take advantage of the fact that a twin chopper TOF spectrometer is being replaced at Harwell and utilise its detector bank, shielding, detectors and electronics.

The monochromator system would need to be specially designed but this should pose few problems as similar bent monochromator systems have already been built in-house(IN8, IN3). A rough layout is studied in Appendix III.

CONCLUSION

26 A case has been made out for a unique instrument which would enhance the facilities at the I.L.L. to the extent that it would offload many experiments from IN5 (Note that 45% of all experiments on IN5 utilise $\lambda < 6.5$ Å) and perhaps even attract new experiments because of its better resolution for higher Q ranges and higher intensity than IN5.

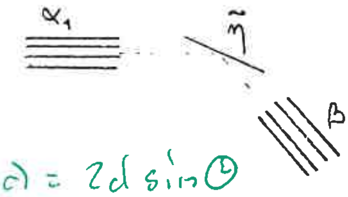
$$\delta f = \left(\frac{\partial^2 f}{\partial x^2} \cdot \delta_x^2 + \frac{\partial^2 f}{\partial y^2} \delta_y^2 + \ldots \right)^{\frac{1}{2}}$$

A P P E N D I X I

RESOLUTION

In the following we derive the basic formulae describing the energy resolution of the spectrometer. This formalism should help to design the machine. For the sake of simplicity we therefore omit higher order effects and regard only the essential contributions.

The wavelength spread:



A static monochromator comprising collimation α, mosaic $\tilde{\eta}$ and collimation β offers neutrons in a wavelength band $\delta\lambda$:

$\lambda = 2d \sin\Theta$

$\frac{d\lambda}{d\Theta} = 2d \cos\Theta = \lambda \cdot \frac{\cos\Theta}{\sin\Theta}$

$$\delta\lambda = \underbrace{\lambda \cdot ctg\,\Theta}_{d\lambda/d\Theta} \cdot \delta\Theta \qquad \text{(A1)}$$

with

$$\delta\Theta = \left(\frac{\alpha_1^2 \tilde{\eta}^2 + \beta^2 \tilde{\eta}^2 + \alpha_1^2 \beta^2}{\alpha_1^2 + \beta^2 + 4\tilde{\eta}^2} \right)^{1/2} \qquad \text{(A2)}$$

$\tilde{\eta}$ means here the width of the angular distribution of reflecting planes i.e. the mosaic spread of a plane crystal. In our case of a curved monochromator assembly we have to include the effect of curving $\frac{\alpha_2}{2}$ as well as the local mosaic η into $\tilde{\eta}$: $\tilde{\eta}^2 = \frac{\alpha_2^2}{4} + \eta^2$.

It is because of the curvature that $\tilde{\eta} \gg \alpha_1$ or β. In this limit eqn. (A2) reduces to

Experiment: 1. + 2. order el. line

$\rightarrow \delta\hbar\omega_1 \simeq 0.06$ meV $\quad \hbar\omega_1 = 0$

$\delta\hbar\omega_2 \simeq 0.93$ meV $\quad \hbar\omega_2 \simeq 14.8$ meV

$$\delta\Theta = \frac{1}{2}\sqrt{\alpha_1^2 + \beta^2} \quad \text{for } \tilde{\eta} > \alpha_1, \beta \tag{A3}$$

It isinteresting to note that we obtain the same result $\delta\theta = \sqrt{\frac{\alpha^2}{2}}$ from (A2) in the limit $\alpha_1 = \beta$ for any $\tilde{\eta}$. So the wavelength spread passing the static chopper is

$$\delta\lambda = \lambda_I \cdot \mathrm{ctg}\,\Theta \cdot \frac{1}{2}\sqrt{\alpha_1^2 + \beta^2} \tag{A4}$$

independent of the mosaic. The local mosaic spread has to be chosen carefully to give maximum intensity (Appendix III).

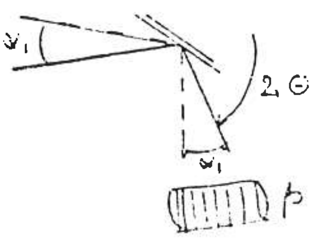
To calculate the energy resolution we calculate pulse width at the detector for a given inelastic process with energy transfer $\hbar\omega$. Using eqn. (15) the time spread due to the wavelength $\delta\lambda$ is:

$$\delta\tau_1 = C\left\{L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2}\right\} \cdot \delta\lambda \tag{A5}$$

insert (A4)

$$\delta\tau_1 = \sqrt{\alpha_1^2+\beta^2} \cdot C \cdot \frac{\lambda_I}{2} \cdot \mathrm{ctg}\,\Theta \left\{L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2}\right\} \tag{A6}$$

Further we may define the <u>sweeptime $\delta\tau_2$</u> as the duration of the pulse of strictly monochromatic neutrons at the location of the chopper. 2θ being well-defined, these neutrons have an angular distribution of α_1 provided $\eta > \alpha_{1/2}$. The monochromatic sweeptime is then:



$$\delta\tau_2 = \frac{\sqrt{\alpha_1^2 + \beta^2}}{2\pi\nu} \tag{A7}$$

ν = chopper speed

The chopper speed ν is still a free parameter. If we request time focussing just for the energy transfer $\hbar\omega_F$ under consideration we insert (18) into (A7) and get

$$\delta\tau_2 = C\cdot d \cos\Theta \left\{ L_{23} + L_{34}\left(1 - \frac{\hbar\omega_F}{E_I}\right)^{-3/2} \right\} \sqrt{\alpha_1^2 + \beta^2} \qquad (A8)$$

or

$$\delta\tau_2 \geq \delta\tau_1 \quad !!$$

The static or, what is the same, the instantaneous λ-resolution is identical to the burst time of monochromatic neutrons . That is the reason why only one of them, $\delta\tau_1$ and not $\delta\tau_2$ contributes to the final resolution eqn. (A12).

<u>The sample size $\delta\tau_3$.</u>

A very thin plate is oriented at the angle ψ with resp... beam. Le... w. The pulse width at the detector caused by the path difference between left and right is /5/

$$\delta\tau_{3_1} = \frac{W}{2\sin\psi}\left[\frac{\cos\psi}{v_I} - \frac{\cos(\psi-\phi)}{v_F}\right] \qquad (A9)$$

$\delta\tau_{3_1} = 0$ for symmetric reflection geometry $\psi = \frac{\phi}{2}$ in the case of elastic scattering.

/5/ Carlile, Ross see page 6.

The thickness d_3 of the sample plate adds another contribution:

$$\delta\tau_{32} = 0.68 \frac{d_3}{\sin\psi}\left[\frac{1}{v_I} - \frac{\cos\phi}{v_F}\right] \qquad \text{(A10)}$$

The factor 0.68 is introduced to describe the fact that the sample thickness is a rectangular distribution rather than a Gaussian.

Detector thickness d_4

$$\delta\tau_4 = C \cdot \lambda_F \cdot d_4 \qquad \text{(A11)}$$

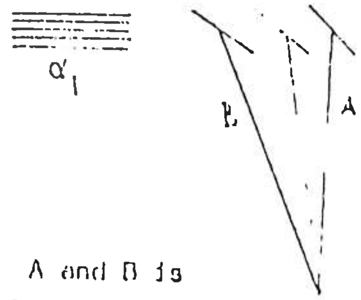
It is worth mentioning that the effective detector thickness is a function of λ_F so that in first order, $\delta\tau_4$ is a constant rather than $\alpha\lambda_F$.

In the case of perfect time focussing i.e. if eqn.(13) is fulfilled, the pulsewidth at the detector is then:

$$\delta\tau^2 = \delta\tau_1^2 + \delta\tau_{31}^2 + \delta\tau_{32}^2 + \delta\tau_4^2 \qquad \text{(A12)}$$

MISMATCH OF TIME FOCUSSING $\Delta\tau$

We now calculate the pulse width at the detector coming from an inelastic process $\hbar\omega \neq \hbar\omega_f$, the focussed energy transfer. We start from the assumption that both the guide collimation α_1 and the chopper collimation β are small compared with the acceptance angle α_2, offered by the monochromator assembly



$$\alpha_2 > \alpha_1, \beta$$

The wavelength variation between ray A and B is

$$\Delta\lambda = \lambda_A - \lambda_B = \lambda_I \cdot \mathrm{ctg}\,\Theta \quad \frac{\alpha_2}{2} \qquad \text{(A13)}$$

Analog to (A6) this leads to a difference of flight time

$$\Delta T = \frac{\alpha_2}{2} \cdot C \cdot \lambda_I \cdot \mathrm{ctg}\,\Theta \left\{ L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2} \right\} \qquad \text{(A14)}$$

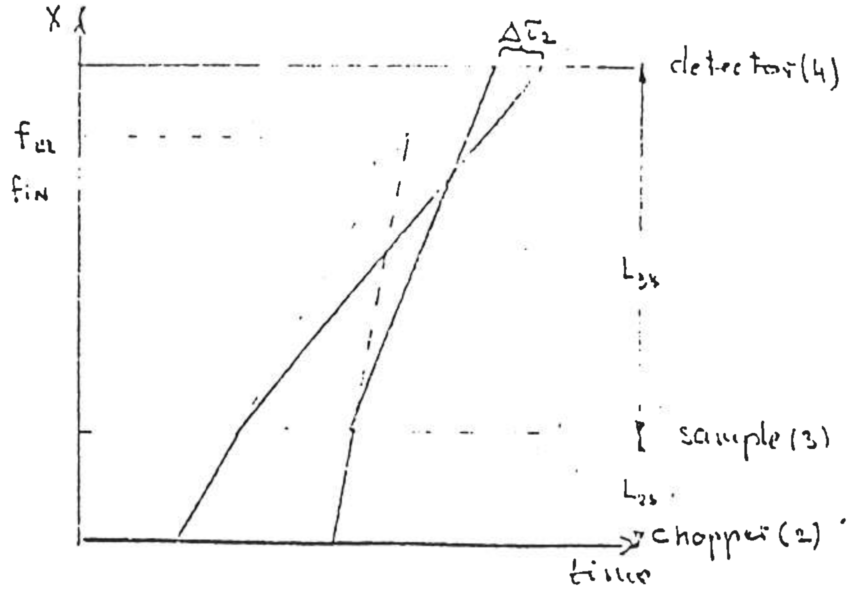
This, however, is more or less compensated by the difference in start time at the chopper spinning at the speed ν

$$\Delta t = \frac{\alpha_2}{2\pi\nu} \qquad \text{(A15)}$$

to give $\Delta\tau = \Delta T - \Delta t$

$$\Delta\tau_2 = \alpha_2 \left[C \frac{\lambda_I}{2} \mathrm{ctg}\,\Theta \left\{ L_{23} + L_{34}\left(1 - \frac{\hbar\omega}{E_I}\right)^{-3/2} \right\} - \frac{1}{2\pi\nu} \right] \qquad \text{(A16)}$$

Setting $\Delta\tau = 0$ immediately gives the focussing condition (18), or (9) for the case of elastic scattering.



Finally the pulse width at the detector is given as the sum of the squares of the individual contributions:

$$\Delta\tau^2 = \delta\tau_1^2 + \delta\tau_{31}^2 + \delta\tau_{32}^2 + \delta\tau_4^2 + \Delta\tau_2^2 \qquad \text{(A17)}$$

It should be mentioned that this result was derived with the following approximations: a) no distinction was made between Gaussian and rectangular distributions. The contributions $\delta\tau_3$ and $\Delta\tau_2$ are probably more rectangular. This can be accounted for by multiplying them by 0.68 . b) The formalism fails in the limit $\alpha_2 \leqslant \beta$. c) The sample width term $\delta\tau_{31}$ was taken to be uncorrelated with $\delta\tau_1$. Meister (private communication) pointed out that in fact the left and righthand sides of the sample correspond to different path lengths as given in (A9) but they see as well different wavelengths coming from one small spot of the monochromator. This effect tends to be unimportant in the case of exact focussing. However it needs to be included in a more rigorous treatment.

APPENDIX II.

INTENSITY CALCULATION

In the comparison of different types of TOF instruments, intensity considerations are important in connection with a given resolution. We compared the focussing chopper with a Fermi chopper and a rotating cyrstal TOF spectrometer. Both chopper instruments offer the advantage of the use of crystals bent vertically to the scattering plane.

The number of neutrons/sec. with energies in the interval ΔE_F counted in the detector is given by (e.g. Gläser et al. 1967):

$$\Delta I = \frac{\partial^2 \phi}{\partial \Omega_I \partial \lambda_I} \cdot \Delta\Omega_I \cdot \delta\lambda_I \cdot f_I \cdot f_t \cdot F \left[N d_3 \frac{\sigma}{4\pi} \frac{k_I}{k_F} e^{-\frac{\hbar\omega}{2kT}} \tilde{S}(Q,\omega) \right] \cdot d\Omega_F \cdot f \cdot \Delta E_F \qquad \text{(A18)}$$

$\frac{\delta^2 \phi}{\delta\Omega\delta\lambda}$	Flux in the cold neutron guide (1.35 $10^{12} \left[\frac{1}{\text{sterad cm}^2 \text{sec Å}}\right]$)
$\Delta\Omega_I \Delta\Omega_F$	incoming and outgoing solid angle seen from the sample
f_I	attentuation factor between neturon source and sample (cut in neutron guide, crystal reflectivity, chopper transmission)
f_t	duty cycle
F	sample area
N	number density of sample
σ	scattering cross section of sample material
$\tilde{S}(Q,\omega)$	symmetrized scattering law
f	attenuation factor between sample and detector (efficiency, attenuation on the flight path).

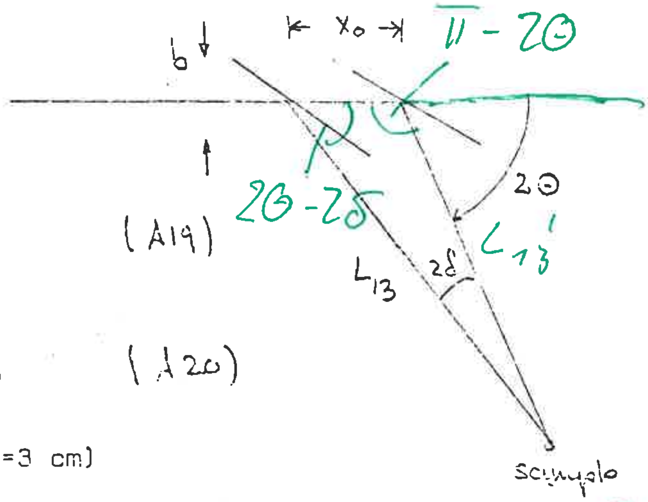
Except for the monchromators, the calculations were performed for identical spectrometers at a cold neutron guide position. 1 m^2 He^3 detectors with a mean efficiency of 0.9 were assumed to be installed at a distance of 2 m from a 3 cm wide and 1 cm thick sample with $0.01 \cdot 10^{24}$ atoms/cm^3 and a scattering cross section of 6.2 barn. For the rotating crystal a radius of 1.3 cm and a mosaic spread of 0.8° was assumed, and for the chopper a transmission of 0.75. All other parameters are identical to the ones of the resolution calculations. Focussing on $\hbar\omega = 0$ and two pulses per revolution were taken into account. The scattering law of the sample was assumed to be $\tilde{S}(q,\omega) = 1(1/\mathrm{meV})$, so that the results must be multiplied by the value of the symmetrized scattering law to get the final intensity expected from the sample. For the energy interval ΔE_F the resolution width was taken, so that one has to multiply the results by $\Delta E(\mathrm{Channel})/\Delta E_F$ (resolution) to get the number of counts in one time channel summed over all detectors.

The calculated intensities for the differents spectrometers are compared with values calculated for IN5 in Table III in §19.

$\frac{x_0}{\sin 2\delta} = \frac{L_{13}}{\sin(\pi - 2\Theta)}$ $\frac{L_{13}'}{\sin(2\Theta - 2\delta)}$

APPENDIX III

The Monochromator Assembly



Geometrically

$$\frac{x_0}{L_{13}} = \frac{\sin 2\delta}{\sin(\pi - 2\Theta - 2\delta)} \qquad (A19)$$

or

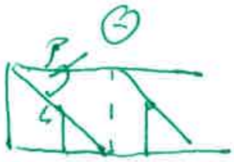
$$\delta \approx \frac{x_0}{2L_{13}} \cdot \sin 2\Theta \qquad (A20)$$

designating the guide width b(=3 cm)

we get

$$x_0 = b \cdot ctg\,\Theta \qquad \frac{x_0}{b} = \frac{\cos\Theta}{\sin\Theta} \qquad (A21)$$

$$\delta = \frac{b}{2L_{13}} \cdot ctg\,\Theta \cdot \sin 2\Theta$$



$\cos\Theta = \frac{P}{...}$ x_0

$\sin\Theta = 3/L$ $P = x_0$

The second crystal can only fully reflect if the first one has

not yet removed the corresponding wavelength of the beam i.e.

$$\eta \leq \delta$$

$2d \sin\vartheta = \lambda$

In the case of $\eta = \delta$ the

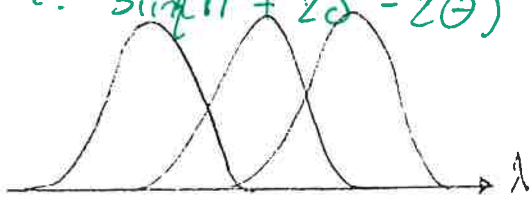
1. $\sin(\Theta \pm \eta) = \Delta\lambda$

successive cystals reflect

2. $\sin(\pi + 2\delta - 2\Theta)$

just adjacent wavelength

bands.



On the other hand it is essentially the mosaic which determines

the size of the spot in the focus

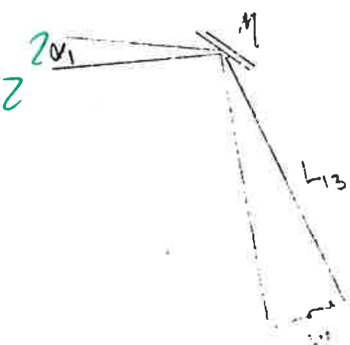
$$W = L_{13} \cdot \sqrt{\alpha_1^2 + 4\eta^2} \qquad (A22)$$

this might lead to

$\frac{W^2}{L_{13}^2} = \alpha_1^2 + 4\eta^2$

the request

$$\eta < \delta$$



Assuming $\eta = \delta$ substitute (A21) in (A22) to get the beam width

$$W = \left(L_{13}^2 \, \alpha_1^2 + (b \, \mathrm{ctg}\,\Theta \cdot \sin 2\Theta)^2 \right)^{1/2} \qquad (A23)$$

In the vertical direction simply α_1 and $2\eta.\sin\theta$ are responsible for the finite height h of the focussed spot

$$h = L_{13} \sqrt{\alpha_1^2 + 4\eta^2 \sin^2\Theta} \qquad (A\,24)$$

In numbers:

$\lambda_I = 4.5$ Å	$\theta = 42°$	
$L_{13} = 180$ cm	$\alpha_1 = 0.6°$	$b = 3$ cm

yields:

length of 3 crystals	$3X_0 = 10$ cm
mosaic	$\eta = 0.53°$
beam width	$w = 3.8$ cm
beam height	$h = 2.9$ cm