AN INSTRUMENT CONCEPT FOR DYNAMICS OF COMPLEX (BIO-) SYSTEM FROM ELASTIC SCATTERING

ANTONIO BENEDETTO
UNIVERSITY COLLEGE DUBLIN & PSI

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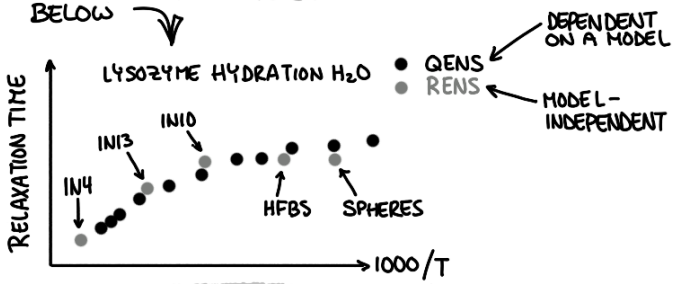
THERE IS NO AD-HOC TECHNIQUE TO MEASURE COMPLEX SYSTEMS (e.g. BIO-MOLECULES

BENEDETTO DEVELOPED **RESOLUTION ELASTIC NEUTRON SCATTERING (RENS)** AND WITH DON KEARLEY DEVELOPED AN INSTRUMENT DEDICATED TO RENS

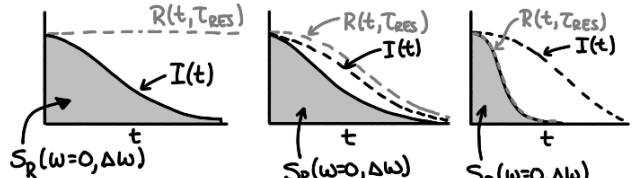
RENS IS A MODEL-FREE WAY TO EXTRACT τ_{RELAX}

AND THE AGREEMENT WITH QENS IS EXCELLENT IN THE CASE SHOWN BELOW

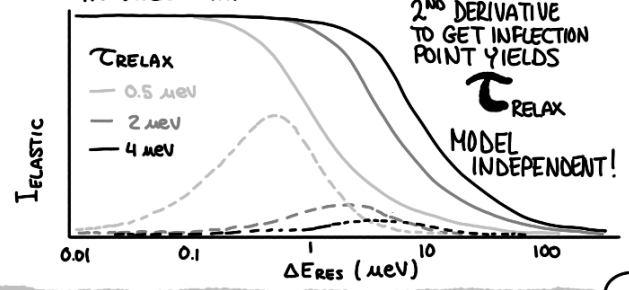


$$S_R(Q,\omega=0;\tau_{RES}) = \int_{-\infty}^{\infty} dt\, I(Q,t)\, R(t;\tau_{RES})$$

- $S_R(Q,\omega=0;\tau_{RES})$: MEASURED ELASTIC SCATTERING
- $I(Q,t)$: SYSTEM DYNAMICS
- $R(t;\tau_{RES})$: RESOLUTION FUNCTION



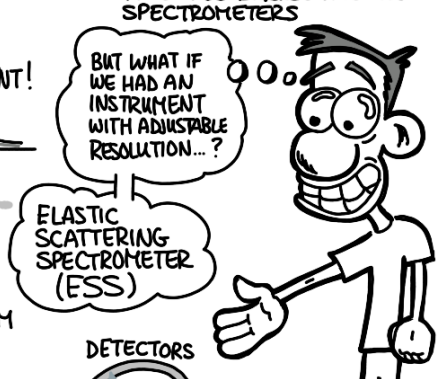
IN THEORY....



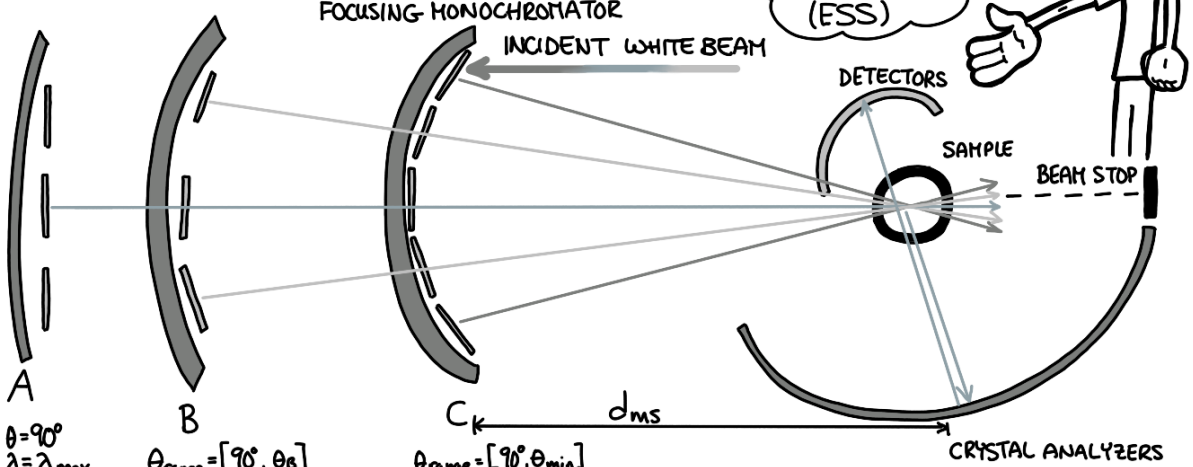
2ND DERIVATIVE TO GET INFLECTION POINT YIELDS τ_{RELAX}

MODEL INDEPENDENT!

BUT.... **INEFFICIENT!** SINCE IT REQUIRES MULTIPLE BACKSCATTERING SPECTROMETERS



CONSTANT WAVELENGTH SETUP (CW SOURCE)



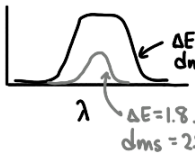
A	B	C
$\theta = 90°$	$\theta_{range} = [90°, \theta_B]$	$\theta_{range} = [90°, \theta_{min}]$
$\lambda = \lambda_{max}$	$\lambda_{range} = [\lambda_B, \lambda_{max}]$	$\lambda_{range} = [\lambda_{min}, \lambda_{max}]$
$\Delta\lambda = \Delta\lambda_{min}$	$\Delta\lambda_{range} = [\Delta\lambda_{min}, \Delta\lambda_B]$	$\Delta\lambda_{range} = [\Delta\lambda_{min}, \Delta\lambda_{max}]$

VARYING MONOCHROMATOR–SAMPLE DISTANCE AND MONOCHROMATOR CURVATURE YIELDS DIFFERENT INSTRUMENTAL ENERGY RESOLUTIONS

$$\lambda = d \sin\theta \rightarrow \frac{\Delta\lambda}{\lambda} = \frac{\Delta\theta}{\tan\theta} + \frac{\Delta d}{d}$$

AB ALSO DESCRIBED A ESS INSTRUMENT CONCEPT EXPLOITING TOF BUT I HAVEN'T SHOWN IT HERE

McSTAS SIMULATIONS



ESS-TO-I(t)

$$\frac{d}{d\tau_{RES}} S_R(\tau,\tau_{RES}) = \int_{\tau_{RES}}^{\tau_{RES}+\delta\tau_{RES}} I(t,\tau)\, R(t,\tau_{RES})\, dt \simeq I(\tau_{RES},\tau)\, R(\tau_{RES},\tau_{RES})$$

$$NORM\left[\frac{d}{d\tau_{RES}} S_R(\tau,\tau_{RES})\right] = I(\tau_{RES},\tau)$$

ESS VS. QENS ➡ $\Delta\tau/\tau = 5\%$

PROTEINS IN WATER (AS MEASURED WITH $\Delta E = 0.3$ meV ON IN16B)

→ "KINK" SHIFTS TO LOWER T
→ H_2O DYNAMICS FASTER THAN PROTEIN

SKETCHNOTES: