



INVESTIGATION OF MONTE CARLO TRANSPORT FOR MEDICAL POSITRON EMISSION TOMOGRAPHY (PET)

P.W. Chin¹, N.M. Spyrou², D.G. Lewis¹

¹Dept of Medical Physics, Velindre Cancer Centre, Cardiff, UK

²Dept of Physics, University of Surrey, Guildford, UK

MONTE CARLO SIMULATION OF PET

1. WHERE DO WE BEGIN?

Positron source or photon source



inelastic scattering
elastic scattering
bremsstrahlung



PHOTON
PHOTON

MONTE CARLO SIMULATION OF PET

1. HOW DO WE BEGIN?

Positron source or photon source

2. HOW DETAIL MUST WE GO?

Annihilation in-flight

Rayleigh

Spin

Bound Compton

Relaxations

Angular Sampling

Bethe-Heitler / NIST

1. ANNIHILATION

overview

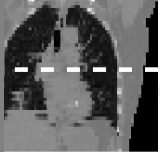
e⁺ POSITION
B
e⁺

γ - γ ANGLE

TEXTBOOKS SAY $180 \pm 0.25^\circ$

WE FOUND 79 to 180°

WHY!



2. TRANSPORT SETTINGS

PATIENT



DETECTOR

LSO

BGO

Rayleigh On / Off

Spin On / Off

Bound Compton On / Off

Relaxations On / Off

Angular Sampling Detailed / Simple

Bethe-Heitler / NIST

e⁺ source / 511 keV γ source

CLOSE-UPS

1. ANNIH AT REST

2. ANNIH IN FLIGHT

Positron will annihilate at rest	1	0.010	1	-0.059,0.131,500.106	0.143,-0.362,-0.921
Positron annihilates at rest	1	0.511	0	-0.059,0.131,500.106	-0.329,-0.620, 0.712
	2	0.511	0	-0.059,0.131,500.106	0.329, 0.620,-0.712

CONDENSED HISTORY THRESHOLD
 - CAN'T GO ANY LOWER!
 BACK TO BACK

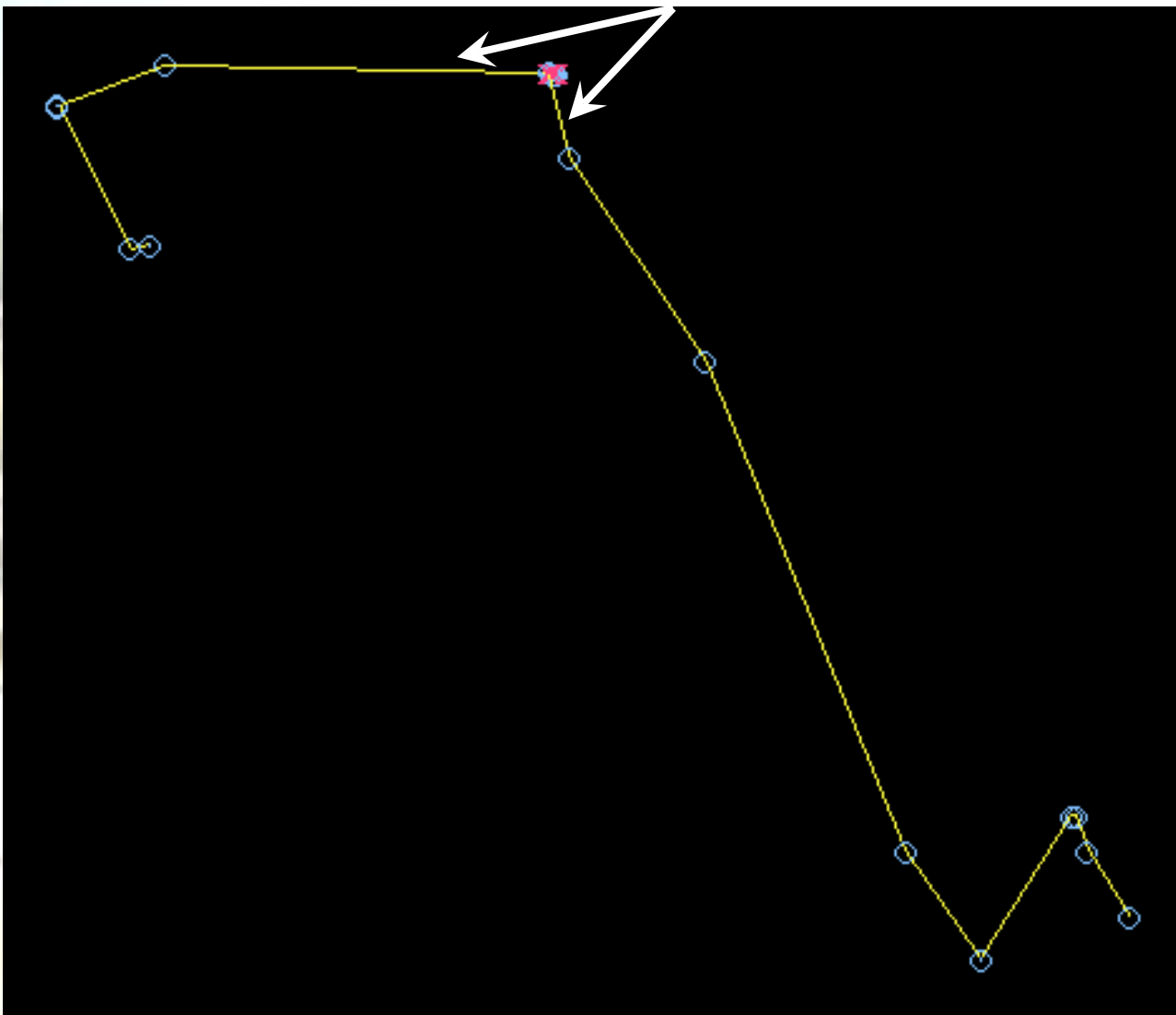


Positron about to decay in flight	1	0.606	1	2	0.155,0.023,500.314	-0.122,-0.592, 0.797
Resulting photons	1	0.979	0	2	0.155,0.023 500.314	-0.311, 0.020, 0.950
		0.649	0	2	0.155,0.023 500.314	0.282,-0.935,-0.213

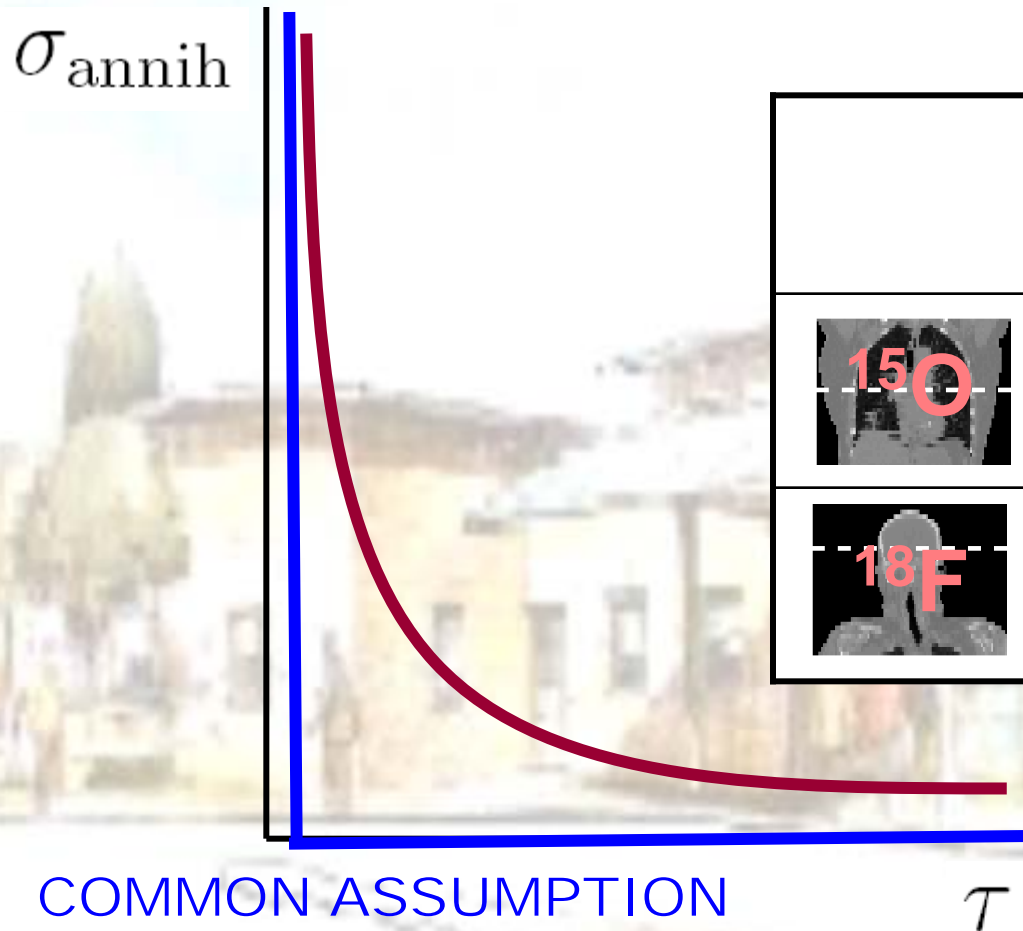
NOT THERMALISED?



$0.606 + 0.511$
 $= 0.979 + 0.649$

NOT BACK-TO-BACK!



TO INFINITY: LOW ENERGY e^+ MUST
 ANNIHILATE (AT REST)



	Annih in flight	Annih at rest
	1	39
	1	124

$$\sigma_{annih} = \frac{\pi r_0^2}{\tau + 2} \left[\frac{\tau^2 + 6(\tau + 1)}{\tau(\tau + 2)} \ln(\tau + 1 + \sqrt{\tau(\tau + 2)}) - \frac{\tau + 4}{\sqrt{\tau(\tau + 2)}} \right]$$

HEITLER

POSITRONS

PHOTONS

\log_{10} (counts)

RANGE

γ - γ ANGLE

ENERGY

ENERGY

COMMON ASSUMPTION

1.7 MeV e^+

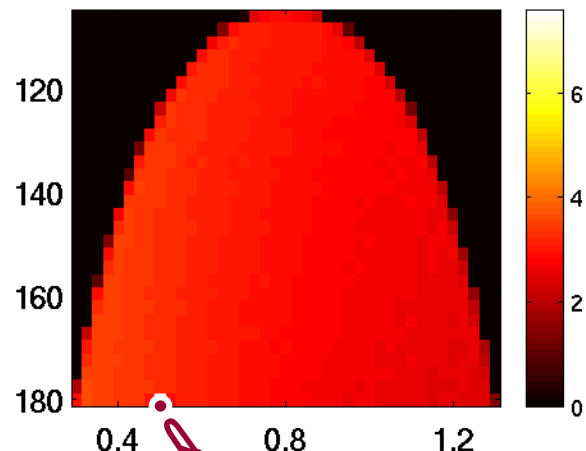
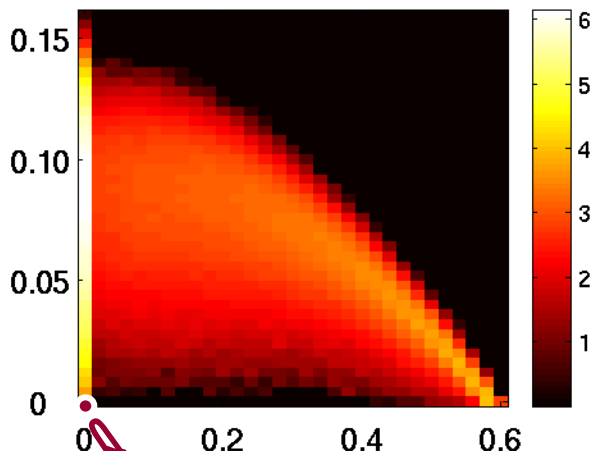
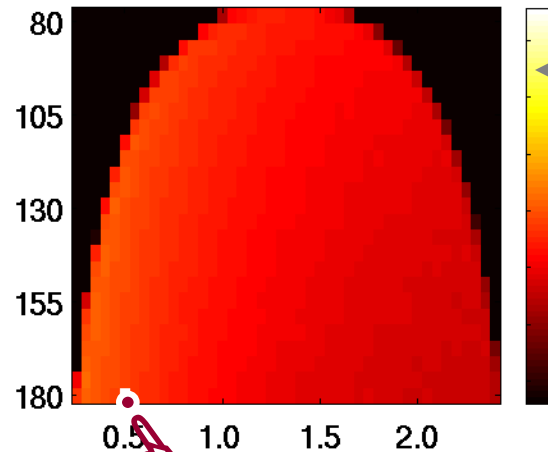
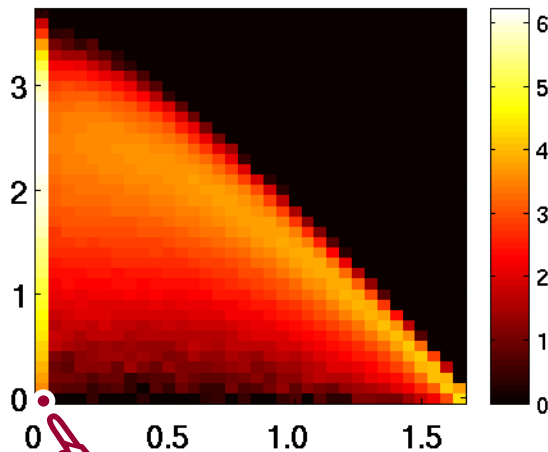
End-point energy of ^{15}O

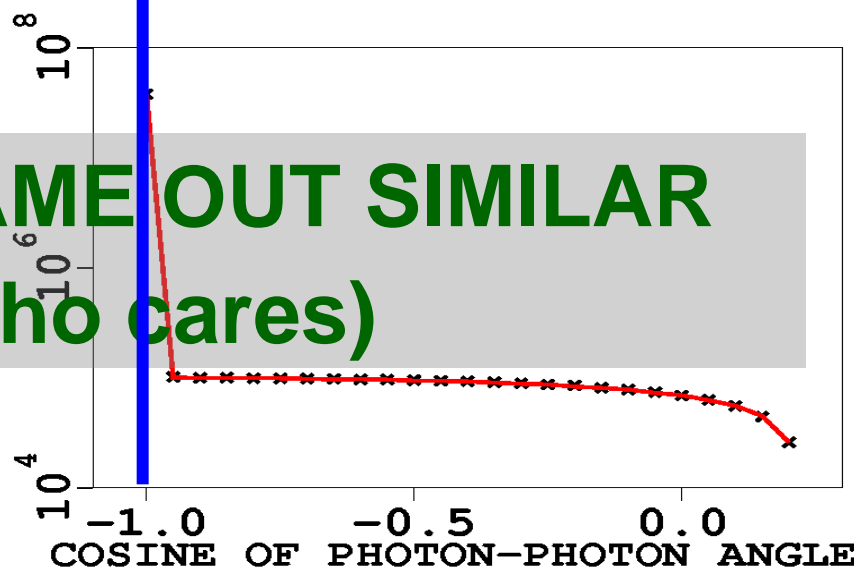
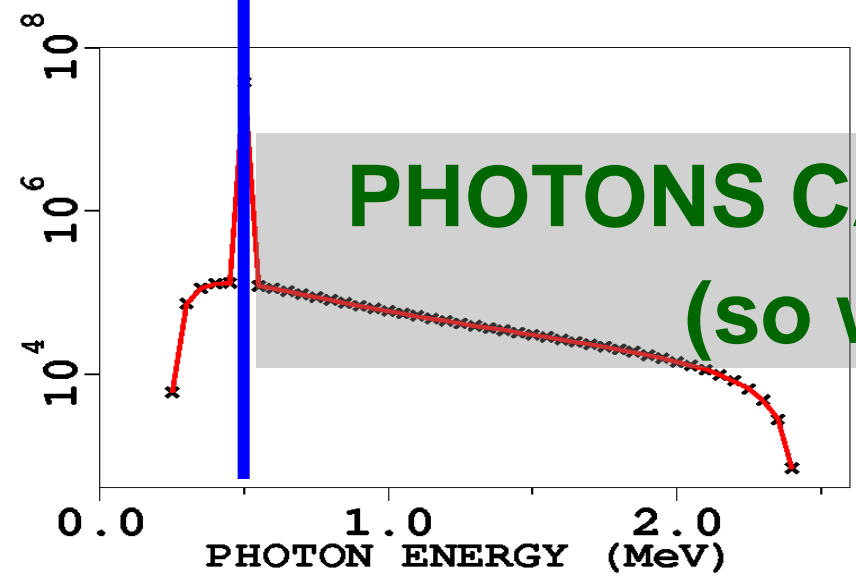
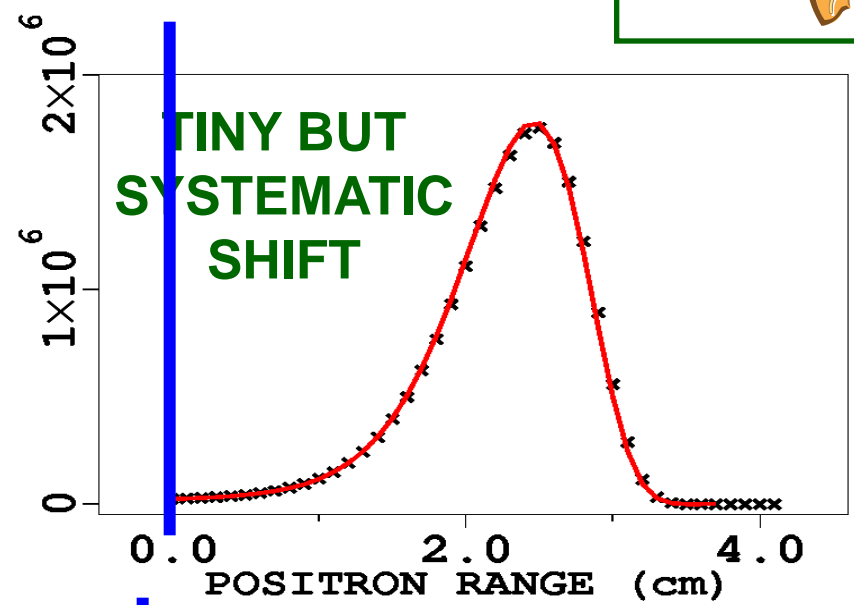
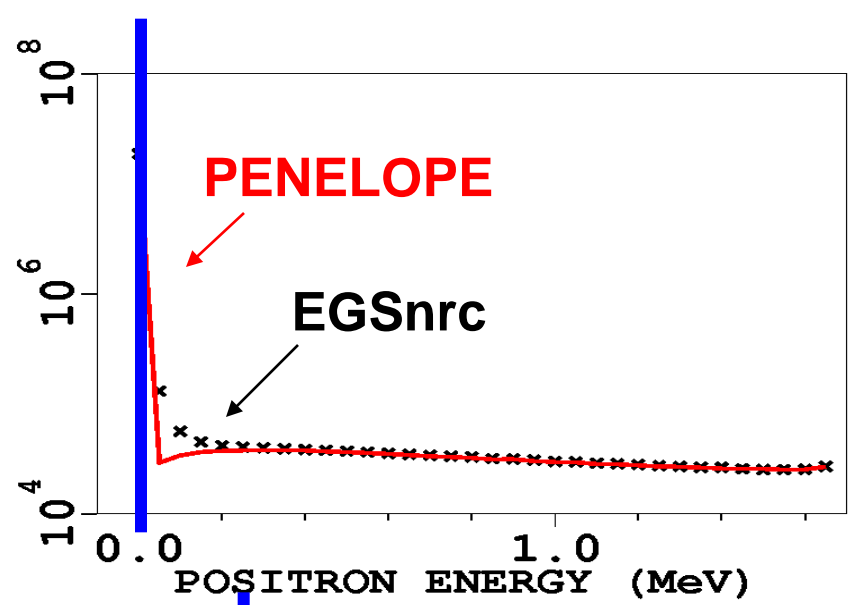
0.6 MeV e^+

End-point energy of ^{18}F

HOMOG

HOMOG

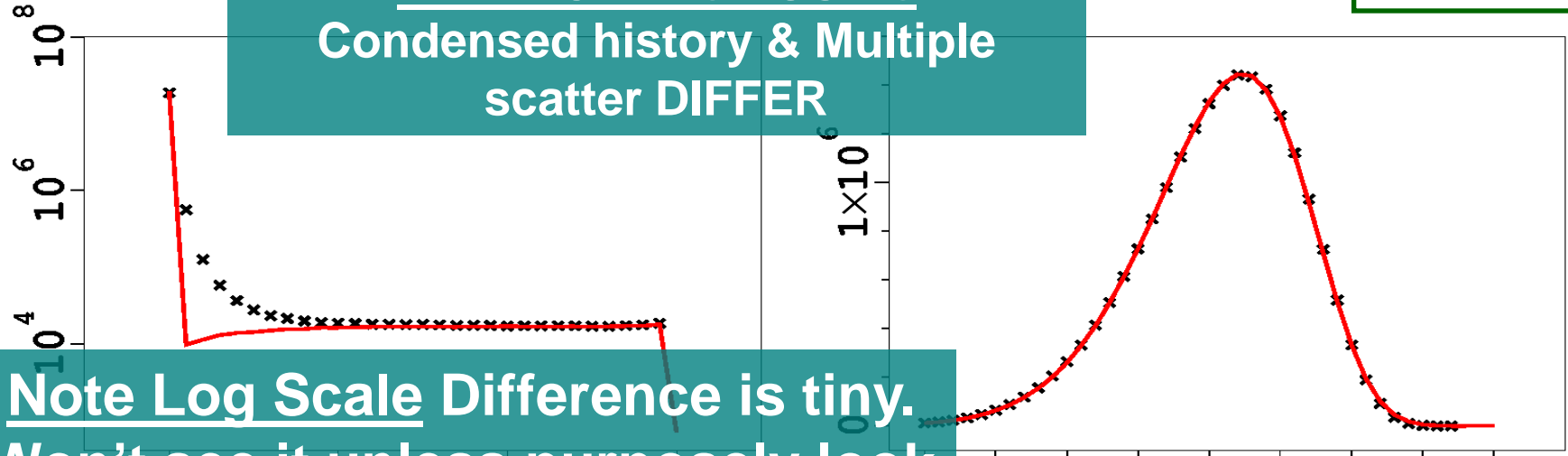




PHOTONS CAME OUT SIMILAR (so who cares)

COMMON ASSUMPTION

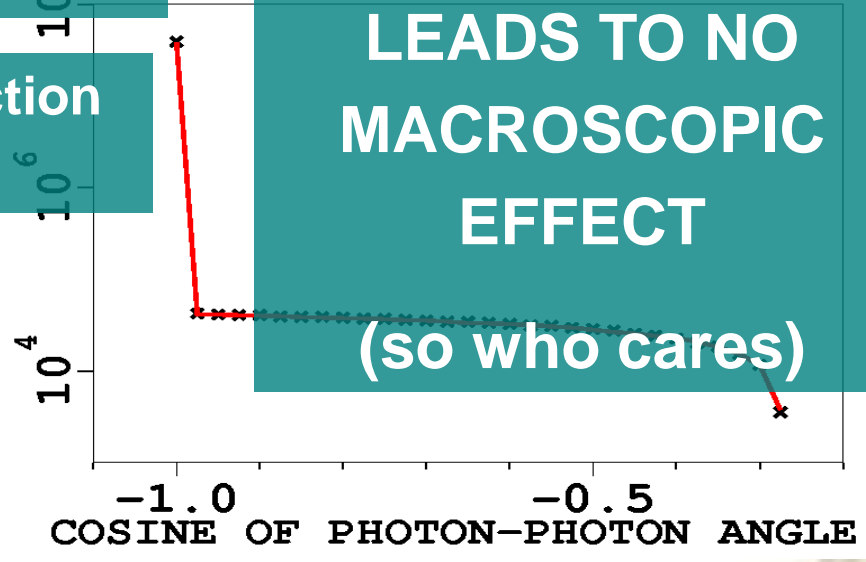
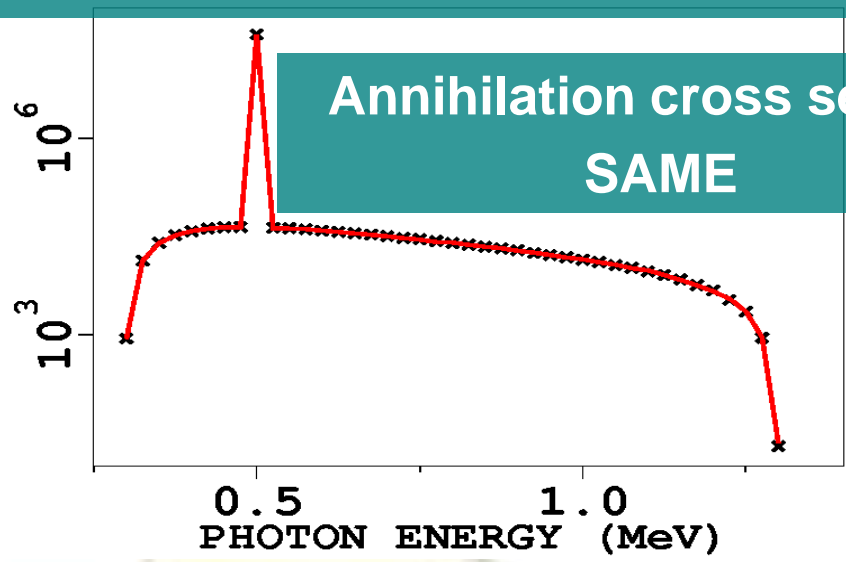
PENELOPE vs EGSnrc
Condensed history & Multiple scatter DIFFER



Note Log Scale Difference is tiny.
Won't see it unless purposely look for it.

DIFFERENCE LEADS TO NO MACROSCOPIC EFFECT (so who cares)

Annihilation cross section SAME



THAT'S

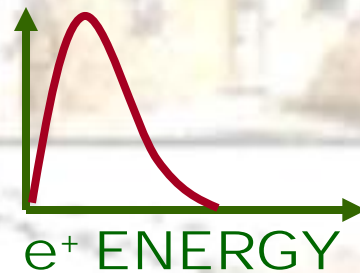
1.7 MeV e⁺  HOMO

&

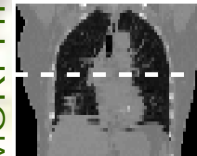
0.6 MeV e⁺  HOMO

WHAT ABOUT

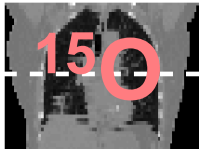
IN



ANTHROPOMORPHIC



COMMON ASSUMPTION



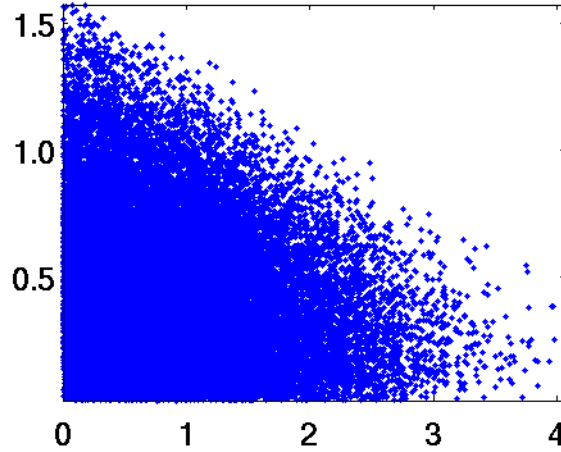
15



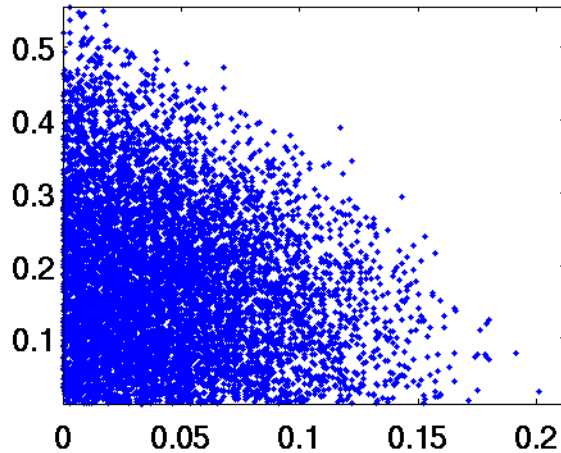
18

ENERGY

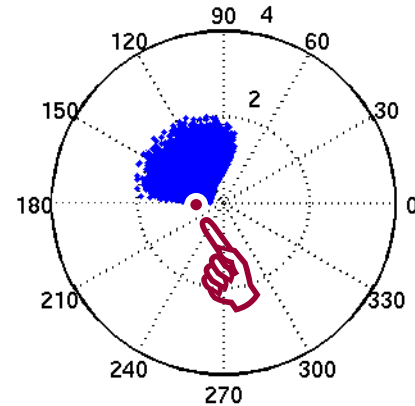
POSITRONS



RANGE

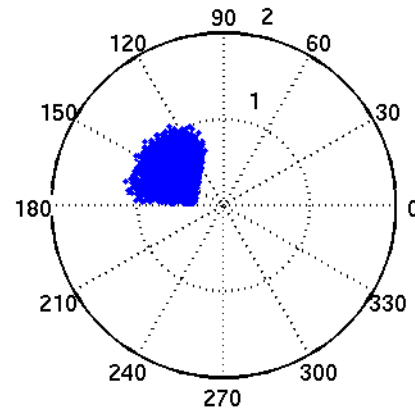


PHOTONS



$\Theta = \gamma\text{-}\gamma \text{ ANGLE}$

$R = \gamma \text{ ENERGY}$



IN FACT DOWN TO 79°

POLAR PLOTS SIMILAR WHETHER

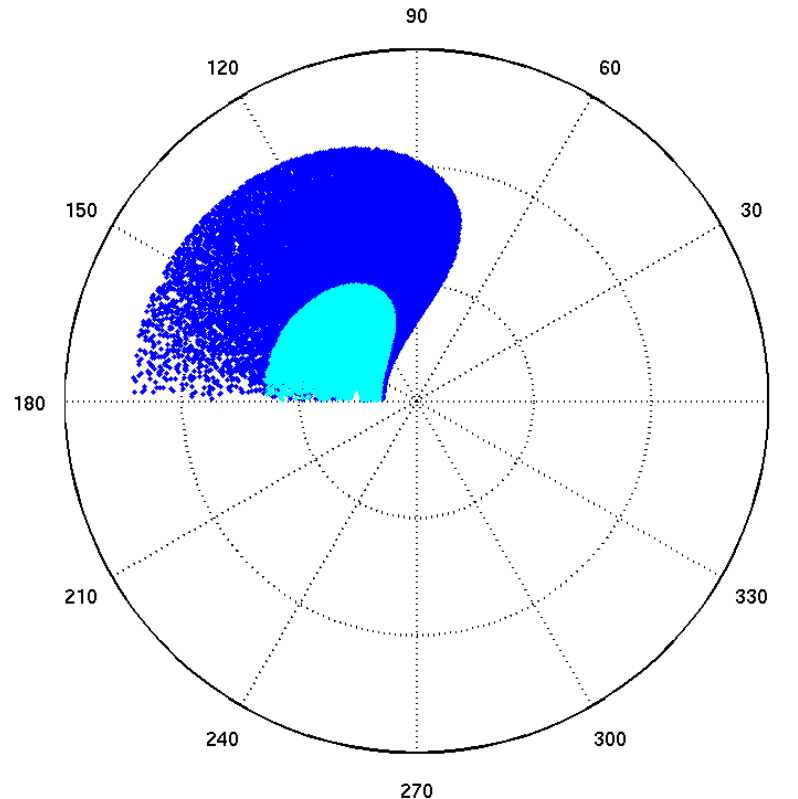


OR



1.7 MeV incident

0.6 MeV incident



$\Theta = \gamma$ - γ ANGLE

R = γ ENERGY

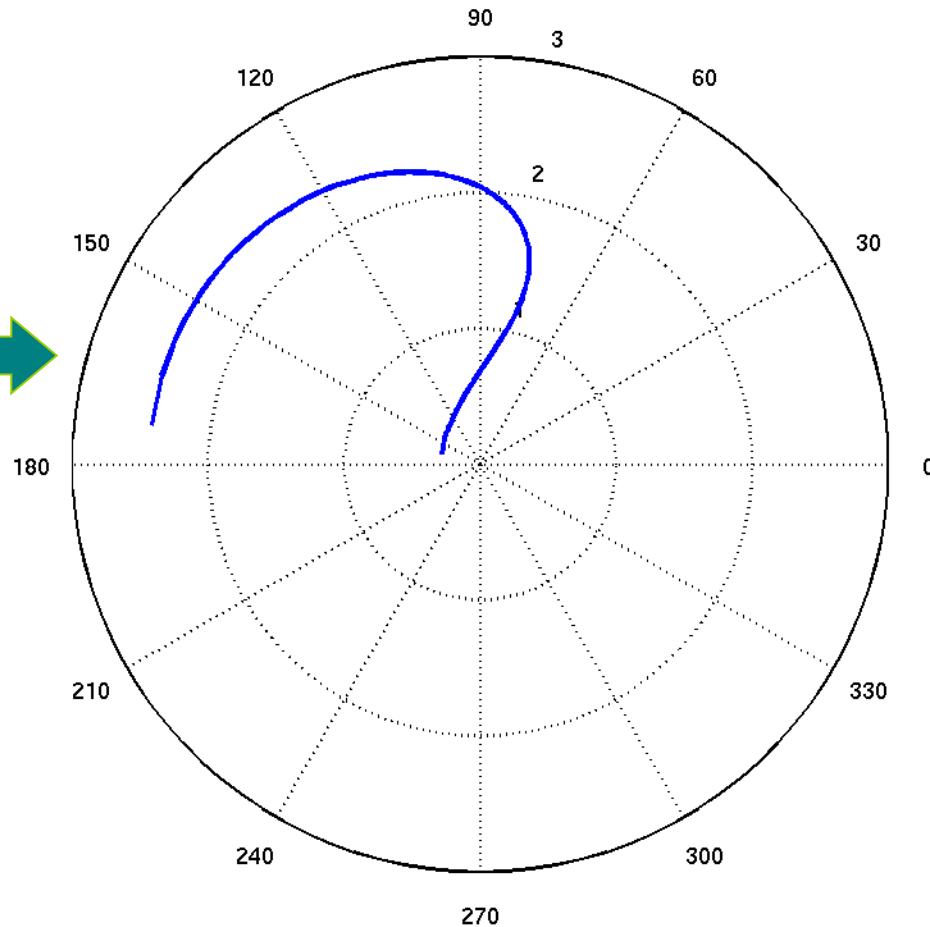
GOVERNED BY RELATIVISTIC KINEMATICS

$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.7 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$



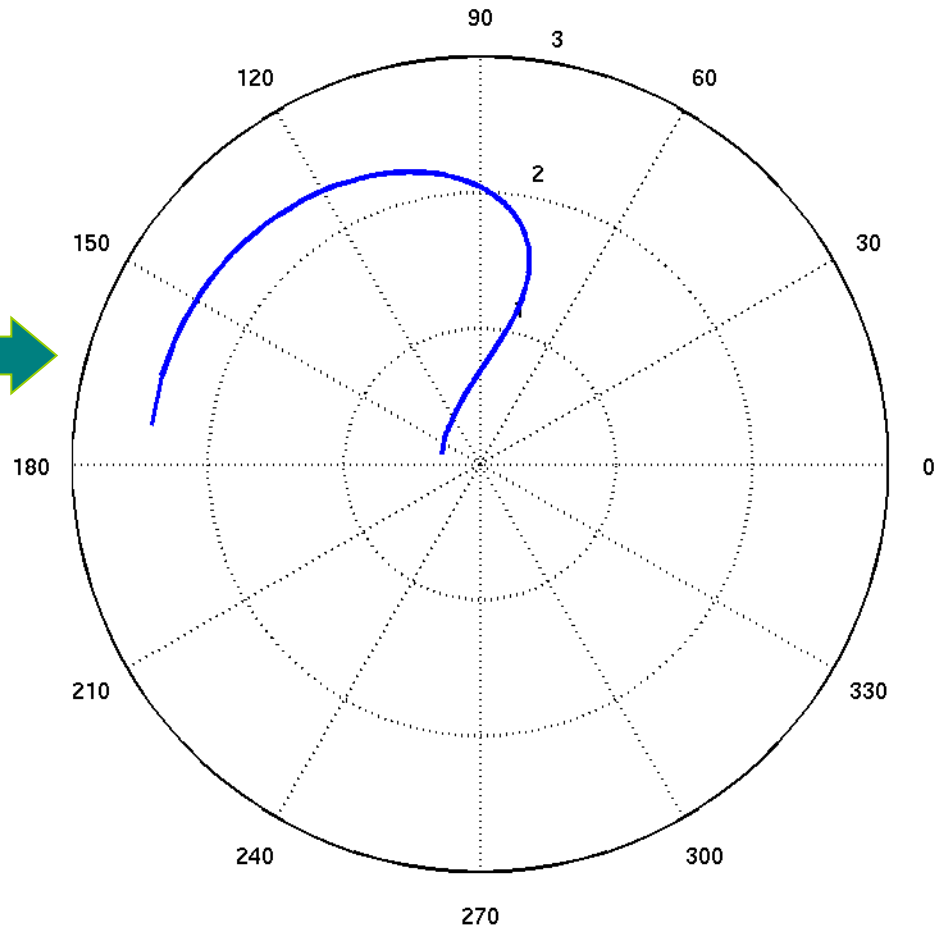
NOT FORGETTING ANNIH OF SLOWING DOWN e^+ ...

$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.6 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

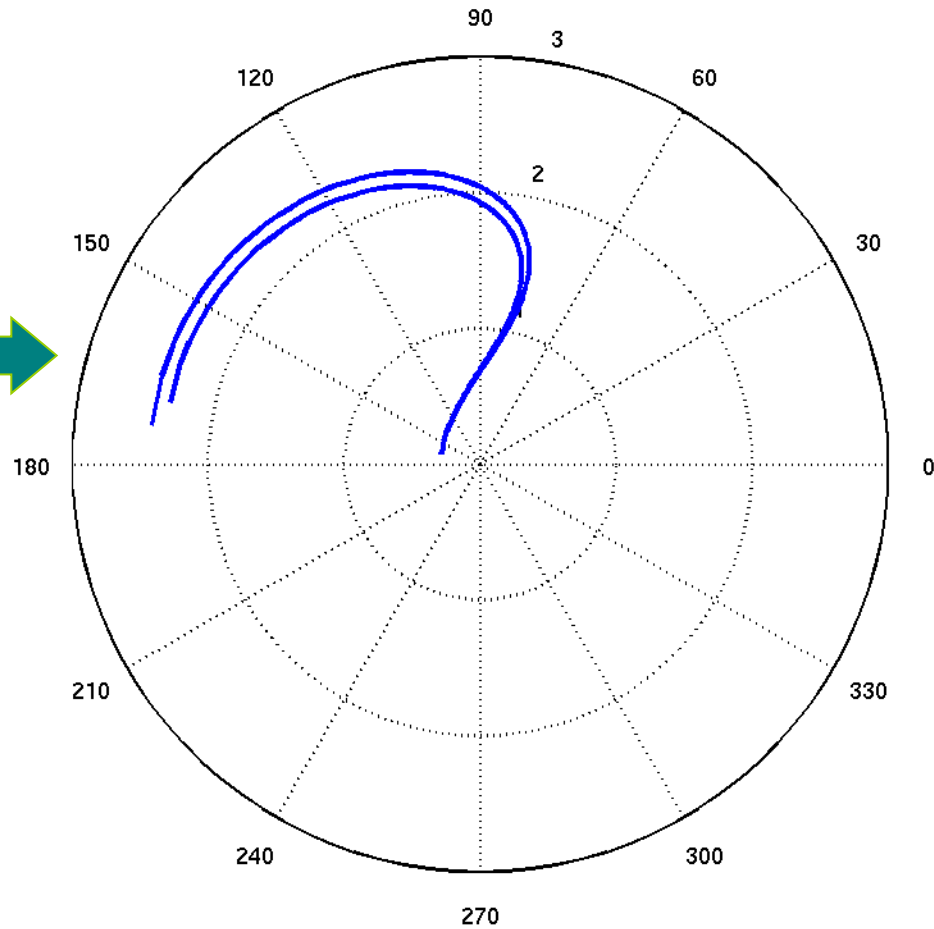


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.5 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

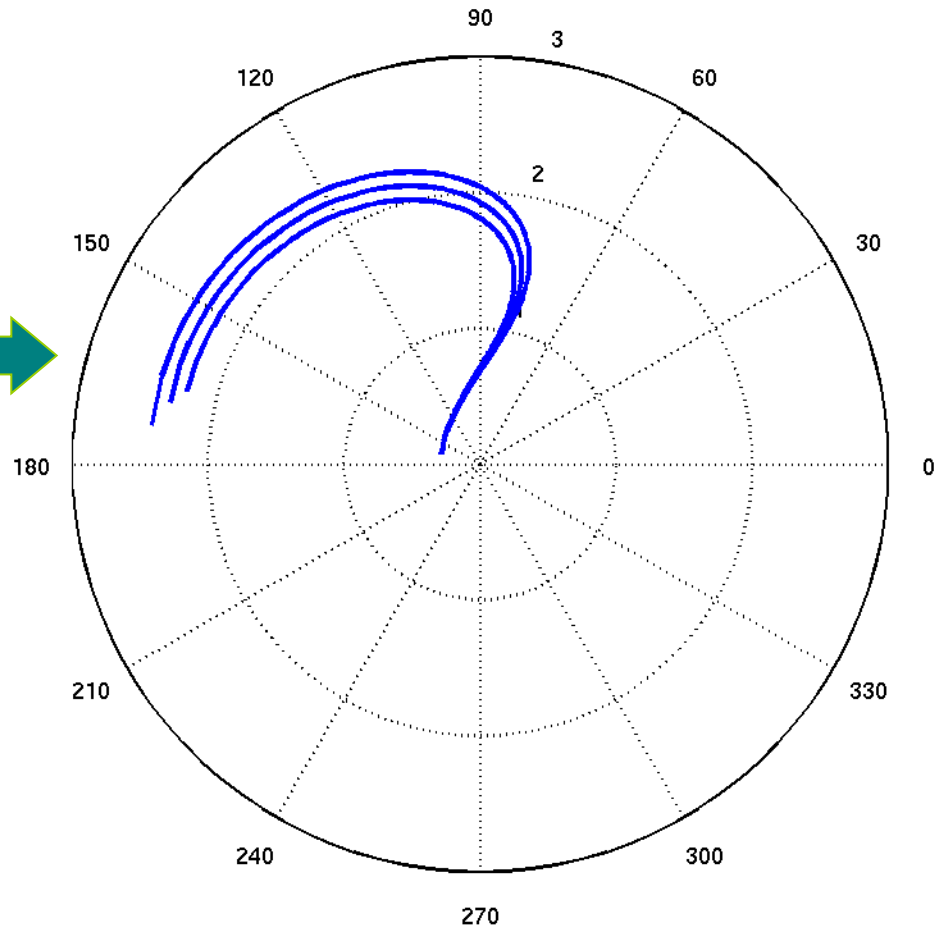


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.4 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

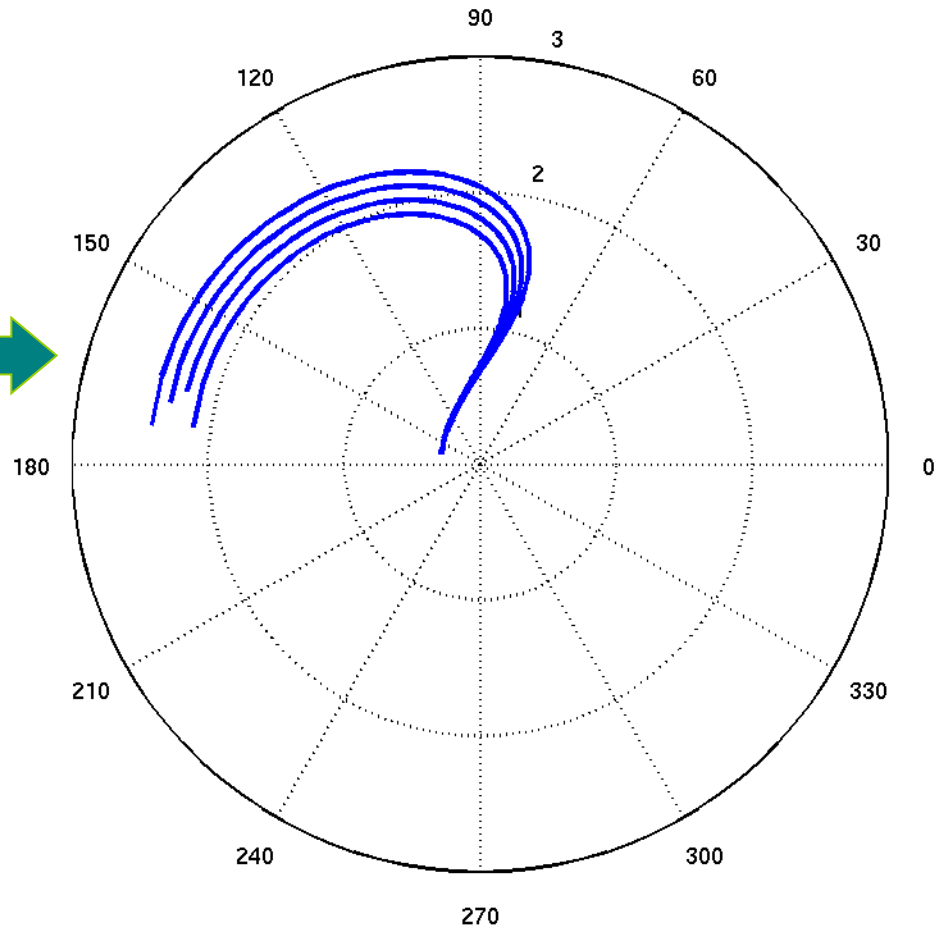


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.3 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

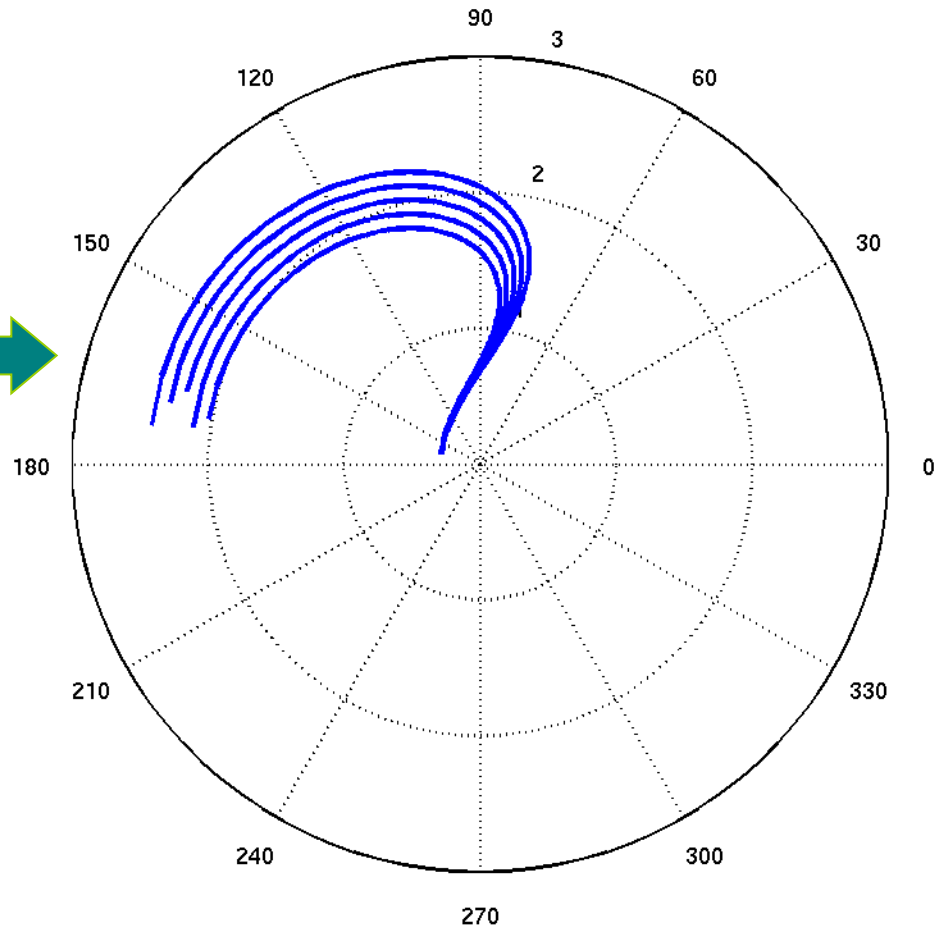


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.2 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

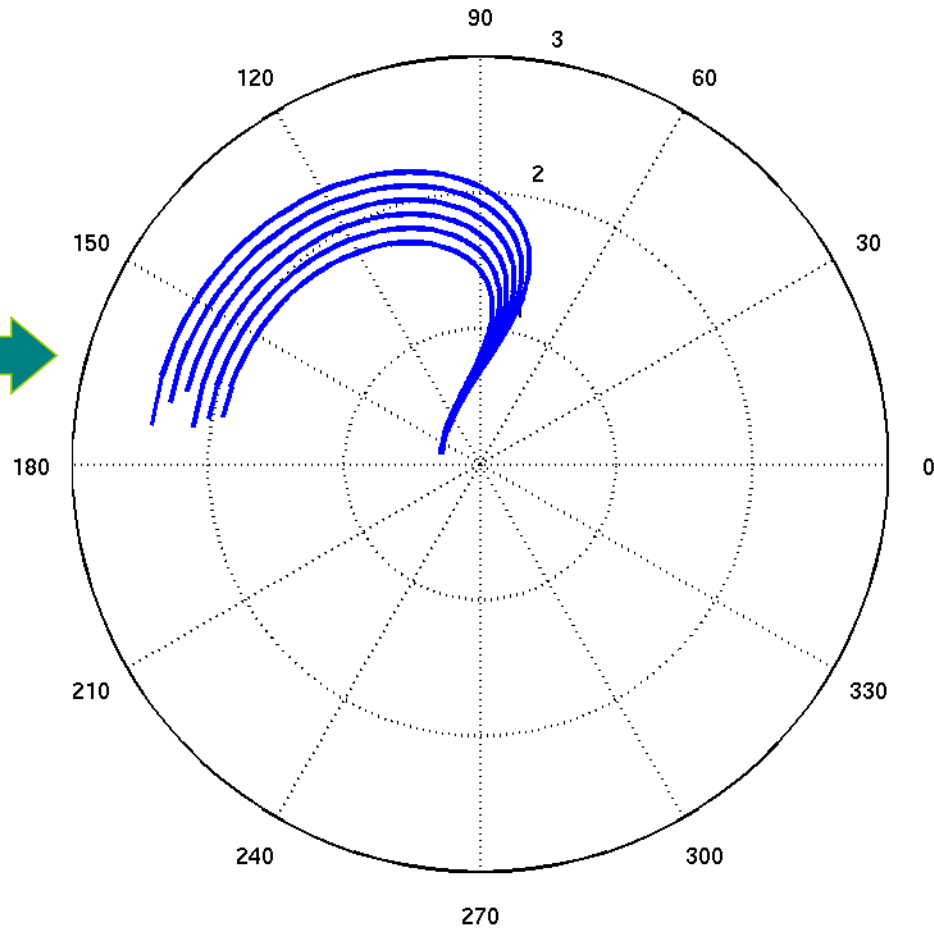


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.1 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

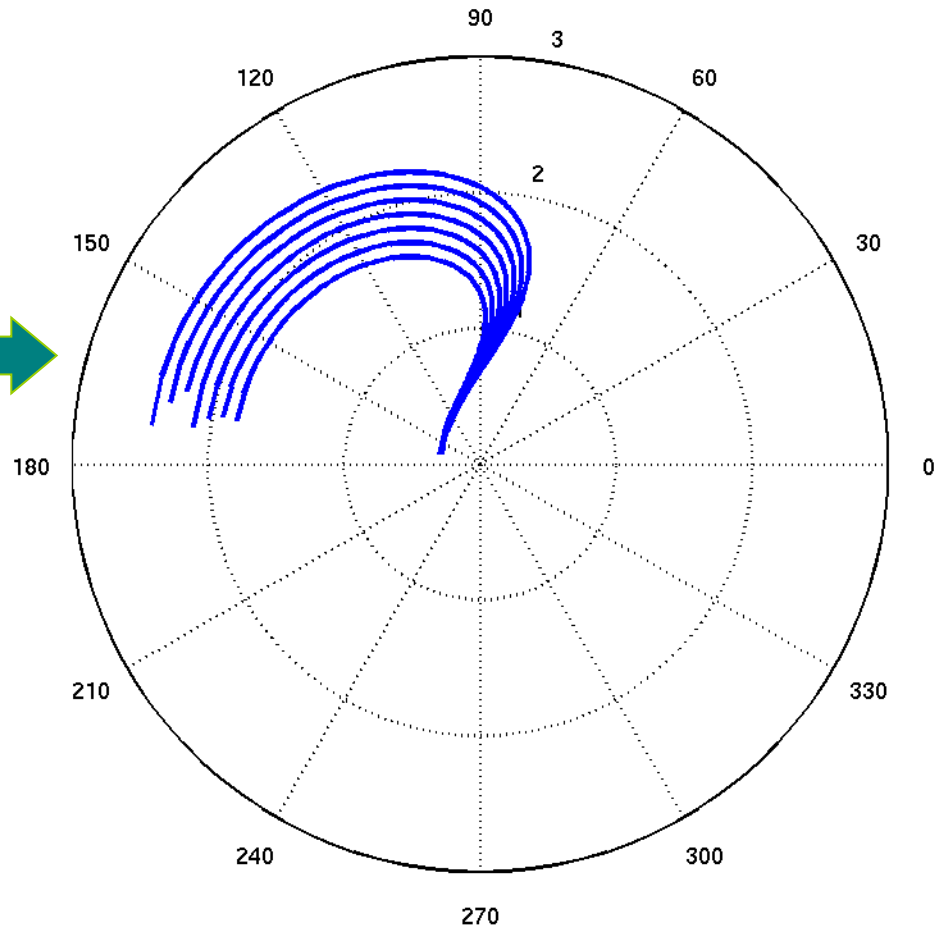


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 1.0 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

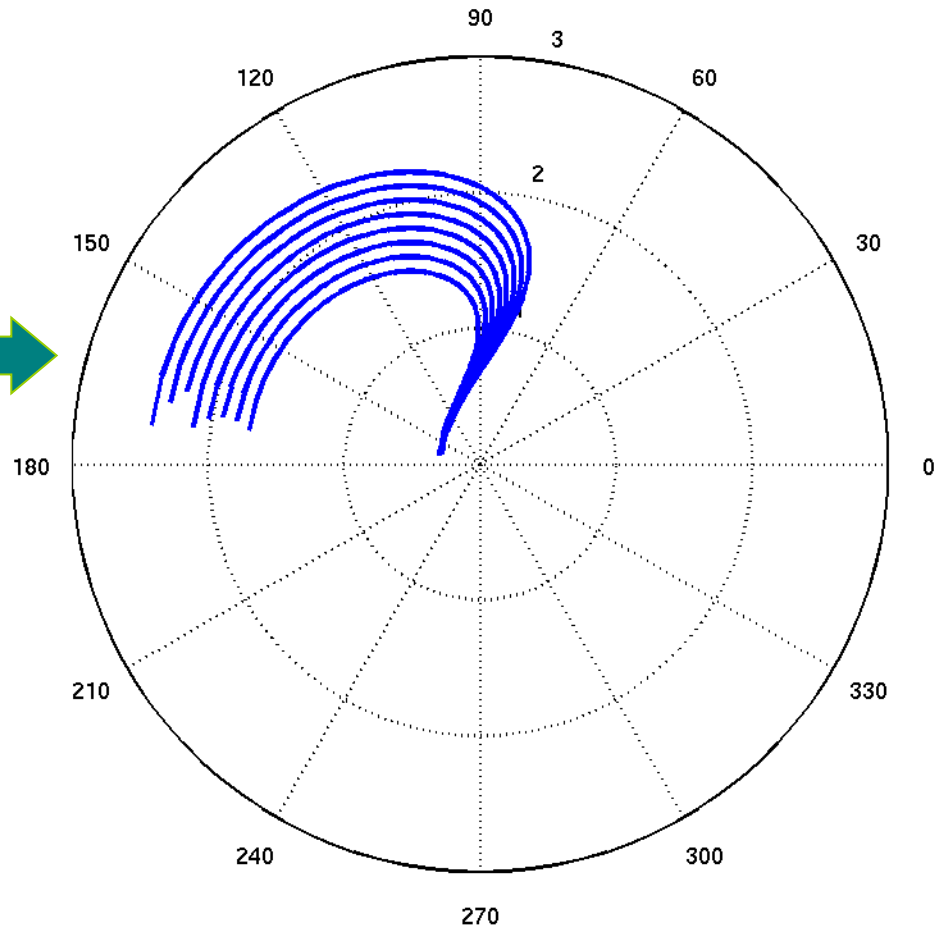


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.9 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

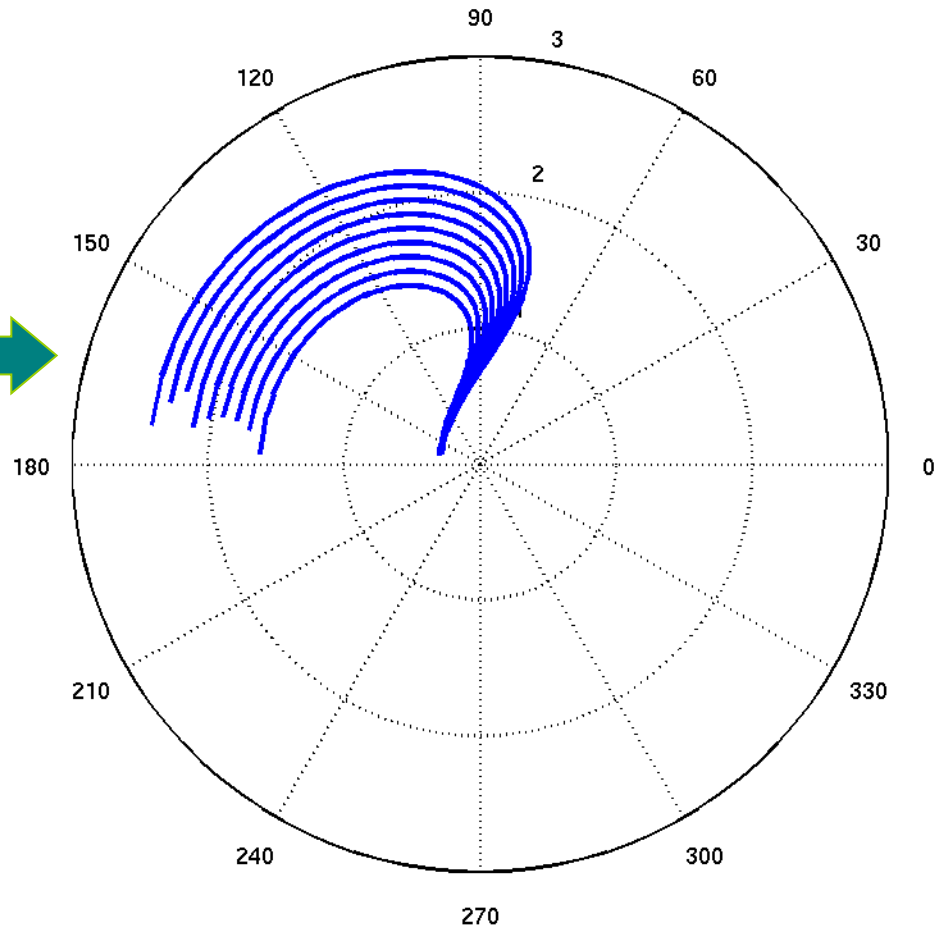


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.8 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

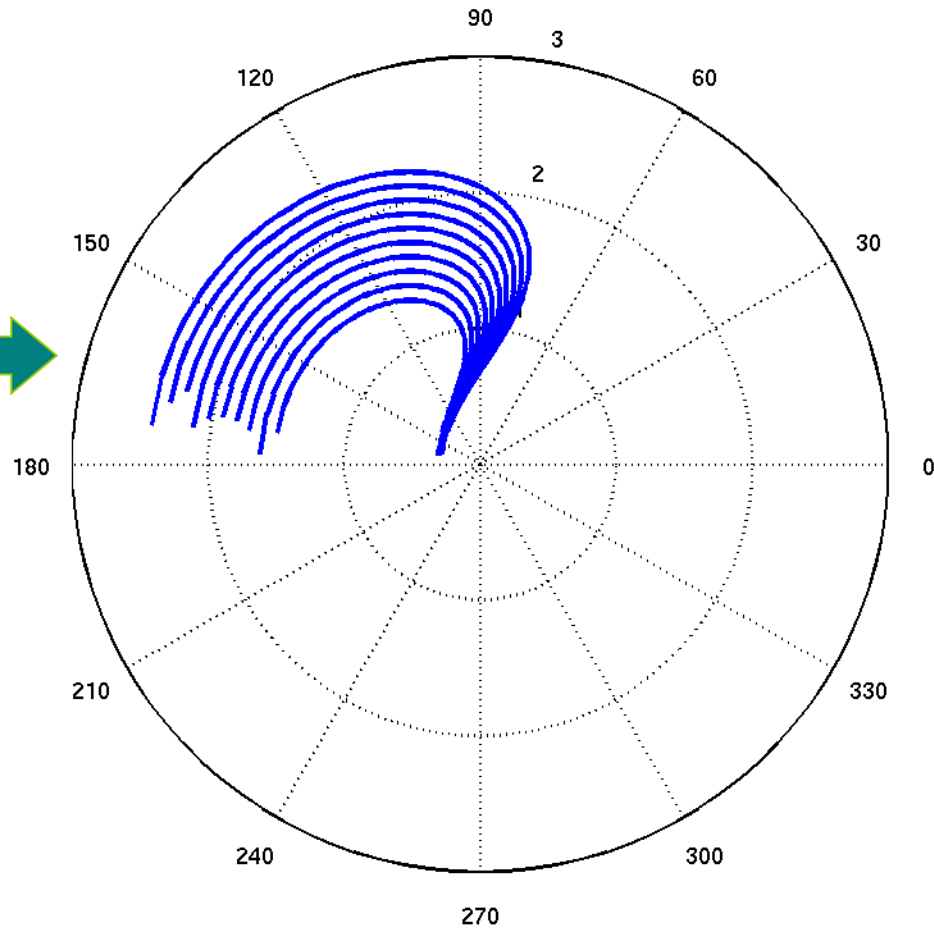


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.7 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

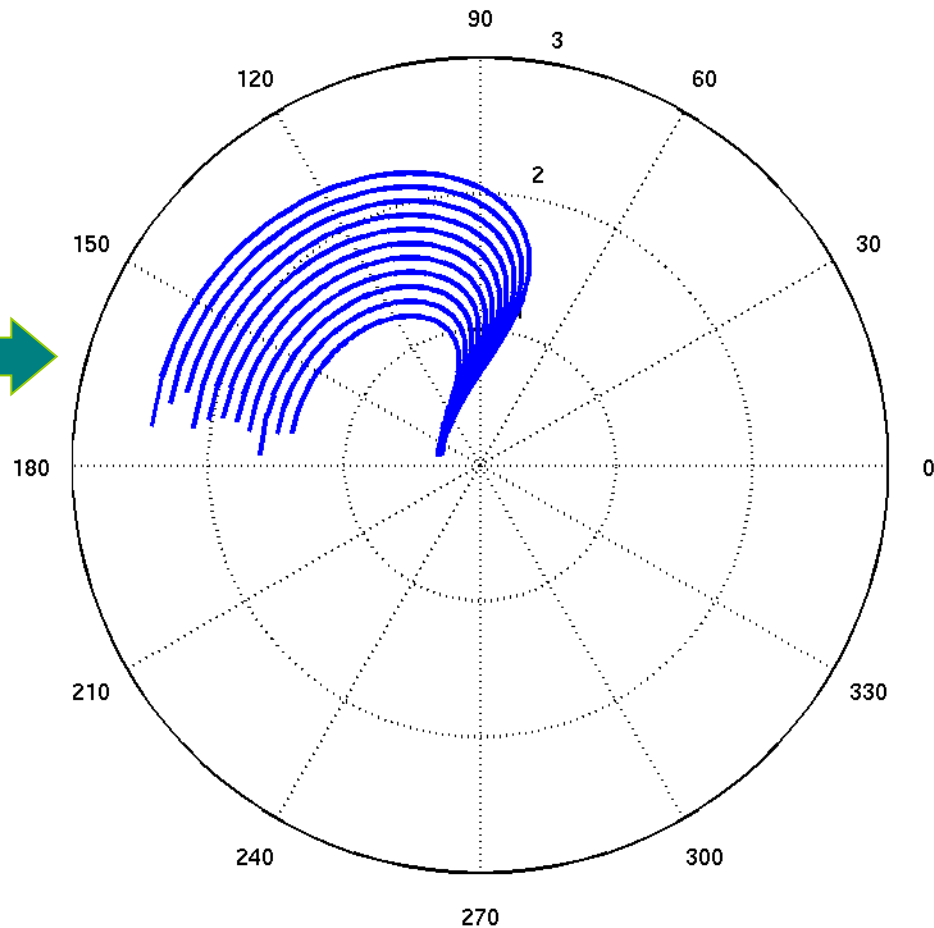


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.6 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

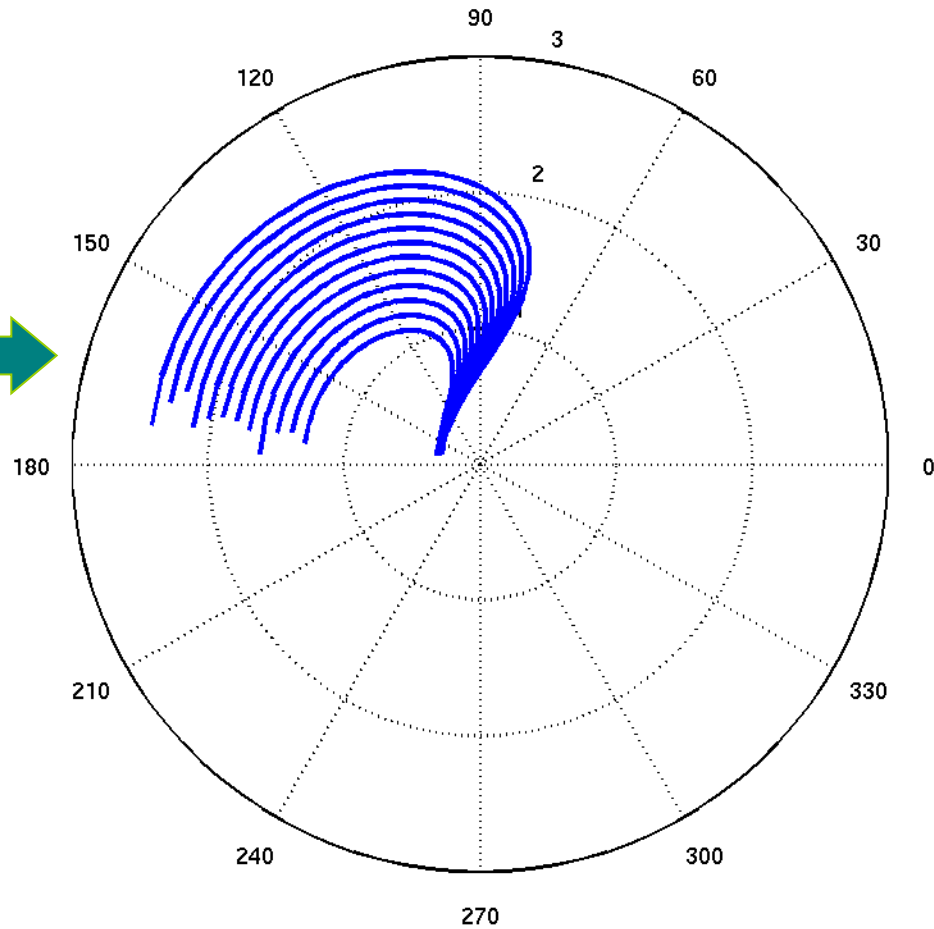


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.5 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

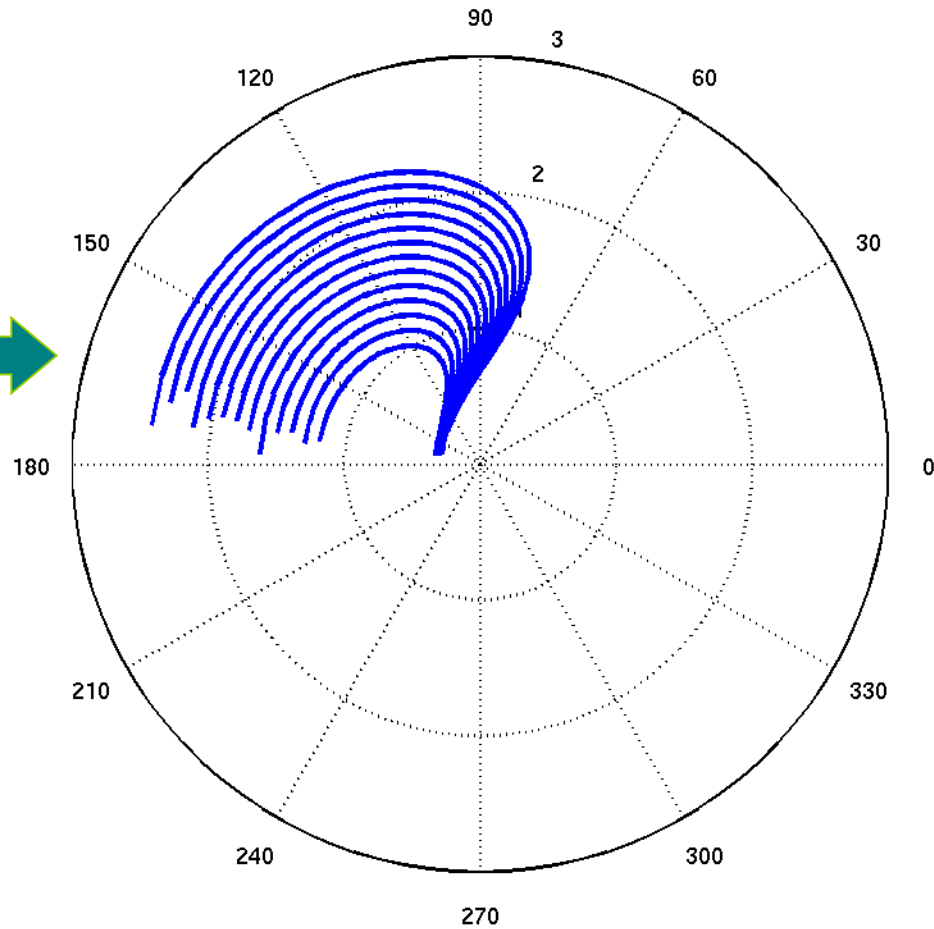


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.4 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

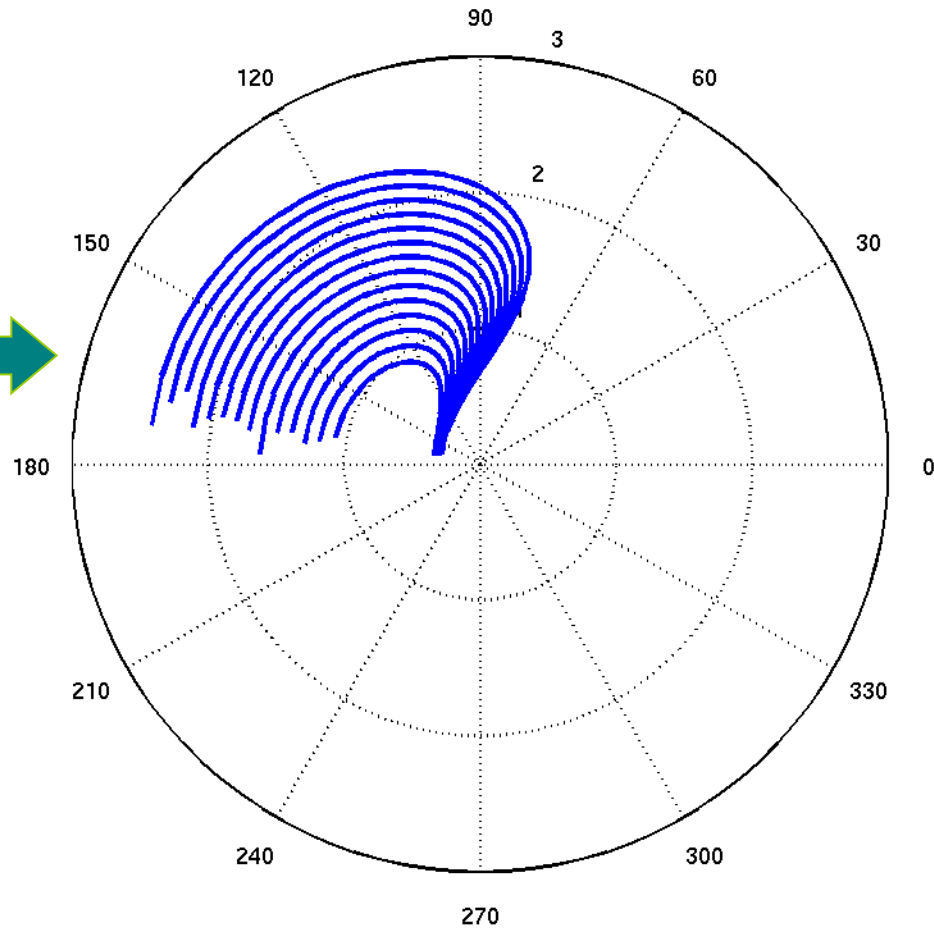


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.3 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

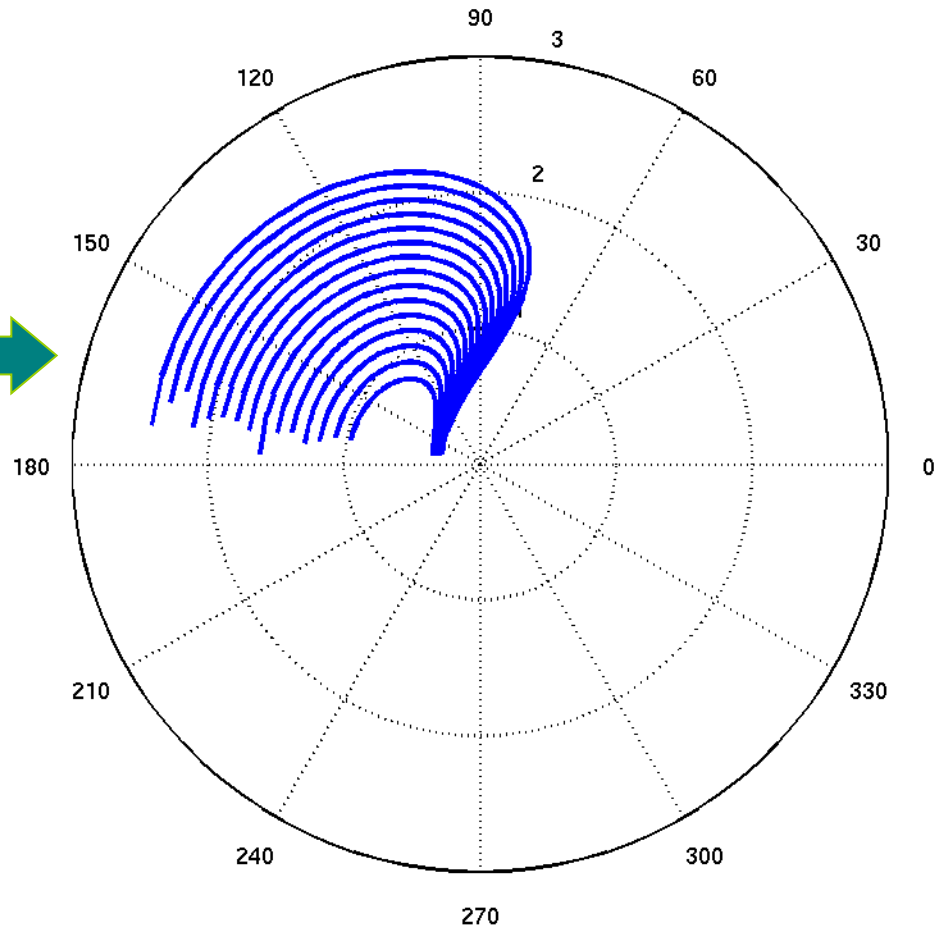


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.2 \text{ MeV}$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$

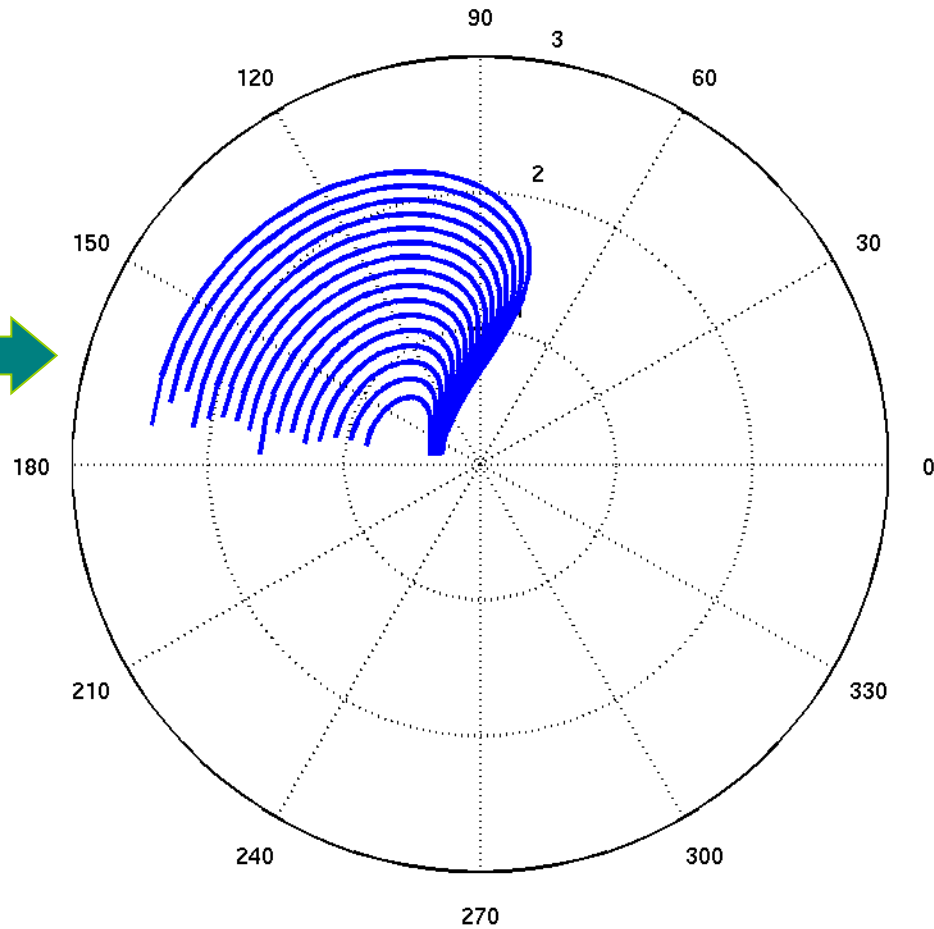


$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

← $\tau = 0.1 \text{ MeV}$


$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

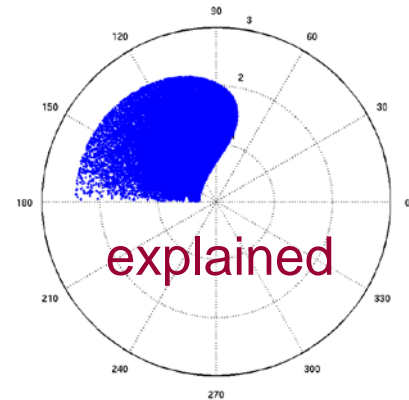
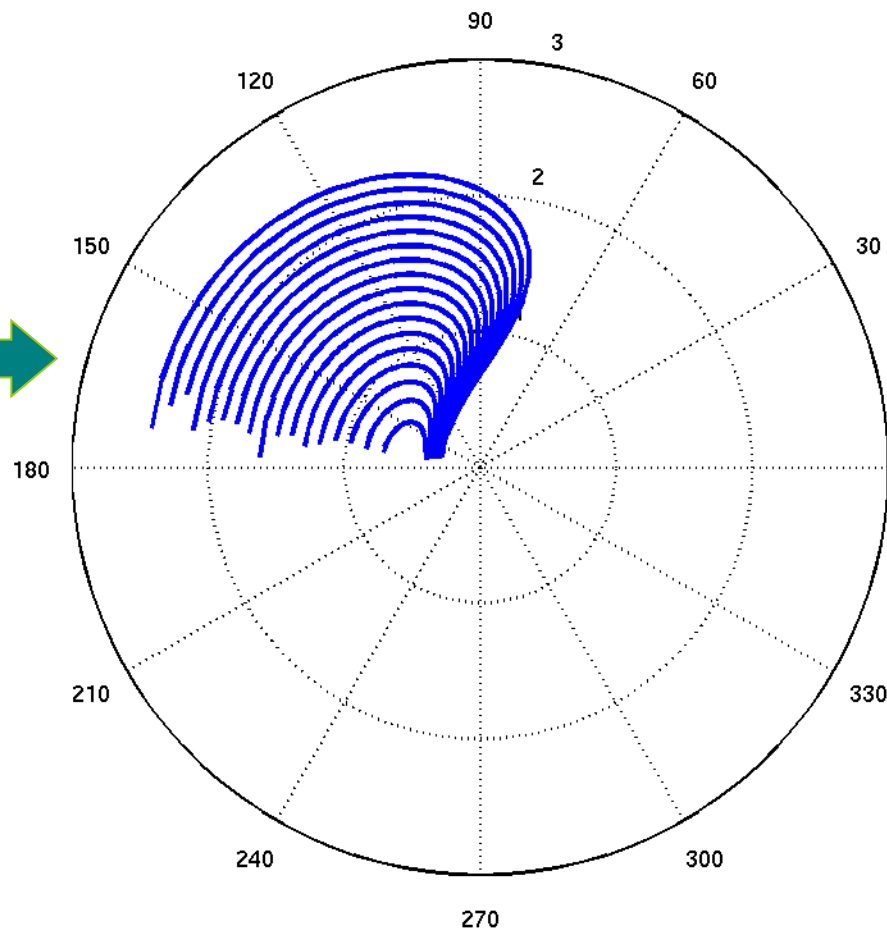
$\rightarrow \text{polar}(\theta_1 + \theta_2, \kappa_1)$



$$\cos \theta_1 = \frac{\kappa_1 - m}{\kappa_1 \sqrt{\frac{\tau}{\tau + 2}}}$$

$$\cos \theta_2 = \frac{\kappa_2 - m}{\kappa_2 \sqrt{\frac{\tau}{\tau + 2}}}$$

$polar(\theta_1 + \theta_2, \kappa_1)$ 



our understanding

WHEN

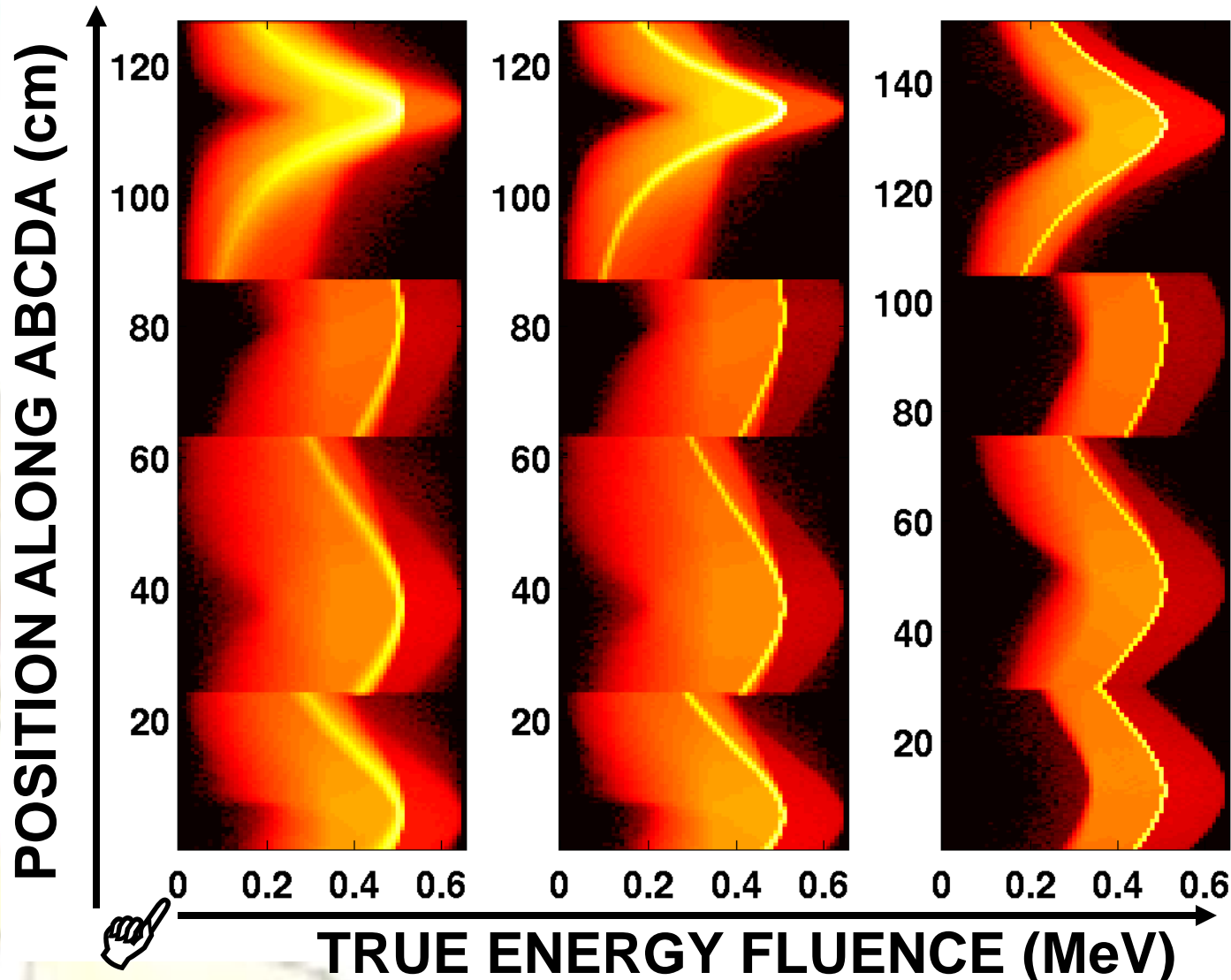
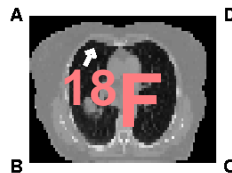
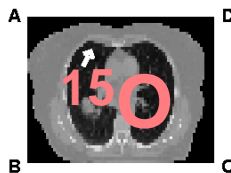
TEXTBOOKS SAY

$180 \pm 0.25^\circ$ OR $180 \pm 0.5^\circ$

THEY ACCOUNTED FOR

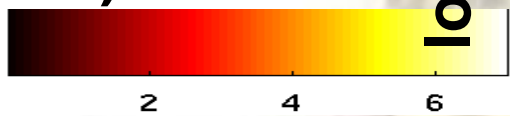
NON-ZERO e^- MOMENTUM, BUT

NOT ANNIHILATION IN-FLIGHT.



Means grazing fluence component, not zero energy.

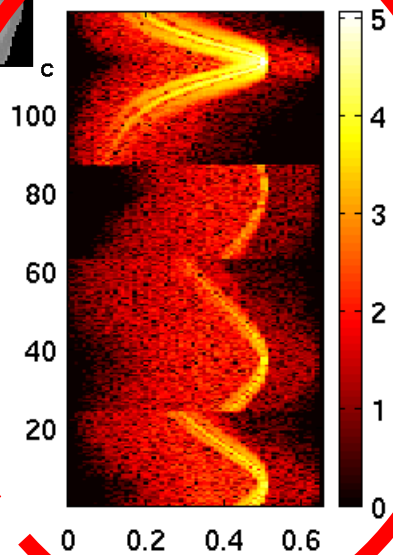
Only 350 ~ 650 keV photons were tallied



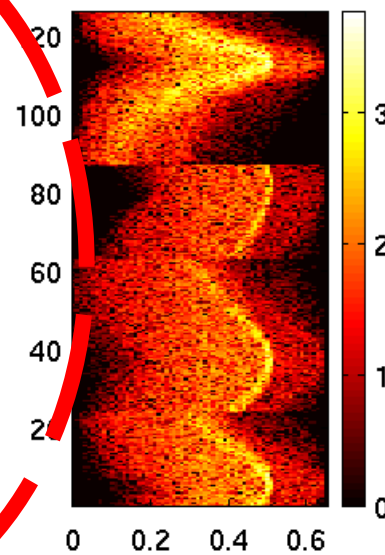
log₁₀ (counts)



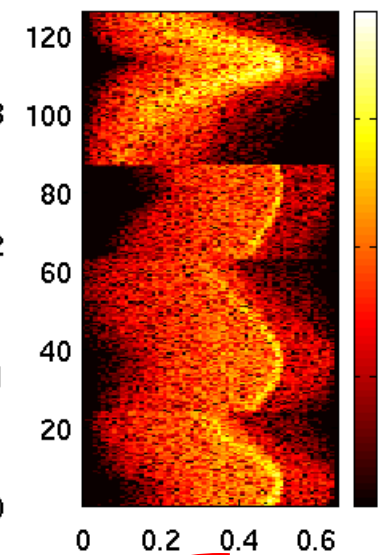
SPIN



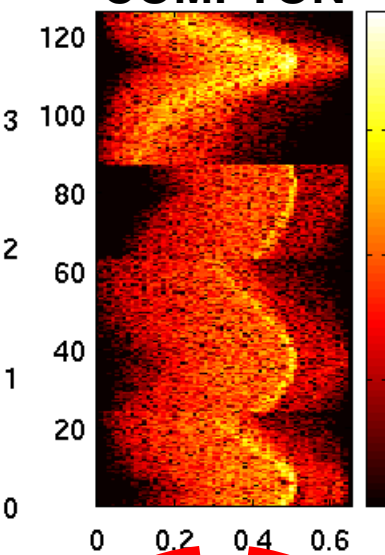
RAYLEIGH



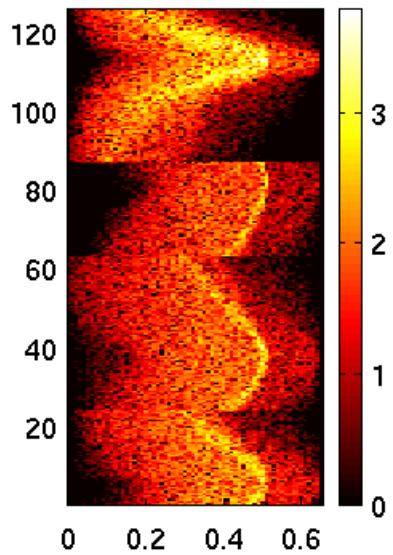
NIST



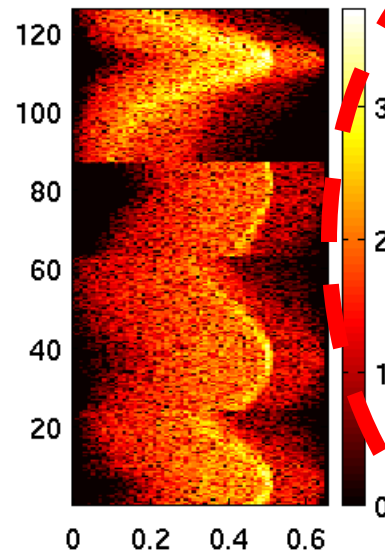
**RADIATIVE
COMPTON**



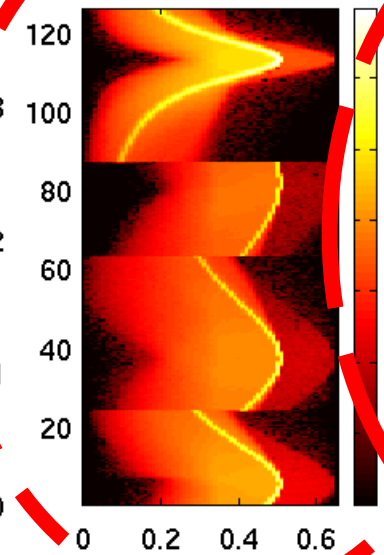
**BOUND
COMPTON**



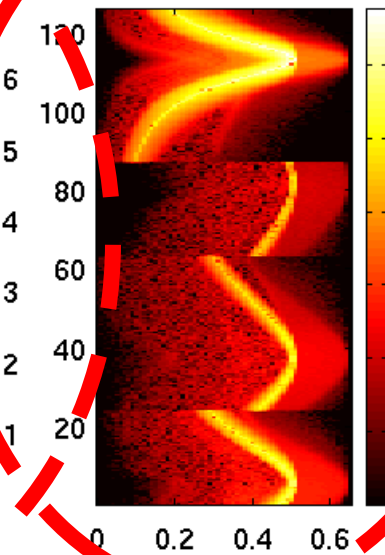
**BREM ANGULAR
SAMPLING**



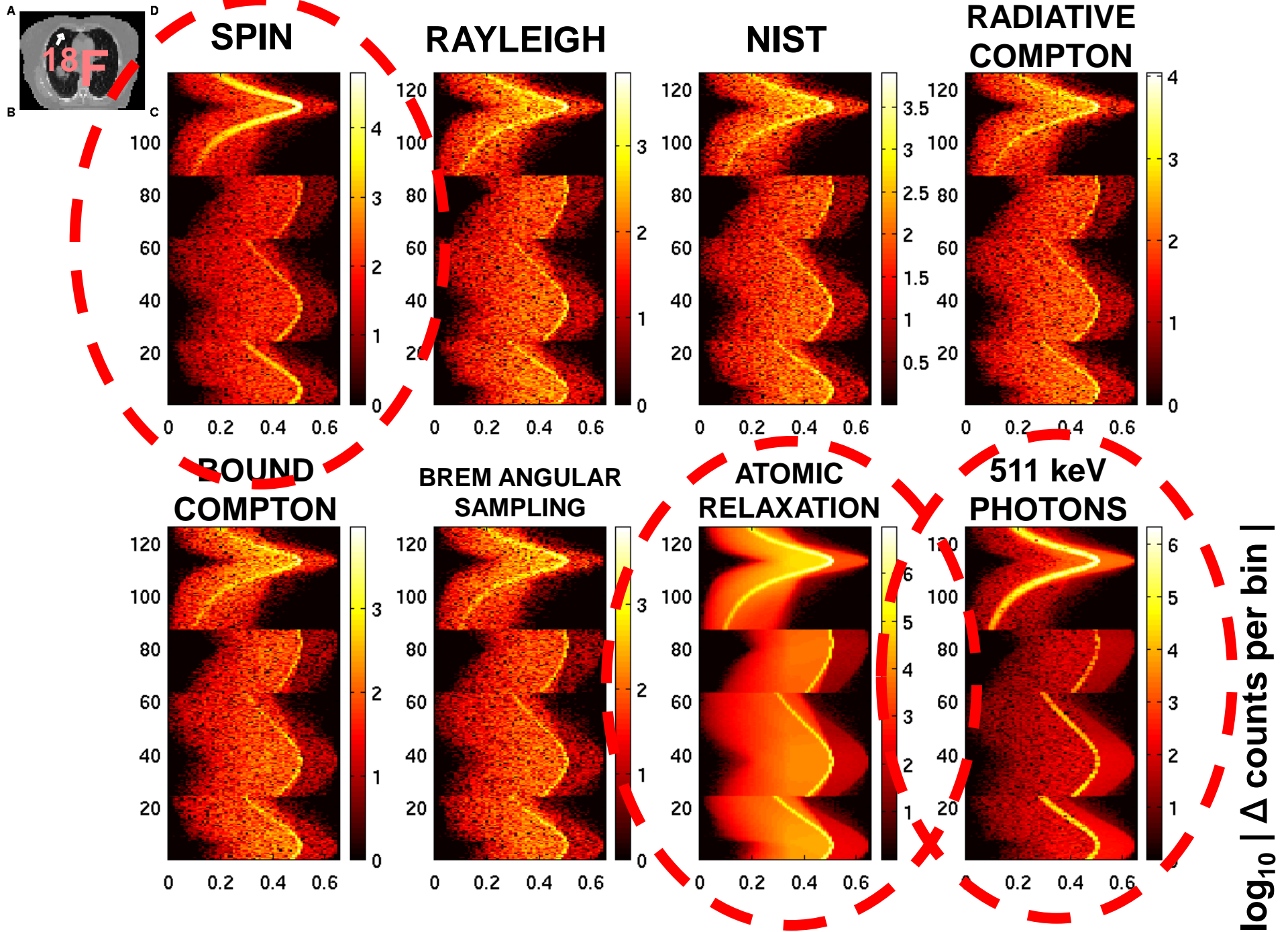
**ATOMIC
RELAXATION**



**511 keV
PHOTONS**



$\log_{10} |\Delta \text{ counts per bin}|$



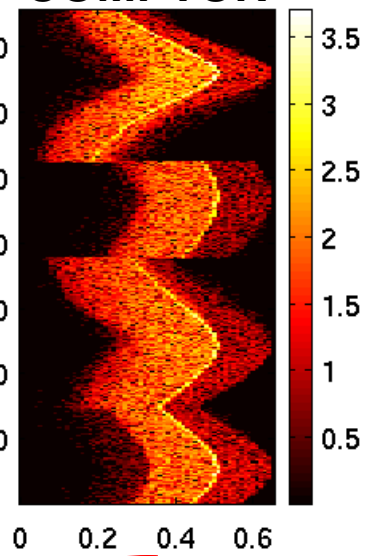
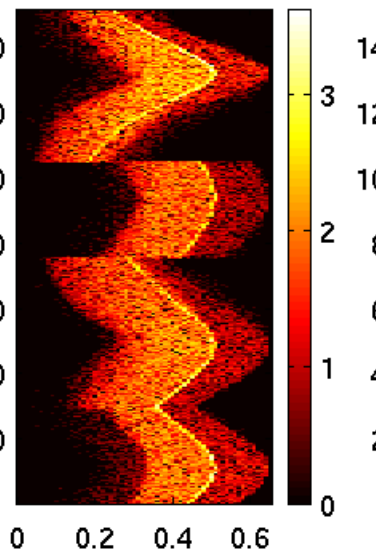
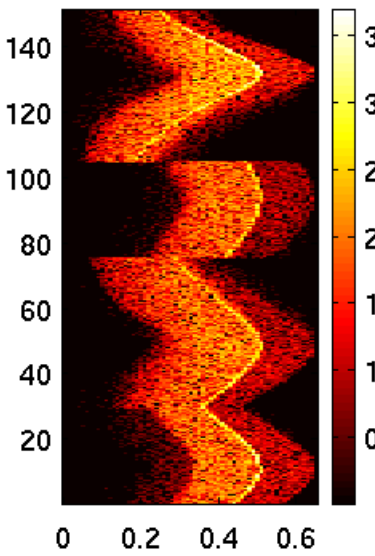
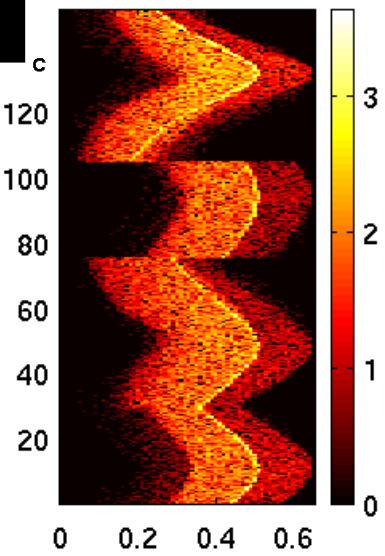


SPIN

RAYLEIGH

NIST

**RADIATIVE
COMPTON**

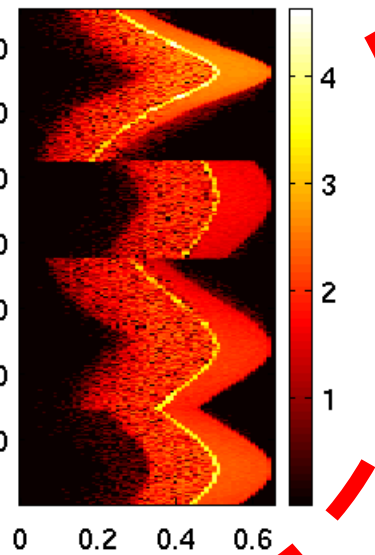
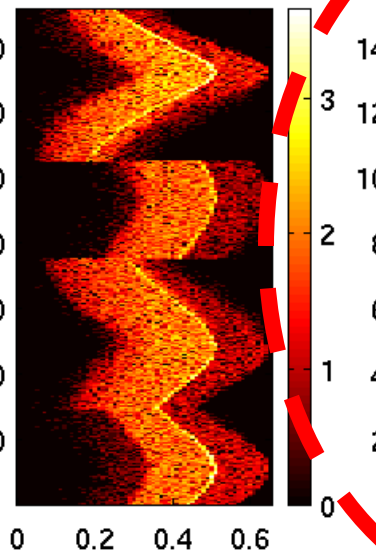
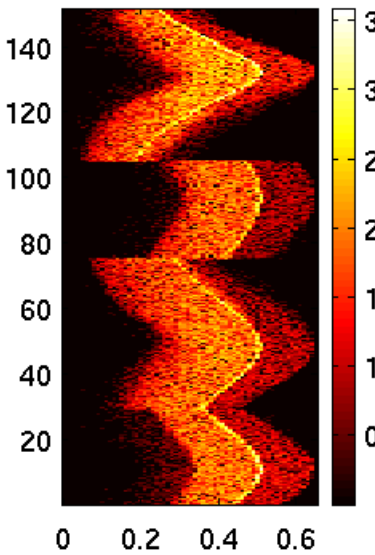
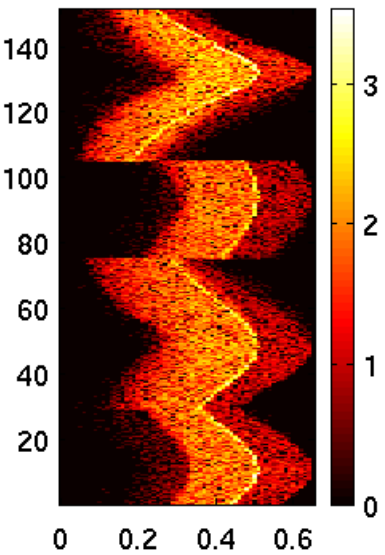


**BOUND
COMPTON**

**BREM ANGULAR
SAMPLING**

**ATOMIC
RELAXATION**

**511 keV
PHOTONS**

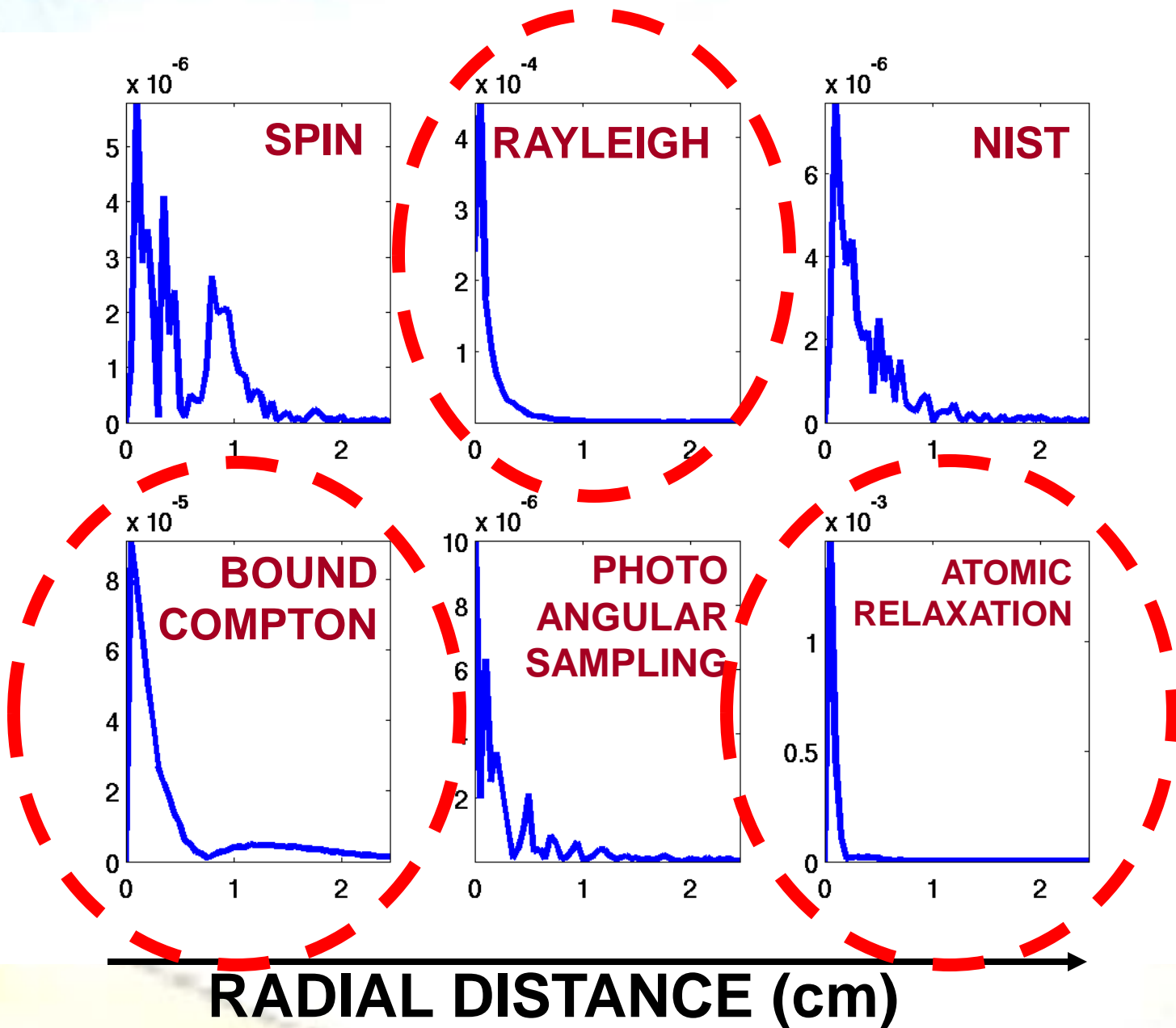


$\log_{10} |\Delta \text{ counts per bin}|$

LSO

History-by-history stats. All bins < 0.5% standard error.

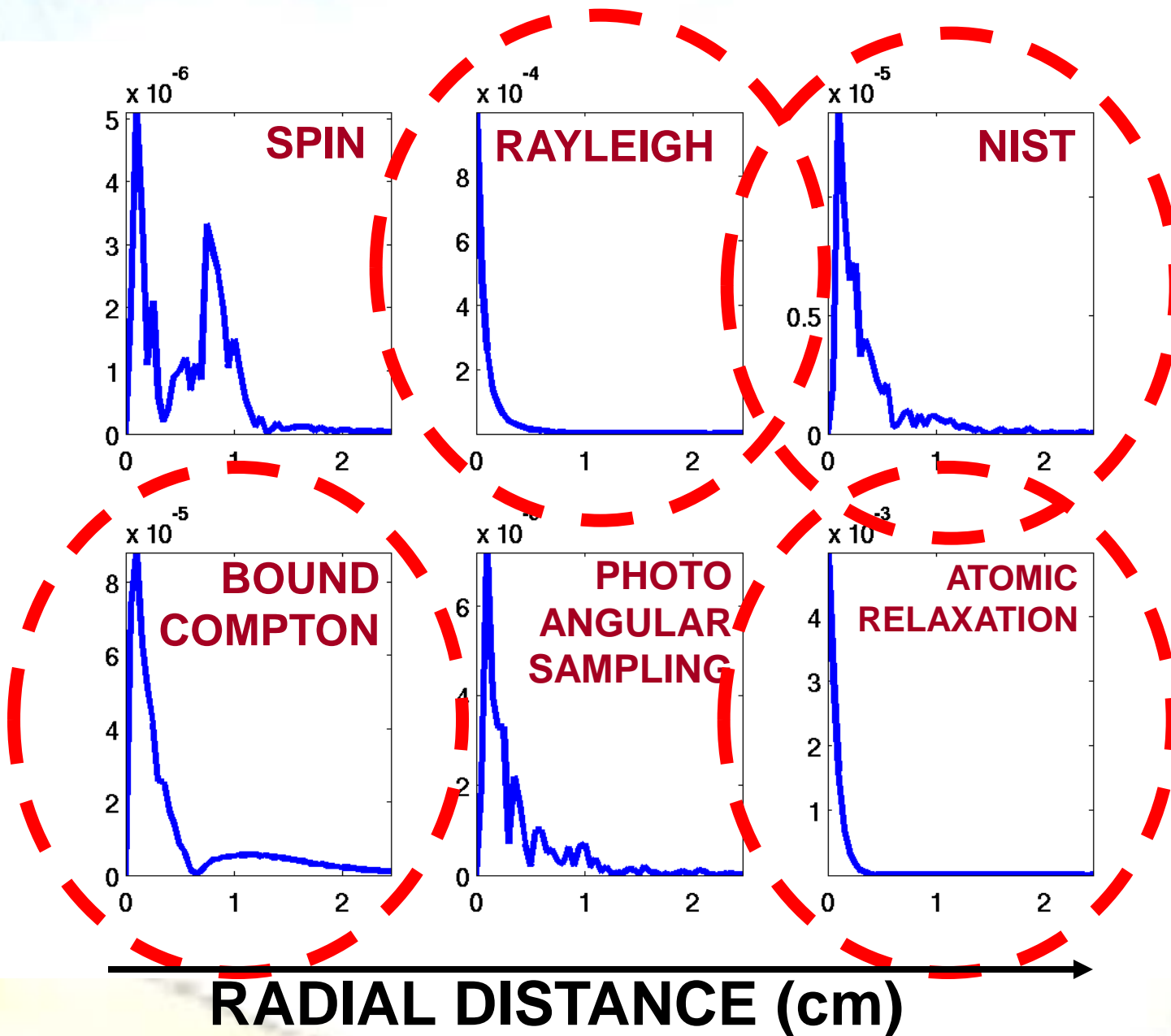
**| Δ EDEP/hist |
(MeV)**

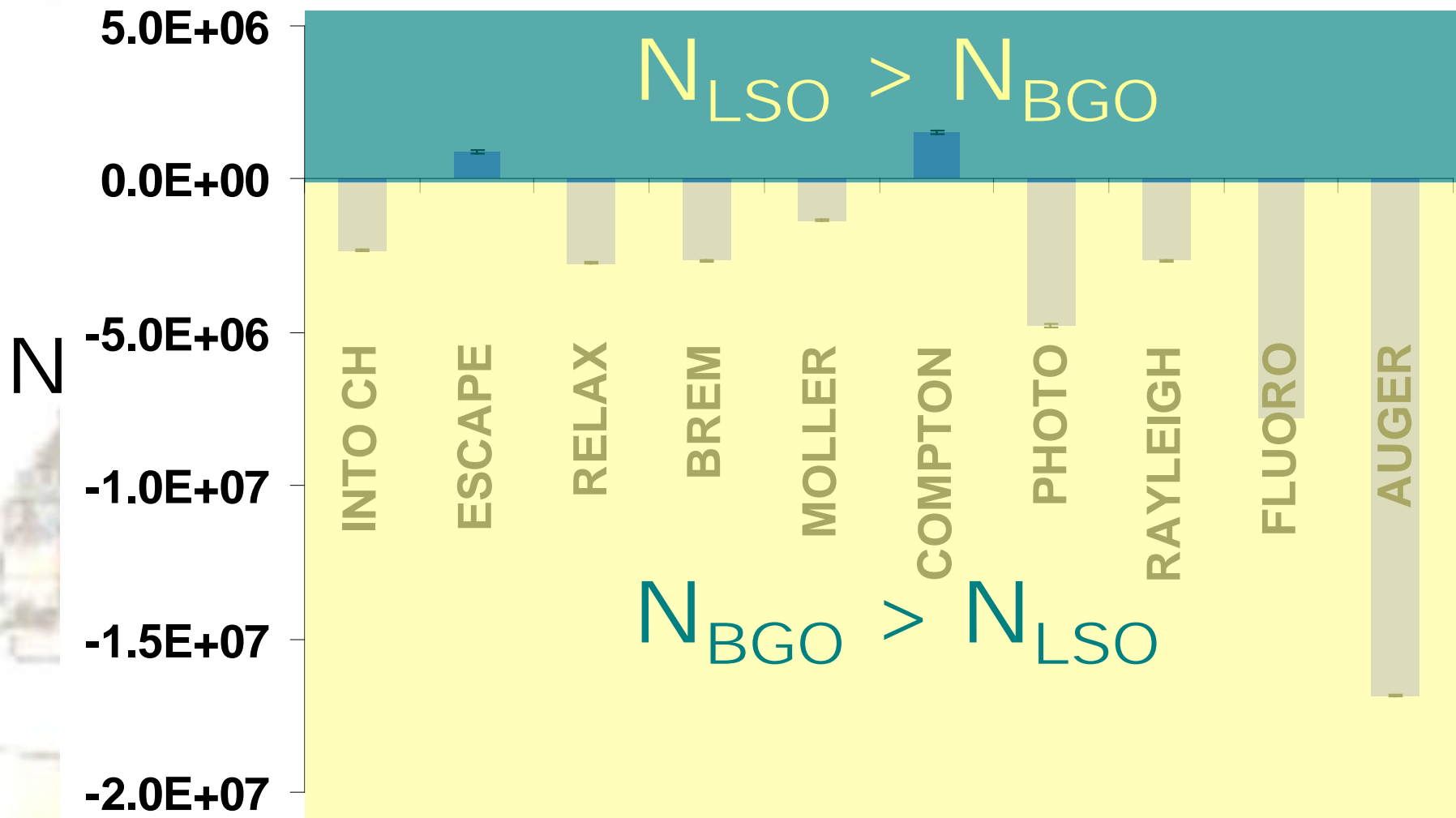


BGO

History-by-history stats. All bins < 0.5% standard error.

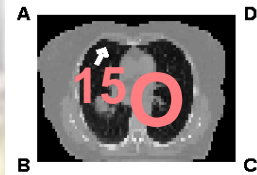
$|\Delta \text{EDEP}/\text{hist}|$
(MeV)





PENELOPE vs EGSnrc

Similar annihilation photon outcome despite different condensed history & multiple scatter.




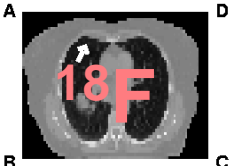

e^+ annihilated at up to 1.58 MeV, producing 0.30 to 2.20 MeV photons 79° to 180° apart.



e^+ annihilated at up to 0.56 MeV, producing 0.33 to 1.18 MeV photons 109° to 180° apart.

RESULTS vs TEXTBOOKS

Textbooks under-estimate deviation from 180° 511 keV. Annihilation in-flight not accounted for.

	SPIN	RAYLEIGH	NIST	BOUND COMPTON	ANGULAR SAMPLING	ATOMIC RELAX
	!				!	!
	!				!	!
						!
LSO		!		!		!
BGO		!	!	!		!



me@marychin.org