

Time-of-flight and backscattering neutron spectrometers

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Orphée reactor : 14 MW D₂0 moderated reactor





T. Perrin



R. Pynn





TOF and BS



Principle of inelastic neutron scattering



Quasi-elastic or inelastic scattering experiment:

- Measure the number scattered of neutrons as a function of \vec{Q} and ω ($\hbar\omega \approx 0.01$ to few meV, Q ≈ 0.05 to few Å⁻¹)
- The aim is to extract from the measure the dynamical structure factor S(Q,ω) which depends on the properties of the sample *only* (microscopic structure and dynamics)
- Time-of-flight techniques : TOF-TOF, cristal-TOF (TOF-cristal) and backscattering spectrometers

Neutrons

Mass : $m_N = 1.675 \ 10^{-27} \text{ kg}$ Charge=0; s=1/2; $\gamma = -2913 \ 2\pi \text{ (Gs)}^{-1}$

$$E = \frac{\hbar k^2}{2m} = \frac{1}{2}mv^2$$

Neutrons

Mass : m_N =1.675 10⁻²⁷ kg Charge=0; s=1/2; γ =-2913 2 π (Gs)⁻¹

$$E = \frac{\hbar k^2}{2m} = \frac{1}{2}mv^2 \quad v = \frac{d}{t} \approx \frac{3950}{\lambda(\text{\AA})}m.s^{-1}$$

 $\lambda = 5 \text{\AA} \quad \mathbf{V} \approx 800 \ \mathbf{ms}^{-1}$ $\lambda = 10 \text{\AA} \quad \mathbf{V} \approx 400 \ \mathbf{ms}^{-1}$





Same scattering angle : different wavevectors Q (and energy)

Energy – wavevector plot



Energy – wavevector plot









IN5 Xcrystal mode Full S(Q,ω) in 2 days

« However »

One λ One T One H

S. Petit, et al



V. Simonet, R. Ballou, unpublished results obtained on IN5 on Ba₃NbFe₃Si₂O₁₄ (BNFS) Measured quantity : double differential cross section

Number of neutrons per unit of time dt and solid angle $d\Omega$

 $\frac{\partial \sigma}{\partial \Omega \partial t}$

Measured quantity : double differential cross section

Number of neutrons per unit of time dt and solid angle $d\Omega$

$$\frac{\partial^2 \sigma}{\partial \Omega \partial t} \rightarrow \frac{\partial^2 \sigma}{\partial \Omega \partial \omega} = N \frac{k_f}{k_i} \frac{\sigma}{4\pi} S(Q, \omega)$$

$$TOF \rightarrow Energy$$



- 5 Å v≈800 m.s⁻¹ TOF of a few msec
- repetition rates

50-150 Hz Depending on λ and $\Delta\lambda$

Direct chopper spectrometer: TOF-TOF (reactor time - distance diagram based) Δλ d detector -sd Sample **└**ms M-chop ∟ pm P-chop ▶ time

Chopper system versus cristal monochromatisation

- No high order
- Clean and well-defined shape
- Tunable resolution
- 100% transmission at the centerline

5 Å v≈800 m.s⁻¹ TOF of a few msec

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50-150 Hz Depending on λ and $\Delta\lambda$

time - distance diagram



time - distance diagram



time - distance diagram

Time overlap

d



time - distance diagram



Direct chopper spectrometer: TOF-TOF







Energy Resolution (R.E. Lechner)





Hypothesis of non correlated variables : δ

$$\partial \hbar \omega = \left[\sum_{i} \left(\frac{\partial \hbar \omega}{\partial t_{i}}\right)^{2} \delta t_{i}^{2}\right]^{\frac{1}{2}}$$





Hypothesis of non correlated variables : δ

4

$$\delta\hbar\omega = \left[\sum_{i} \left(\frac{\partial\hbar\omega}{\partial t_{i}}\right)^{2} \delta t_{i}^{2}\right]^{\frac{1}{2}}$$

$$l_m - l_p = \alpha L_{pm} \lambda_i$$

$$t_d - t_m = \alpha (L_{ms} \lambda_i + L_{sd} \lambda_f)$$

$$t_d - t_s = \alpha L_{sd} \lambda_f$$

+ - 1)

$$\delta\hbar\omega = \frac{m}{\alpha^{3}L_{pm}L_{sd}\lambda_{f}^{3}} \begin{bmatrix} L_{ms} + L_{sd}\left(\frac{\lambda_{f}}{\lambda_{i}}\right)^{3} \right]^{2} \tau_{p}^{2} + \\ L_{pm} + L_{ms} + L_{sd}\left(\frac{\lambda_{f}}{\lambda_{i}}\right)^{3} \right] \tau_{m}^{2} + \\ L_{pm}^{2}\delta t_{d}^{2} \end{bmatrix}$$

Hypothesis of non correlated variables :

$$\delta\hbar\omega = \left[\sum_{i} \left(\frac{\partial\hbar\omega}{\partial t_{i}}\right)^{2} \delta t_{i}^{2}\right]^{\frac{1}{2}}$$

 $t_m - t_p = \alpha L_{pm} \lambda_i$ Time opening of the pulsing chopper $t_d - t_m = \alpha (L_m \lambda_i + L_{sd} \lambda_f)$ $t_{d} - t_{s} = \alpha L_{sd} \lambda_{f}$ $\delta\hbar\omega = \frac{m}{\alpha^{3}L_{pm}L_{sd}\lambda_{f}^{3}} \begin{bmatrix} L_{pm} + L_{sd}\left(\frac{\lambda_{f}}{\lambda_{i}}\right)^{3} (\tau_{p}^{2} + \tau_{p}^{2}) \\ L_{pm} + L_{ms} + L_{sd}\left(\frac{\lambda_{f}}{\lambda_{i}}\right)^{3} (\tau_{m}^{2} + \tau_{m}^{2}) \\ L_{pm}^{2} (\lambda_{i}^{2} - \tau_{m}^{2}) \end{bmatrix}$

Hypothesis of non correlated variables : $\delta\hbar$

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+ - 1)

Time opening of the monochromating chopper

$$\delta\hbar\omega = \frac{m}{\alpha^{3}L_{pm}L_{sd}\lambda_{f}^{3}} \begin{bmatrix} L_{ms} + L_{sd}\left(\frac{\lambda_{f}}{\lambda_{i}}\right)^{3} \right]^{2} \tau_{p}^{2} + \\ L_{pm} + L_{ms} + L_{sd}\left(\frac{\lambda_{f}}{\lambda_{i}}\right)^{3} \tau_{m}^{2} \\ L_{pm}^{2} \delta t_{d}^{2} \end{bmatrix}^{2}$$

Hypothesis of non correlated variables : δ

$$\delta\hbar\omega = \left[\sum_{i} \left(\frac{\partial\hbar\omega}{\partial t_{i}}\right)^{2} \delta t_{i}^{2}\right]^{\frac{1}{2}}$$

$$t_{d} - t_{m} = \alpha (L_{ms}\lambda_{i} + L_{sd}\lambda_{f})$$
$$t_{d} - t_{s} = \alpha L_{sd}\lambda_{f}$$

 $t - t = \alpha I - \lambda$

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Resolution : convolution of 3 uncertainties



IN5

$$\delta\hbar\omega = \frac{m}{\alpha^3 L_{sd}\lambda_f^3} \begin{bmatrix} \delta t_p^2 + \\ \delta t_m^2 + \\ \delta t_d^2 \end{bmatrix}^{\frac{1}{2}}$$

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• The spraid δt_p at the detector due to the pulsing chopper (τ_p)



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$$\delta t_{L} = \alpha \lambda \delta L_{sd}$$
$$\delta L_{sd} \approx \delta L_{s} + \delta L_{d}$$
$$\uparrow$$
$$2 \text{ cm} 2 \text{ cm}$$

 $\Delta \hbar \omega \approx 100 \mu \text{ev } @ \lambda = 5 \text{\AA}$ $\frac{\delta \lambda}{\lambda} \approx 1.5 - 2\%$

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Δħω≈100μev @ λ=5Å
$$\frac{\delta\lambda}{\lambda} ≈ 1.5 - 2\%$$

Keep the possibility to have $\frac{\delta \lambda}{\lambda} \approx 1\%$ $\frac{\delta L_{sd}}{L_{sd}} \approx 1\%$ $L_{sd} \approx 4m$

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Direct chopper spectrometer: TOF-TOF Energy dependence of the resolution



J. Ollivier and J.-M. Zanotti

ESS a 5MW spallation source with 14 Hz and a PW=2.86 ms



K. Anderson (2011), ESS

ESS a 5MW spallation source with 14 Hz and a PW=2.86 ms





 $70 \text{ ms} \approx 1/14 \text{Hz}$

14 Hz (source) versus 50-150 Hz (TOF spectroscopy)

Repetition Rate Multiplication (RRM) = Multi wavelength mode



14 Hz (source) versus 50-150 Hz (TOF spectroscopy)

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Optimized spectrometer @LPSS (ESS)











C-Spec layout





Instrument performance

Estimation of Flux values from McStas (single energy mode)

Chopper and guide settings		Flux ($\lambda_0 = 4 \text{ Å}$)	Flux (λ ₀ = 5 Å)	Flux ($\lambda_0 = 9 \text{ Å}$)	to compare with:
		[n /(s cm ²)]	[n /(s cm²)]	[n /(s cm ²)]	[n /(s cm²)]
N ₁ = 7.5, N ₂ = 10	standard	7.09 [.] 10 ⁶	5.7·10 ⁶	1.49 [.] 10 ⁶	IN5: 6.38·10⁵ (at 5 Å)
	focus	1.68 [.] 10 ⁷	9.4·10 ⁶	1.30 [.] 10 ⁶	TOFTOF: 1.14 10 ⁵ (at 5 Å)
N ₁ = 13.5, N ₂ = 24	standard	2.58·10 ⁶	1.75·10 ⁶	4.97·10 ⁵	LET:5.6 10 ⁴ (at 4 Å)
	focus	5.24 · 10 ⁶	2.98·10 ⁶	4.17·10 ⁵	IN5: 7 10 ⁴ (at 4 Å)

gain factor ~10

Summary C-Spec

	cold source	
	151.4 m	
	≤ 2 Å	
	1.5 – 15 Å	
40 μeV – 170 μeV @ 5Å		
	2 – 7 μeV @ 15 Å	
@ 2 Å: 0.32 – 5.90 Å ⁻¹		
	@ 5 Å: 0.13 – 2.36 Å ⁻¹	
	@ 10 Å: 0.066 – 1.18 Å ⁻¹	
	@ 15 Å: 0.044 – 0.78 Å ⁻¹	
5 Å:	5.7 ·10 ⁶ neutrons /(s cm ²), standard	
	5 Å: 9.4 \cdot 10 ⁶ neutrons /(s cm ²), focus	
standard: 40 x 20 mm ²		
	focus: 10 x 10 mm ²	
	+/- 1 deg	
	4 m	
¹⁰ B converter layers or Helium		
	-30 to 140 deg	
	40 μeV – 1 @ 2 Å: 0.3 5 Å: standard: 4	




IN6 type : 3 single cristals, time focusing (different wavelength arrive together at the detector)





IN6 type : time focusing @ $\hbar\omega \neq 0$



IN6 type : time focusing @ $\hbar\omega \neq 0$



Focus type (PSI-SINQ)



(IRIS and Osiris @ ISIS)

M. Karlsson

Chopper-cristal spectrometers: pulsed sources



M. Karlsson

Backscattering spectrometer

(H. Maier Leibnitz, A. Heidemman)

$$\frac{\Delta k_{div}}{k} = \cot(\theta) \Delta \theta$$
For $\theta \rightarrow \frac{\pi}{2} \quad \frac{\Delta k_{div}}{k} \approx \frac{\left(\Delta \theta\right)^2}{8}$

Backscattering spectrometer

(H. Maier Leibnitz, A. Heidemman)



IN16 (ILL)

Backscattering spectrometer

(H. Maier Leibnitz, A. Heidemman)



R. Lefort et al

Institution	Instrument	Énergie incidente	Géométrie	Source	Gamme d'énergie	Gamme de résolution
ISIS/RAL	HET MAPS MARI PRISMA MERLIN LET IRIS OSIRIS	15meV - 2000meV 15meV - 2000meV 10meV - 1000meV 10meV - 1000meV 1meV - 80meV 0.25meV - 20meV 0.25meV - 20meV	Directe Directe Inverse Directe Directe Inverse Inverse	Spallation	$\begin{split} -\infty > \mathrm{E}_{f} < 0.8\mathrm{E}_{i} \ \mathrm{meV} \\ -\infty < \mathrm{E}_{f} < 0.8\mathrm{E}_{i} \ \mathrm{meV} \\ -\infty < \mathrm{E}_{f} < 0.8\mathrm{E}_{i} \ \mathrm{meV} \\ 3 \ \mathrm{meV} < \mathrm{E}_{f} < 20 \ \mathrm{meV} \\ -\infty < \mathrm{E}_{f} < 0.8\mathrm{E}_{i} \ \mathrm{meV} \\ -\infty < \mathrm{E}_{f} < 0.6\mathrm{E}_{i} \ \mathrm{meV} \\ -\infty < \mathrm{E}_{f} < 0.6\mathrm{E}_{i} \ \mathrm{meV} \\ -\infty < \mathrm{E}_{f} < 0.6\mathrm{E}_{i} \ \mathrm{meV} \\ -0.8 < \mathrm{E}_{f} < 2.2 \ \mathrm{meV} \\ -0.5 < \mathrm{E}_{f} < 0.5 \ \mathrm{meV} \\ -3.5 < \mathrm{E}_{f} < 4.0 \ \mathrm{meV} \end{split}$	$\begin{array}{l} \Delta E/E_i = 1\text{-}2\%(4\text{m}) \\ 2\text{-}3\%(2.5\text{m}) \\ \Delta E/E_i = 2\text{-}5\% \\ \Delta E/E_i = 1\text{-}2\% \\ \Delta E/E_i = 1\text{-}2\% \\ \Delta E/E_i = 2\text{-}5\% \\ 5\mu\text{eV at } E_i = 1 \text{ meV} \\ 260\mu\text{eV at } \\ E_i = 20 \text{ meV} \\ 1, 4.5, 11, 17.5, \\ 54.5 \ \mu\text{eV} \\ 25 \ \mu\text{eV} \\ 90 \ \mu\text{eV} \end{array}$
SNS	ARCS SEQUOIA CNCS HYSPEC	30 meV - 2000meV 30 meV - 2000meV 0.8 meV - 20meV 5 meV - 50meV	Directe Directe Directe Directe	Spallation		$\begin{array}{l} \Delta E/E_i = 2\text{-}5\% \\ \Delta E/E_i = 1\text{-}5\% \\ 10 \text{ - }500 \ \mu\text{eV} \\ \Delta E/E_i = 2\text{-}15\% \end{array}$
PSI-SINQ	FOCUS MARS	3meV - 30meV 3meV - 30meV	Directe Inverse	Spallation continue	$\left -\infty < \mathcal{E}_f < 0.6\mathcal{E}_i \text{ meV} \right $	$7\mu eV < \Delta E < 5meV$ $1\mu eV < \Delta E$ $< 170\mu eV$
LLB (CEA-CNRS)	MIBEMOL	0.8meV - 20meV	Directe	Réacteur	$-\infty < E_f < 0.6E_i \text{ meV}$	$\Delta E/E_i = 1-8\%$
HMI-BENSC	NEAT	0.25meV - 25meV	Directe	Réacteur	$\left -\infty < \mathcal{E}_f < 0.6\mathcal{E}_i \text{ meV} \right $	6μeV< ΔE <5.4meV
ILL	IN4 IN5 IN6	15meV - 80meV 0.2meV - 20meV 2.35meV - 4.8meV	Directe Directe Directe	Réacteur	$ \begin{vmatrix} -\infty < \mathbf{E}_f < 0.8\mathbf{E}_i \text{ meV} \\ -\infty < \mathbf{E}_f < 0.6\mathbf{E}_i \text{ meV} \\ -\infty < \mathbf{E}_f < 0.6\mathbf{E}_i \text{ meV} \end{vmatrix} $	$ \begin{aligned} \Delta E/E_i &= 3\text{-}6\% \\ \Delta E/E_i &= 1\text{-}3\% \\ 50, 80, 120, 170 \ \mu\text{eV} \end{aligned} $
FRM-II	TOFTOF TOPAS	0.3meV - 20meV 20meV -160meV	Directe Directe	Réacteur Réacteur	$\left -\infty < \mathcal{E}_f < 0.6\mathcal{E}_i \text{ meV} \right $	$\begin{array}{l} \Delta \mathrm{E/E}_i = 1\text{-}3\% \\ \Delta \mathrm{E/E}_i = 5\% \end{array}$
IPNS, ANL	HRMECS LRMECS QENS	3meV - 1000meV 6meV - 600meV ?	Directe Directe Inverse	Spallation	0 - 800meV 0 - 500meV -2.5 < E _f < 200 meV	$\begin{array}{l} \Delta \mathrm{E/E}_i = 2\text{-}4\%\\ \Delta \mathrm{E/E}_i = 6\text{-}8\%\\ 90 \ \mu \mathrm{eV} \end{array}$
NIST, NCNR	FCS DCS	2.2meV - 15meV 0.4meV - 13meV	Directe Directe	Réacteur	$\begin{vmatrix} -\infty < \mathbf{E}_f < 0.6\mathbf{E}_i \text{ meV} \\ -\infty < \mathbf{E}_f < 0.6\mathbf{E}_i \text{ meV} \end{vmatrix}$	60 to 1000 μeV $\Delta E/E_i = 1-3\%$
J-PARC	CNDCS	1meV - 80meV	Directe			$\Delta E/E_i \simeq 1\%$
KENS/MLF KEK KENS	LAM-D LAM-40 LAM-80	1meV - 60meV 1meV - 60meV 1meV - 60meV	Inverse Inverse Inverse	Spallation	$-2 < E_f < 60 \text{meV}$ $-2 < E_f < 10 \text{meV}$ $-30 < E_f < 30 \mu \text{eV}$ $-400 < E_f < 500 \mu \text{eV}$ $1 < E_f < 15 \text{meV}$	$(L_i = 20 \text{ meV})$ $350 \ \mu\text{eV}$ $200 \ \mu\text{eV}$ $1.5 \ \mu\text{eV}$ $6.5 \ \mu\text{eV}$ $17 \ \mu\text{eV}$
i sukuda	AMATERA 4SEASONS DNA HRC	1meV - 80meV 5meV - 300meV 1meV - 60meV 1meV - 2000meV	Directe Directe Inverse Directe	Spallation	$-1 < E_f < 1.3 \text{meV}$	$\Delta E/E_i = 1-7\%/$ 0.3-1.5% $\Delta E/E_i = 6\%$ $\Delta E = 1 \mu eV/10 \mu eV$ $\Delta E/E_i = 1\%$

Conclusion

Time-of-flight neutron spectrometers :

• Direct geometry

TOF-TOF (reactor and spallation sources, continuous and pulsed) Cristal-TOF (reactor or continuous sources)

- Indirect geometry TOF-Cristal (spallation or pulsed sources)
- Backscattering spectrometers (reactor and spallation)

Conclusion



Thanks to :

J.Ollivier and J.-M. Zanotti, Collection SFN 10 (2010) 379-423