A Bethe-Heitler, 5D, Polarized, $\gamma \to e^+e^-$ Pair Conversion Event Generator

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2017 Geant4 User Workshop, G4UW
19 - 22 September 2017, Wollongong

`http://llr.in2p3.fr/~dbernard/polar/harpo-t-p.html`

Talk Layout

- The context: HARPO: high-performance γ-ray astronomy and linear polarimetry with conversion to e^+e^- pairs with a gas TPC

telescope performance studies	NIM A 701 (2013) 225
polarimeter performance studies	NIM A 729 (2013) 765
cosmic-rays TPC tracker characterization	NIM A 718 (2013) 395
polarized γ-ray beam data-taking campaign	PoS (ICRC2015) 1016
high dilution factor polarimetry on beam demonstrated	SPIE (2016) 99052R
arXiv:1706.06483	submitted to Astroparticle Physics
Recent Summary	Il Nuovo Cimento 40 C (2017) 117

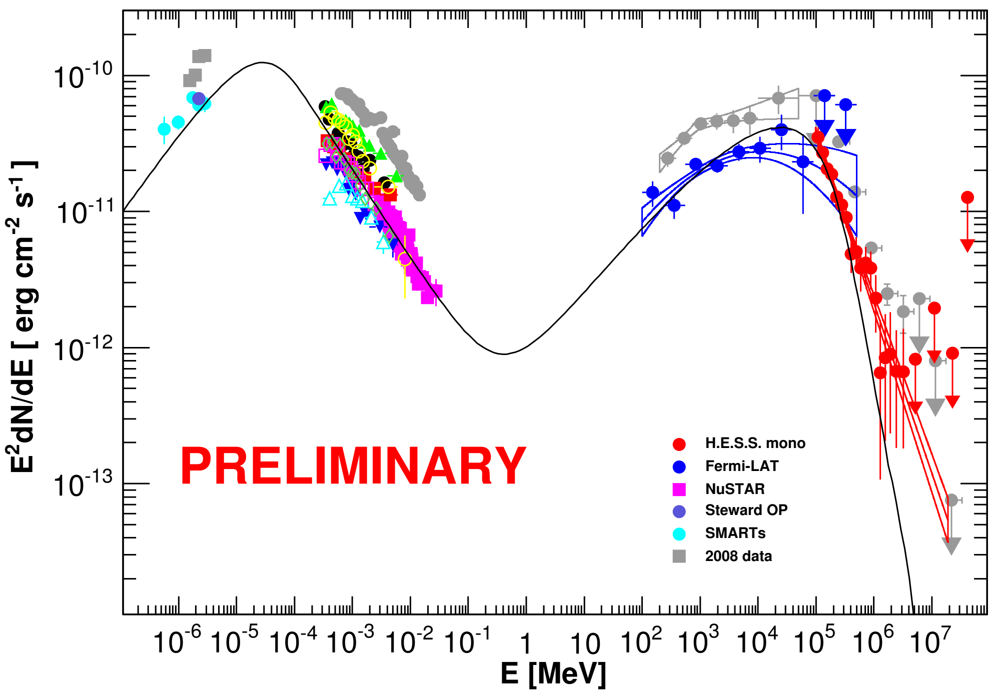
- Event generator:
  - Past achievements: a VEGAS-based generator (FORTRAN)

Exact, 5D, polarized, Event generator	NIM A 729 (2013) 765
Event generator comparison	Astropart. Phys. 88 (2017) 60
	G4SUW, Guildford, April 2017

  - Present activities: towards VEGAS-free generation
  - Perspectives for the future: change it to a private G4EmModel
    - Donation as a public physics model if agreeable by the G4 Coll.

γ-ray sensitivity gap: HBL PKS 2155-304 example

- SED : spectral energy distributions : Flux $\times E^2$



- Grey points: dedicated Multiwavelength campaign 2013:
  - NuSTAR satellite (3-79 keV),
  - the Fermi Large Area Telescope (LAT, 100 MeV-300 GeV)
  - (H.E.S.S.) array phase II

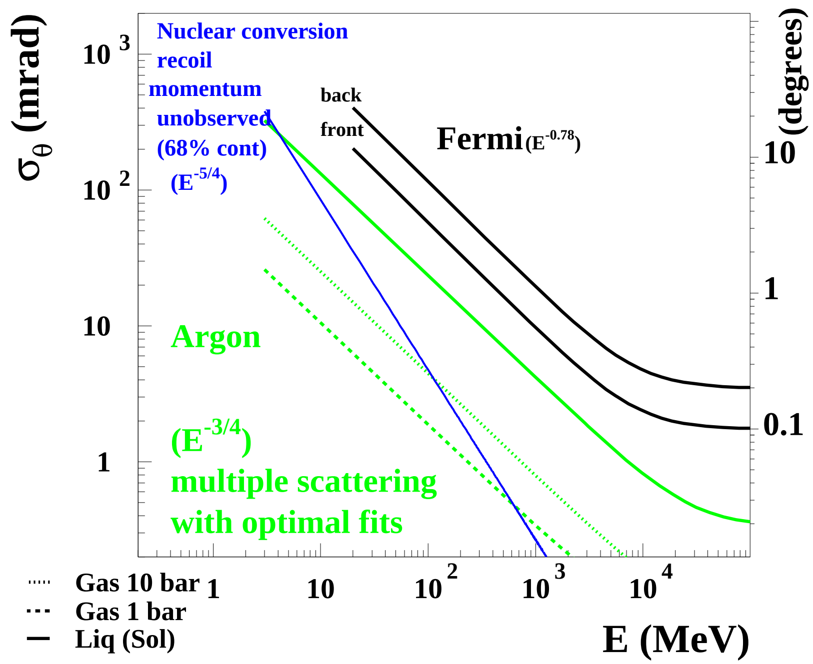
D. A. Sanchez *et al.*, 5th Fermi Symposium: Nagoya, Oct 2014 arXiv:1502.02915v2 [astro-ph.HE]

HARPO: angular resolution and sensitivity

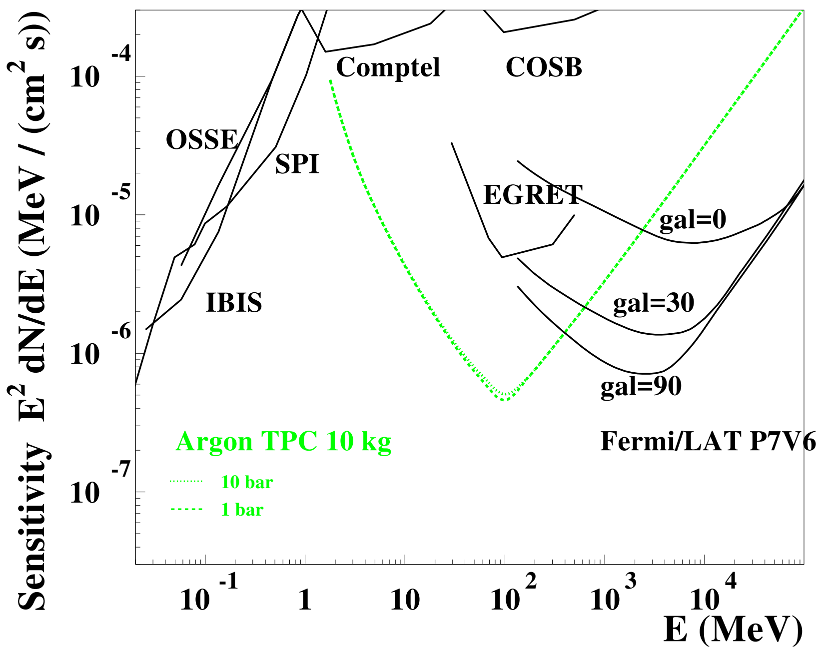
- For $\gamma \to e^+e^-$, the sensitivity wall is mainly an angular resolution wall.

single photon angular resolution
$0.27 \oplus 0.27 = 0.38°$ @ $100\,\mathrm{MeV}$

point-like source sensitivity
(à la Fermi, 3 year, 5σ, $> 10\gamma$ ..)



Nucl. Instrum. Meth. A 701 (2013) 225



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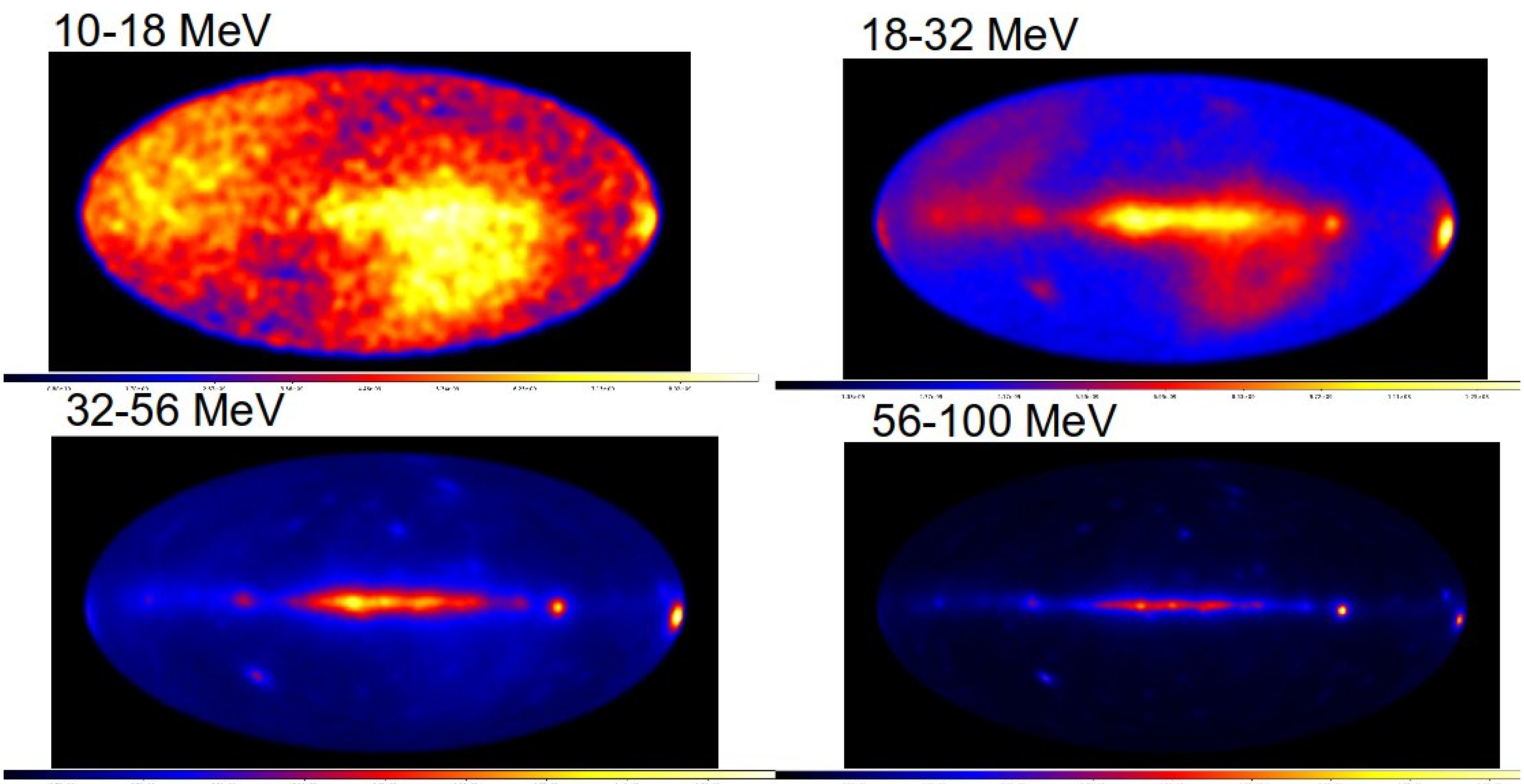
Angular resolution and sensitivity

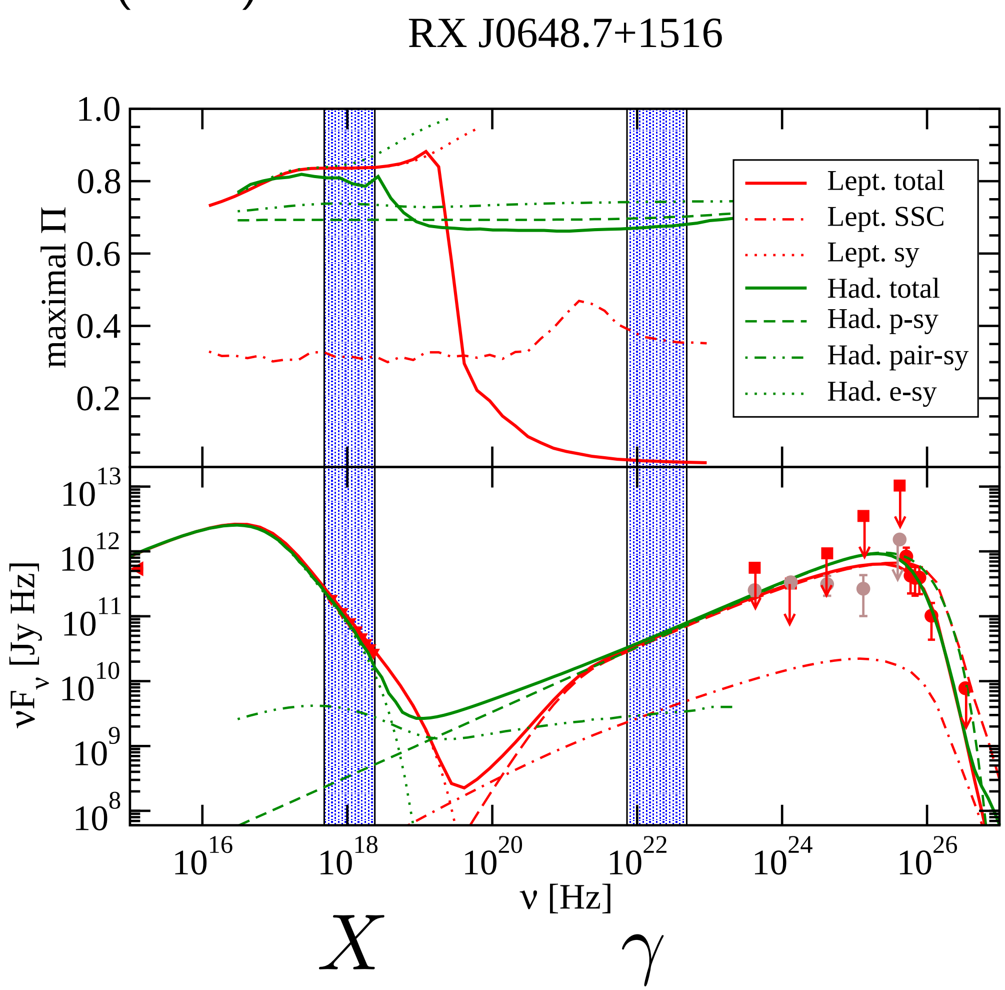
Large Area Telescope on the Fermi space mission, launch 2008



"Fermi-LAT below 100 MeV (Pass8)", J. McEnery, "e-ASTROGAM workshop: the extreme Universe", Padova 2017

Science Case: Polarimetry: Astrophysics

- Blazars: decipher leptonic synchrotron self-Compton (SSC) against hadronic (proton-synchrotron) models
  - high-frequency-peaked BL Lac (HBL)
  - X band: 2 -10 keV
  - γ band: 30 - 200 MeV



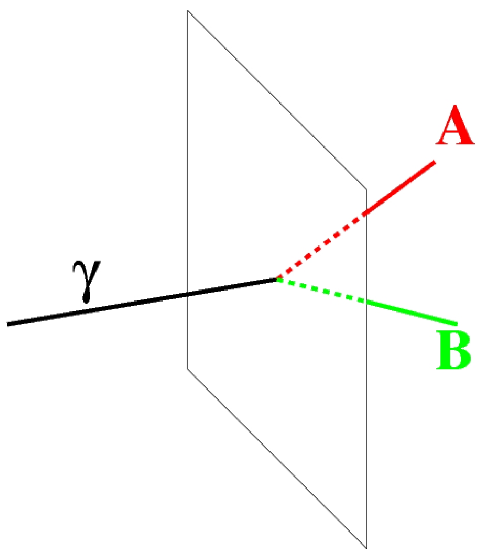
- SED's indistinguishable, but
- X-ray: $P_{\rm lept} \approx P_{\rm hadr}$
- γ-ray: $P_{\rm lept} \ll P_{\rm hadr}$

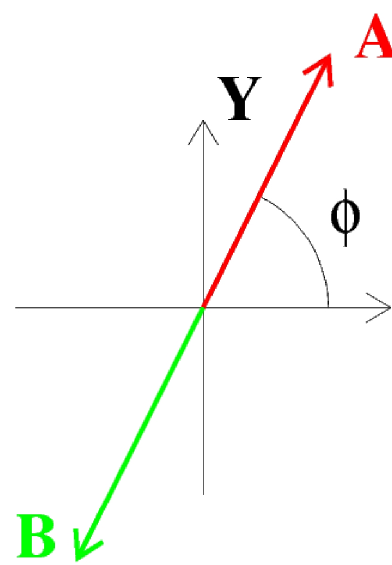
H. Zhang and M. Böttcher,
A.P. J. 774, 18 (2013)

Polarimetry

- Modulation of azimuthal angle distribution

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\phi} \propto (1 + \mathcal{A} P \cos[2(\phi - \phi_0)]), \qquad \sigma_P \approx \frac{1}{\mathcal{A}}\sqrt{\frac{2}{N}},$$



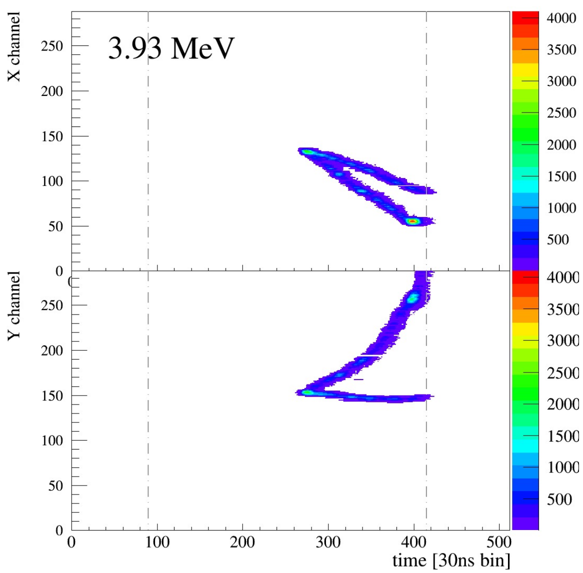


- P source linear polarisation fraction
- $\mathcal{A}$ Polarization asymmetry
- ϕ azimuthal angle

HARPO: Linear polarimetry

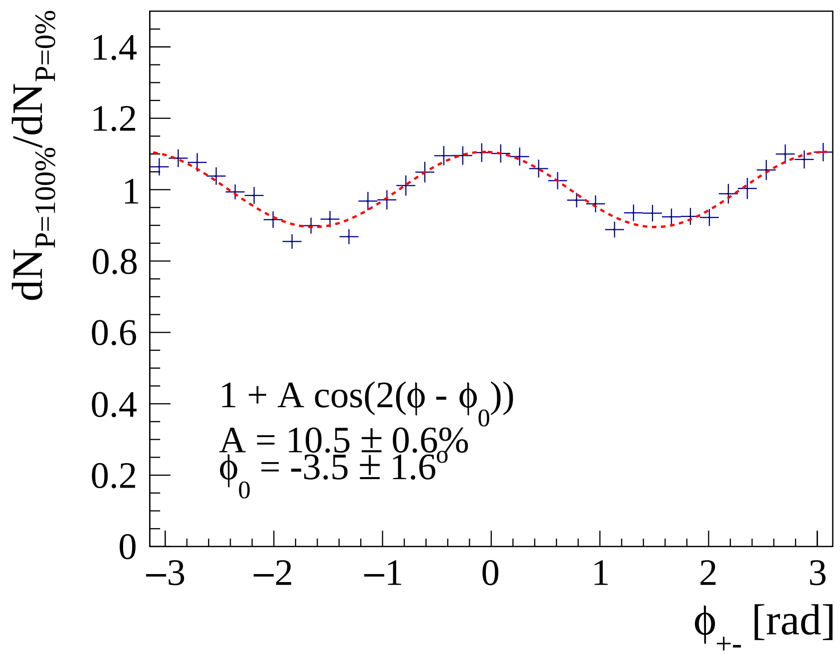
- Polarimetry major diagnostic at low energies (radio - optics - X)
- Missing $E > 1\,\mathrm{MeV}$
- Would enable decipher leptonic/hadronic Blazar models, point to emission region in pulsars, tag the transition energy for magnetars, extend Lorentz invariance violation (LIV) searches sensitivity ...
- Needs large statistics $\longrightarrow$ needs low energies

(x, t) and (y, t) signal maps
$4\,\mathrm{MeV}$ γ in $2.1\,\mathrm{bar}$ Ar-iC4H10 95-5%



SPIE (2016) 99052R

azimuthal angle distribution
$11.8\,\mathrm{MeV}$ γ in $2.1\,\mathrm{bar}$ Ar-iC4H10 95-5%



arXiv:1706.06483, submitted to Astroparticle Physics

An exact, 5D, Polarized Generator

- 5D final state: $\varphi_+, \theta_+, \varphi_-, \theta_-, x_+ \equiv E_+/E_\gamma$
- BASES / SPRING version of the VEGAS method, S. Kawabata, Comp. Phys. Comm. 88, 309 (1995).
- Differential cross section either from:
  - Feyman diagrams (important for low energy triplet) HELAS, H. Murayama, KEK-91-11.
  - Bethe-Heitler approximation (2 dominant diagrams only)
- Exact:
  - no low energy approximation
  - no small angle approximation
  - 5D differential Xsection sampled, no product of 1D differential Xsections
  - strict energy-momentum conservation
- Polarized:
  - linearly polarized photons
  - unpolarized photons
  - partially polarized photons
- Target: nucleus or electron (triplet conversion)
- Atomic electron field screening: form factor $F(q^2)$, coherent (nuclear), incoherent (triplet)
- (2012 - 2013): extensive validations for high-energy photons, $E = 4 - 400, \mathrm{MeV}$

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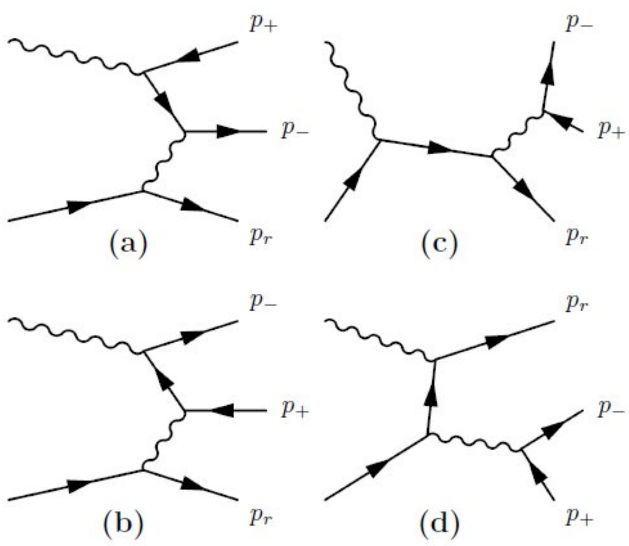
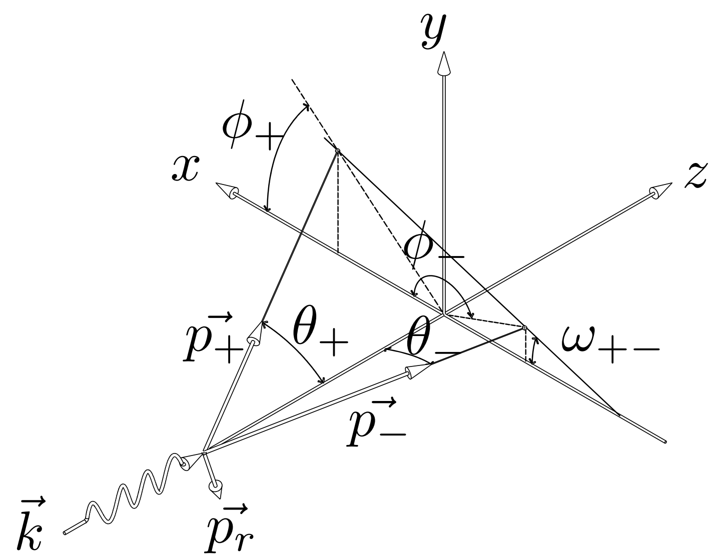
Target, Variables, Feynman diagrams

- Target :

ion	"nuclear conversion"	$\gamma Z \rightarrow e^+ e^- Z$
electron	"triplet conversion"	$\gamma e^- \rightarrow e^+ e^- e^-$

- Variables: azimuthal (ϕ_+, ϕ_-) and polar (θ_+, θ_-) angles of e^+ and e^-, and $x_+ \equiv E_+/E$





- Diagrams
  - (a), (b) dominant, either for nuclear, or triplet at high-energy. (Bethe-Heitler)
  - in addition, for triplet, 4 additional "exchange" diagrams.

Bethe-Heitler differential cross section: 1

- Linearly polarized gamma rays: $(c = 1, \quad \hbar = 1, \quad E = \hbar\omega = \omega)$

$$
\begin{aligned}
\mathrm{d}\sigma \quad = \quad & \frac{-2\alpha Z^2 r_0^2 m^2}{(2\pi)^2\omega^3}\mathrm{d}E_+\mathrm{d}\Omega_+\mathrm{d}\Omega_- \frac{|p_-||p_+|}{|\vec{q}|^4}\left[\left(2E_+\frac{p_-\sin\theta_-\cos(\psi+\phi)}{E_- - p_-\cos\theta_-} + 2E_-\frac{p_+\sin\theta_+\cos\psi}{E_+ - p_+\cos\theta_+}\right)^2\right. \\
& -q^2\left(\frac{p_-\sin\theta_-\cos(\psi+\phi)}{E_- - p_-\cos\theta_-} - \frac{p_+\sin\theta_+\cos\psi}{E_+ - p_+\cos\theta_+}\right)^2 \\
& \left. -\omega^2\,\frac{(p_+\sin\theta_+)^2 + (p_-\sin\theta_-)^2 + 2p_+p_-\sin\theta_+\sin\theta_-\cos\phi}{(E_- - p_-\cos\theta_-)(E_+ - p_+\cos\theta_+)}\right]
\end{aligned}
$$

with: $\quad |\vec{q}|^2 = |\vec{p_+} + \vec{p_-} - \vec{k}|^2, \quad \psi \equiv \varphi^+ \quad$ and $\quad \psi + \phi \equiv \varphi^-$

M. May, Phys. Rev. 84, 265 (1951).
Correction by a factor of 2: Jauch and Rohrlich, *The theory of photons and electrons* (Springer Verlag, 1976).

- Non polarized gamma rays:

$$
\begin{aligned}
& \frac{-\alpha Z^2 r_0^2 m^2}{(2\pi)^2\omega^3}\mathrm{d}E_+\mathrm{d}\Omega_+\mathrm{d}\Omega_- \frac{|p_-||p_+|}{|\vec{q}|^4}\left[\left(\frac{p_+\sin\theta_+}{E_+ - p_+\cos\theta_+}\right)^2(4E_-^2 - q^2) + \left(\frac{p_-\sin\theta_-}{E_- - p_-\cos\theta_-}\right)^2(4E_+^2 - q^2) +\right. \\
& \left.\frac{2p_+p_-\sin\theta_+\sin\theta_-\cos\phi}{(E_- - p_-\cos\theta_-)(E_+ - p_+\cos\theta_+)}(4E_+E_- + q^2 - 2\omega^2) - 2\omega^2\frac{(p_+\sin\theta_+)^2 + (p_-\sin\theta_-)^2}{(E_+ - p_+\cos\theta_+)(E_- - p_-\cos\theta_-)}\right]
\end{aligned}
$$

"The quantum theory of radiation", W. Heitler, 1954.

Bethe-Heitler differential cross section: 2

- That is: $\mathrm{d}\sigma = \Phi(X_u + P \times X_p)\mathrm{d}E_+\mathrm{d}\Omega_+\mathrm{d}\Omega_-$ with $\Phi = \frac{-\alpha Z^2 r_0^2 m^2}{(2\pi)^2\omega^3}\frac{|p_-||p_+|}{|\vec{q}|^4}$
- P the **linear** polarization fraction of the incident photon, And:

$$X_u = \left[\left(\frac{p_+ \sin\theta_+}{E_+ - p_+\cos\theta_+}\right)^2 (4E_-^2 - q^2) + \left(\frac{p_- \sin\theta_-}{E_- - p_-\cos\theta_-}\right)^2 (4E_+^2 - q^2) + \frac{2p_+p_- \sin\theta_+ \sin\theta_- \cos\phi}{(E_- - p_-\cos\theta_-)(E_+ - p_+\cos\theta_+)}(4E_+E_- + q^2 - 2\omega^2) - 2\omega^2 \frac{(p_+\sin\theta_+)^2 + (p_-\sin\theta_-)^2}{(E_+ - p_+\cos\theta_+)(E_- - p_-\cos\theta_-)}\right]$$

$$X_p = \cos 2(\phi+\psi)(4E_+^2 - q^2)\left(\frac{p_-\sin\theta_-}{E_- - p_-\cos\theta_-}\right)^2 + \cos 2\psi(4E_-^2 - q^2)\left(\frac{p_+\sin\theta_+}{E_+ - p_+\cos\theta_+}\right)^2 + 2\cos(\phi + 2\psi)(4E_+E_- + q^2)\frac{p_-\sin\theta_- p_+\sin\theta_+}{(E_- - p_-\cos\theta_-)(E_+ - p_+\cos\theta_+)}$$

- Partial screening effect of (other) atomic electrons parametrized by form factor (fn of q)
- Differential cross section does not depend on **circular** polarization fraction at this first order of Born approximation

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Gears

- Variables that are actually generated:

variable	related to	
$\lambda(1)$	recoil polar angle	in the CMS (center of mass system)
$\lambda(2)$	recoil azimutal angle	
$\lambda(3)$	pair Invariant Mass(MeV)	
$\lambda(4)$	positron polar angle	in the pair CMS frame
$\lambda(5)$	positron azimutal angle	in the pair CMS frame

- Output:
  - e^+, e^- and recoil 4-vectors
  - A series of additional (redundant) information .. pair opening angle, azimutal angle ..

- Photon energy validity range:

real*8	threshold to 100 GeV
real*16	threshold to 1 PeV,

above which the differential cross section becomes negative in some corners of the variable space.

First batch of validations (2012)

- Comparison of the total mass attenuation coefficients (argon; with and without screening; triplet and nuclear) with the data from NIST

  J. H. Hubbell et al., J. Phys. Chem. Ref. Data 9, 1023 (1980).

- Comparison triplet / nuclear q-distribution ratio with analytical calculations

  K. J. Mork, Phys. Rev. 160, 1065 - 1071 (1967).

- Triplet: $\sigma(q > q_0)$, cross section for recoil electron momentum larger than q_0, compared with high-energy asymptotic expression

  M. L. Iparraguirre and G. O. Depaola, Eur. Phys. J. C 71, 1778 (2011).

- Most probable opening compared with $\hat{\theta}_{+-} \approx \dfrac{1.6\,\mathrm{MeV}}{E}$

  H. Olsen, Phys. Rev. 131, 406 - 415 (1963)

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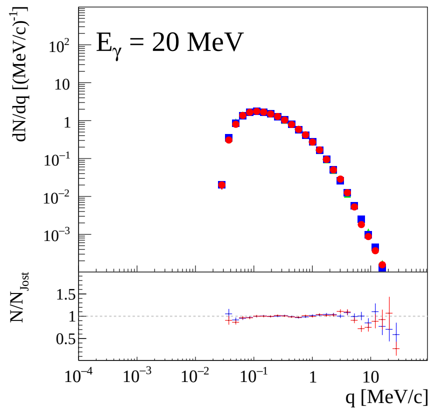
See slides 11-14 of my presentation at G4SUW

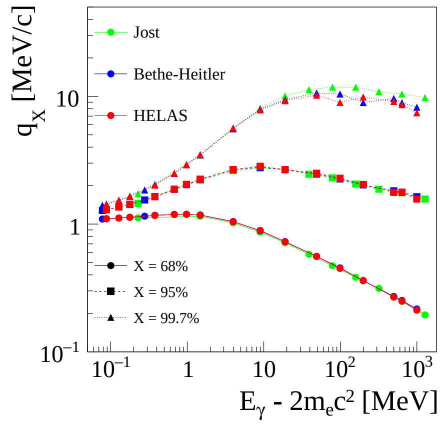
More on validations

- Extend to 1.1 MeV - 1 GeV

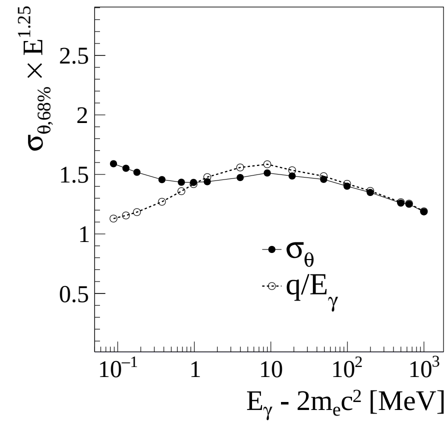
recoil momentum q



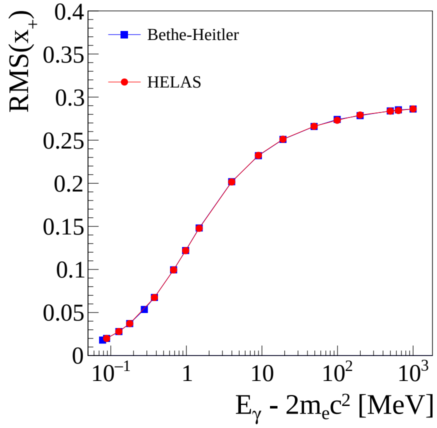
recoil momentum q containment



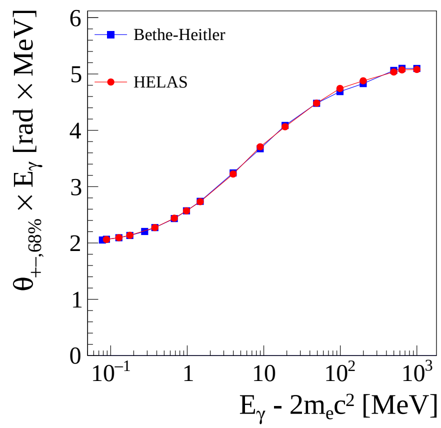
angular resolution containment



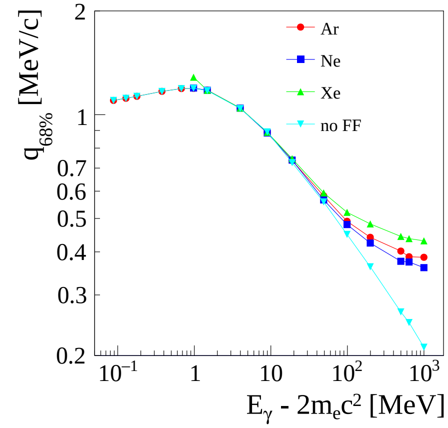
R.M.S. of $x_+ \equiv E_+/E$



opening angle containment



recoil momentum containment



R. Jost, "Distribution of Recoil Nucleus in Pair Production by Photons," Phys. Rev. 80, 189 (1950).

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γ *Conversion Event Generators: A Comparison*

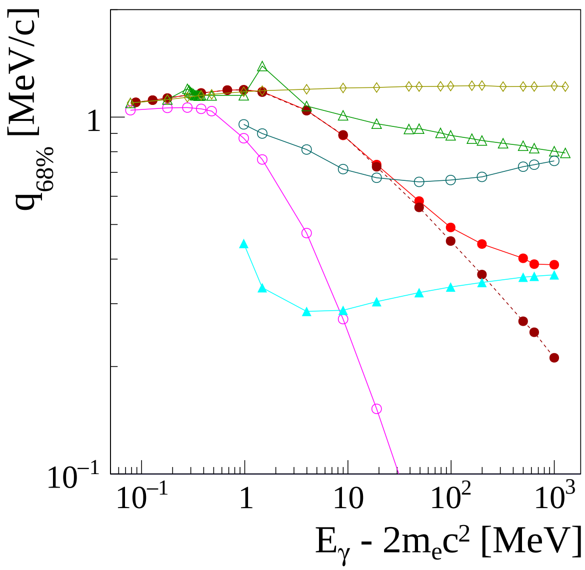
Name	Model	Generator
HELAS	HELAS Feynman amplitudes	BASES/SPRING
Bethe-Heitler	Bethe-Heitler	BASES/SPRING
G4:emstandard	G4BetheHeitler	Geant4 10.02.01
G4:livermorepola	G4LivermorePolarizedGammaConversion	Geant4 10.02.01
G4:penelope	G4PenelopeGammaConversion	Geant4 10.02.01
EGS0	egs5, IPRDST$= 0$	egs5 1.0.6
EGS2	egs5, IPRDST$= 2$	egs5 1.0.6

- *G4:livermore* has same kinematics as *G4:emstandard* : not shown here
- Vladimir has "fixed Livermore and standard pair production below 50 MeV in the Geant4 10.4beta release".

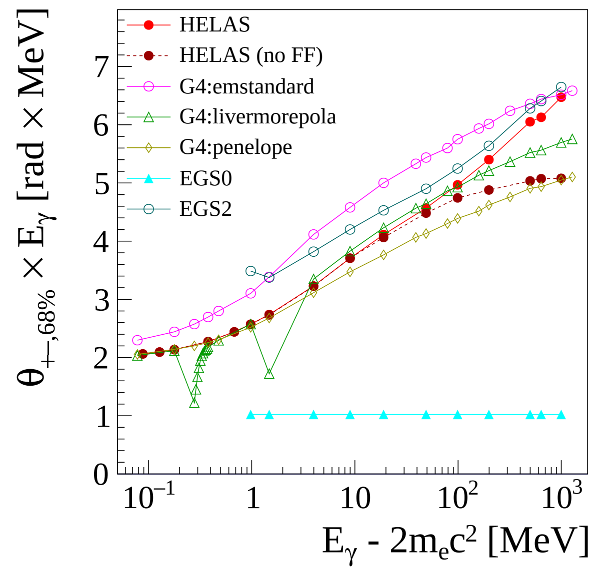
  The modified version is being tested. Not in this talk

Event Generator Comparison: Kinetic Variables

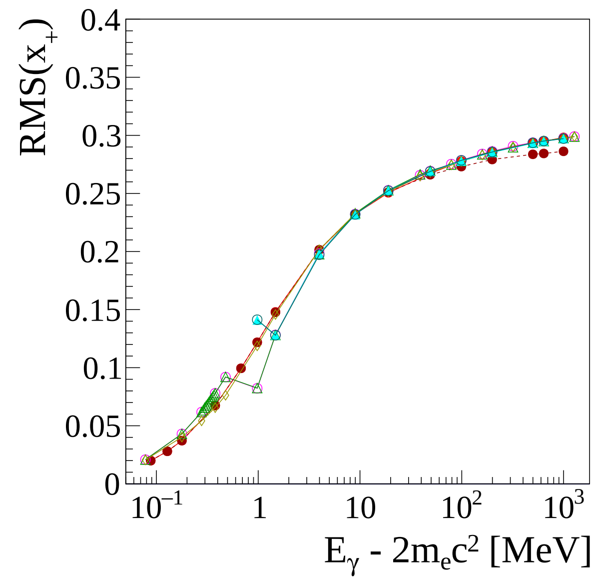
recoil momentum containment



opening angle containment



R.M.S. of $x_+ \equiv E_+/E$



- Recoil momentum incorrectly simulated by G4 and EGS5 physics models
- Inspection of code and/or documentation shows that they (most often) don't even conserve energy-momentum.

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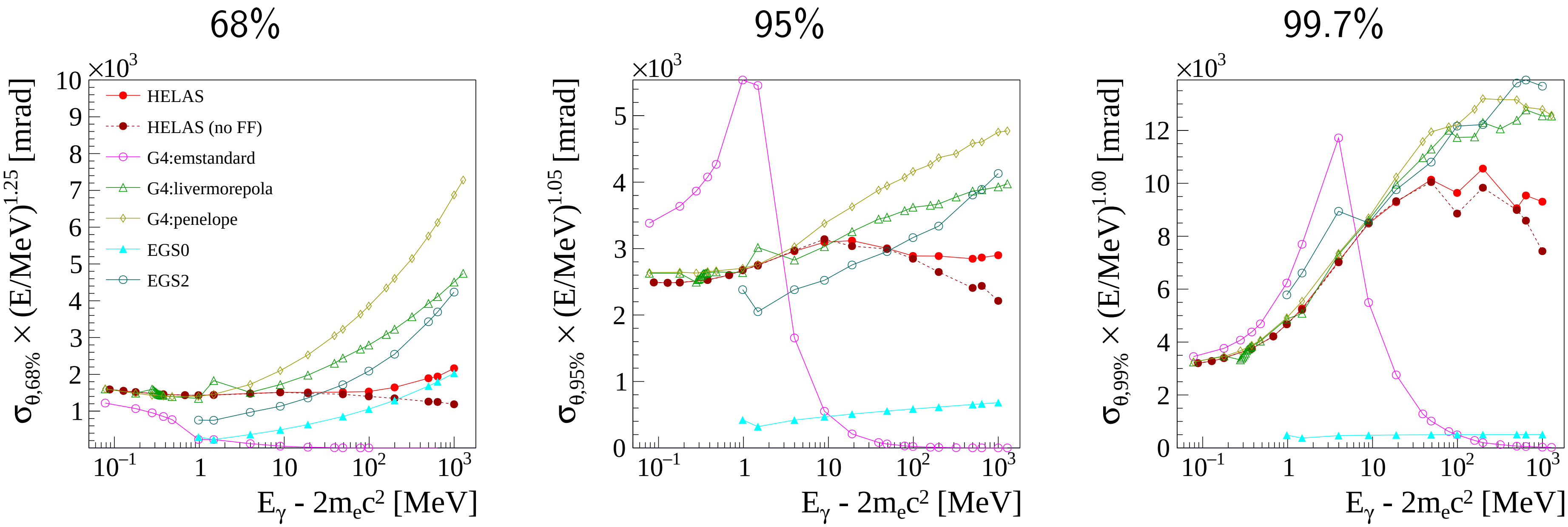
Event Generator Comparison: Angular Resolution



- HELAS: Form Factor (argon): an effect for $E > 100\mathrm{MeV}$
- HELAS: parametrization of σ_θ:

68%	$1.5\,\mathrm{rad}\,(E/\mathrm{MeV})^{-1.25}$
95%	$2.9\,\mathrm{rad}\,(E/\mathrm{MeV})^{-1.05}$
99.7%	$4-9\,\mathrm{rad}\,(E/\mathrm{MeV})^{-1.00}$

- G4 and EGS5 models have 68% angular resolution crazy.
  - Most often, e^+ and e^- generated back-to-back and polar angles generated independently: does not conserve energy-momentum.

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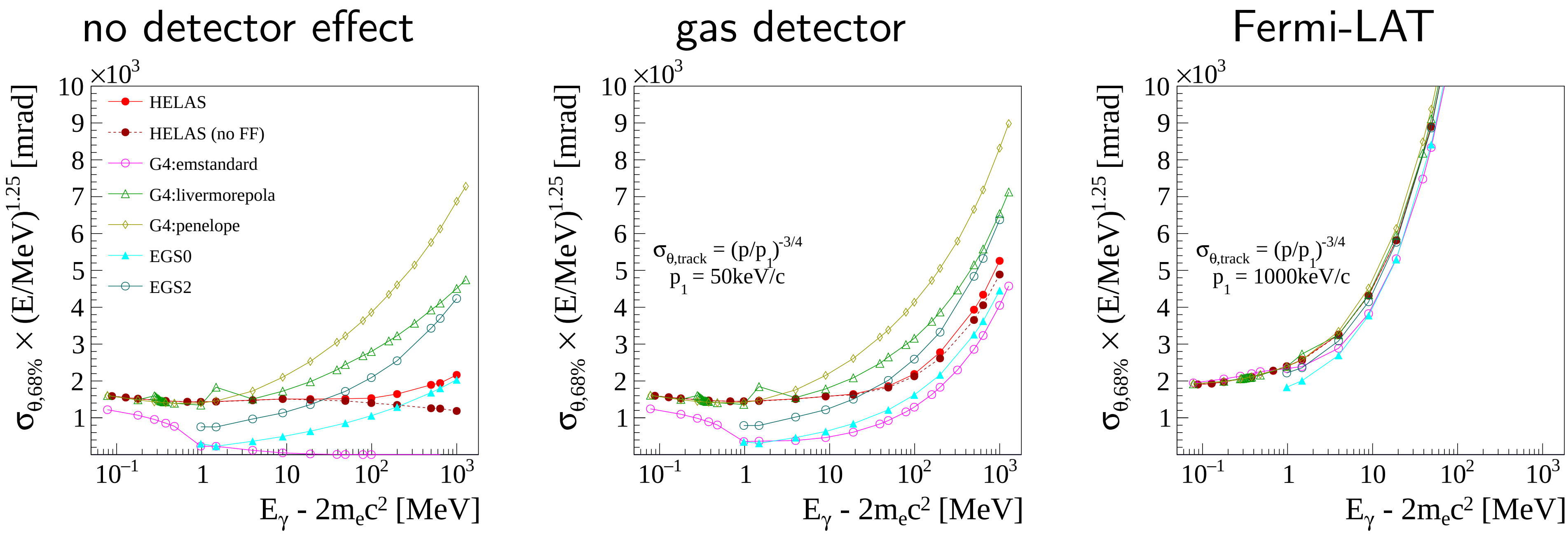
Event Generators and Telescopes



- For dense, high-Z telescopes, the multiple scattering washes out track correlations and therefore the event generator differences

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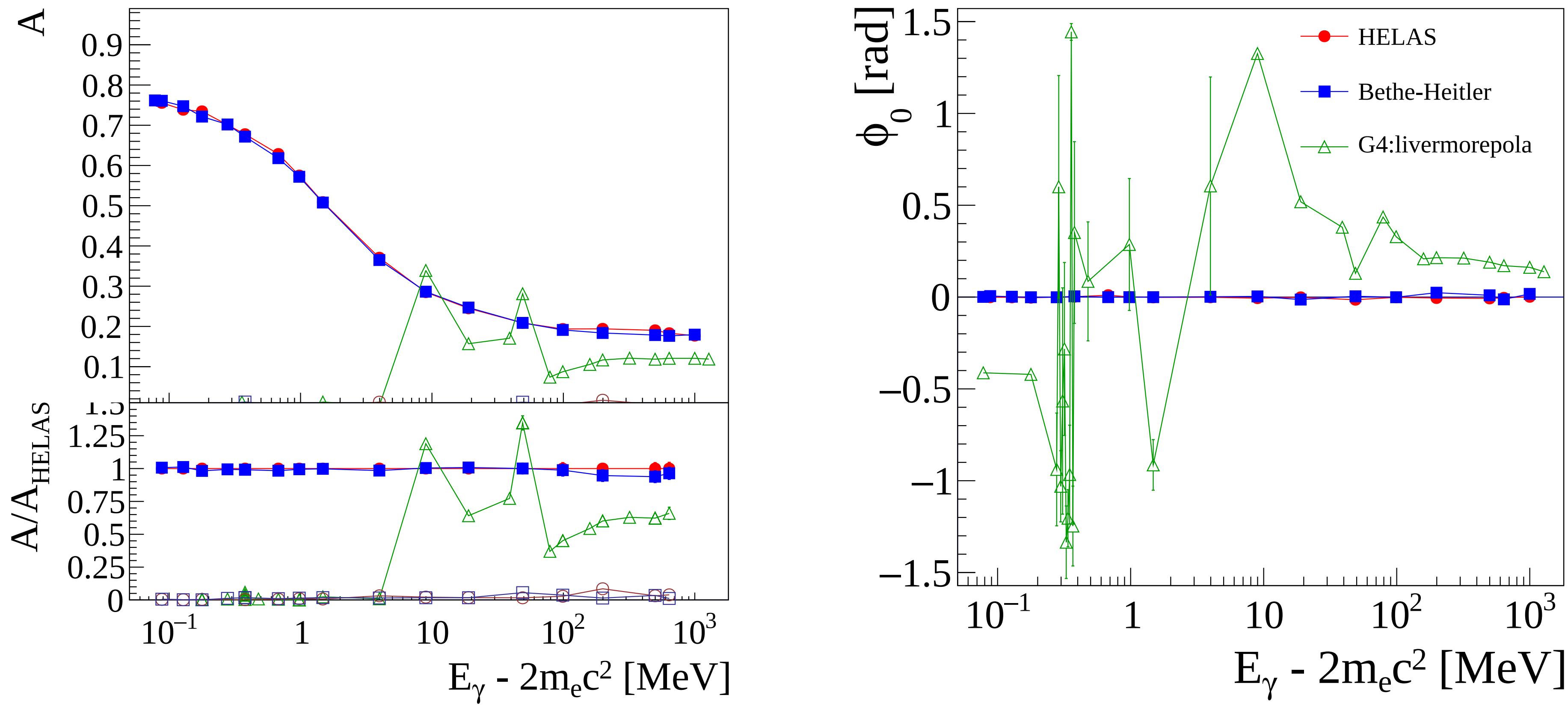
Event Generators and Photon Linear Polarization



- Simulation of polarized γ conversion to pairs by G4:livermorepola surprising (polarisation asymmetry and polarisation angle)

@ 100 MeV, $$\frac{\mathcal{A}_{(\text{HELAS or BH})}}{\mathcal{A}_{\text{G4:livermorepola}}} = \frac{(19.1 \pm 0.4)\%}{(8.7 \pm 0.6)\%} \approx 2.2$$

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VEGAS: Multi-dimensional integration and event generation with package BASES/SPRING

- Method: The VEGAS algorithm, due to G. P. Lepage (J. Comput. Phys. 27 (1978) 192)
- Instantiation: BASES/SPRING (S. Kawabata, Comput. Phys. Commun. 88 (1995) 309.)
- Integration:
  - n-D hyper-volume first segmented in identical cells (n-dimensional bins);
  - pdf and its variance evaluated in each cell, by shooting a number of points;
  - hyper-volume segmentation then tuned iteratively, so as to minimize the variance;
  - upon convergence, an optimal tabulation of the pdf is obtained.
- Event generation:
  - an "exact" generation from $f(\lambda)$ is then obtained easily from the tabulated $f_0(\lambda)$ the acceptance-rejection method
- The pdf depends on photon energy E (and target nature through $F(q^2)$)
  - the integration step is time consuming (few seconds)
  - generation of batches of zillions events with same energy easy.

Towards a VEGAS-free version

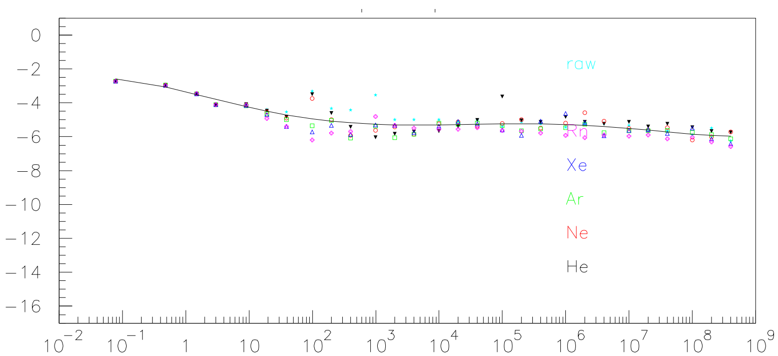
- No sign of (Bethe-Heitler)-HELAS difference: **HELAS dropped**
- **VEGAS dropped**
  - 3 variables taken flat.
  - variables related to
    - the pair Invariant Mass
    - the recoil polar angle

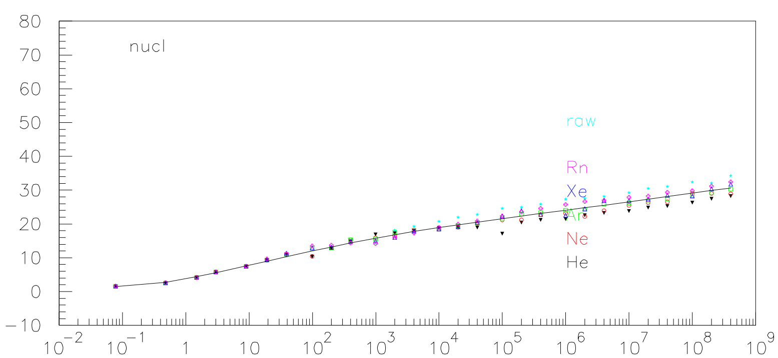
    each taken after a parametrized 1D pdf.
- p_0 pdf of the Ansatz known, product of the 1D ingredients.
- Exact Bethe-Heitler pdf p generated with acceptance-rejection method

Example: variable related to the pair Invariant Mass

- variation with remaining kinetic energy of the 2 parameters of the pdf model

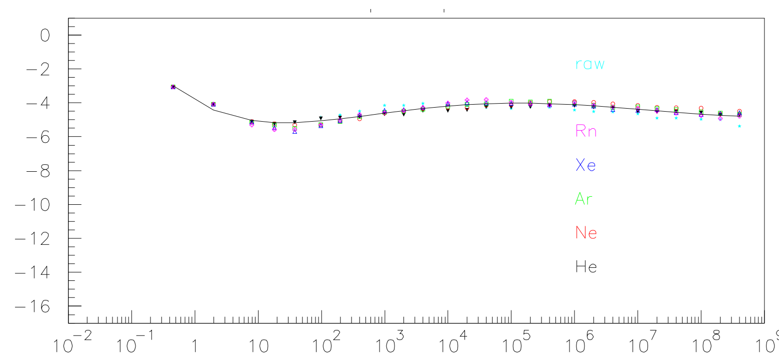
nuclear conversion

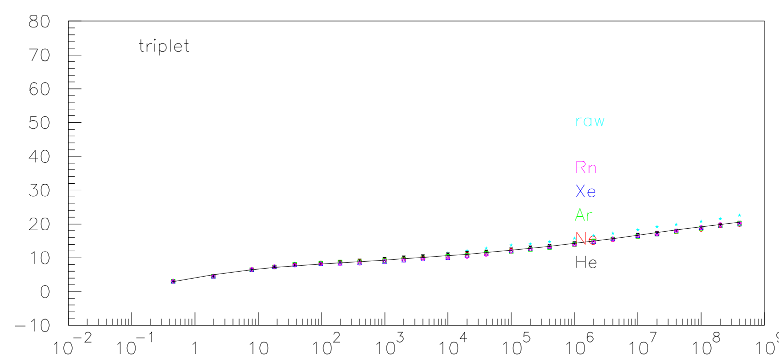




$$E_{kin} = E - 2mc^2 \text{ (MeV)}$$

triplet conversion



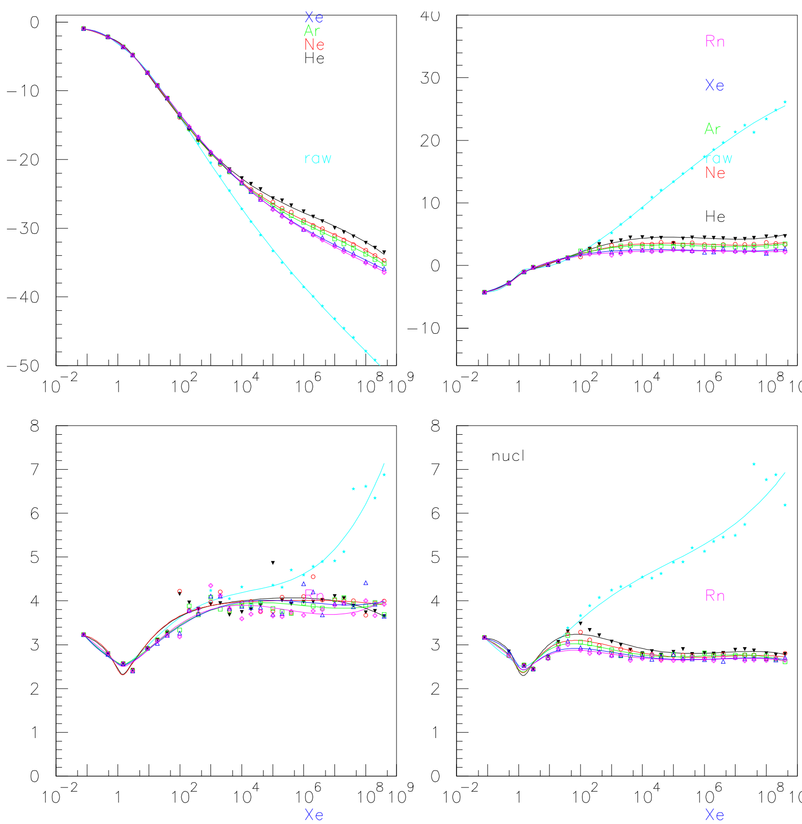


$$E_{kin} = E - 4mc^2 \text{ (MeV)}$$

Example: variable related to the recoil polar angle

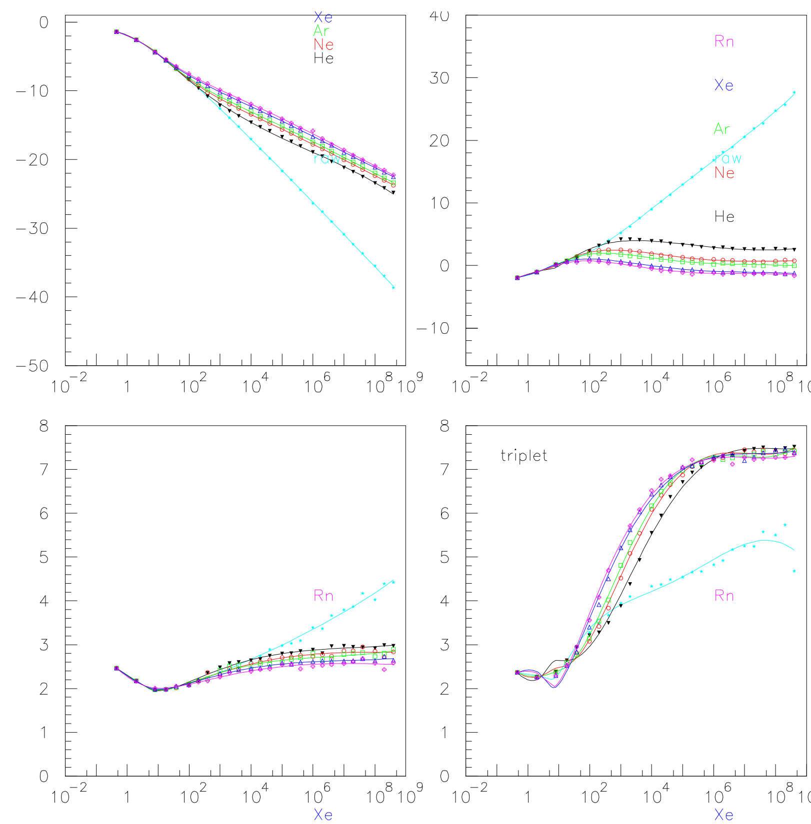
- variation with remaining kinetic energy of the 4 parameters of the pdf model

nuclear conversion



$E_{kin} = E - 2mc^2$ (MeV)

triplet conversion



$E_{kin} = E - 4mc^2$ (MeV)

Perspectives for the future: a Geant4 Physics Model

- Still some tuning to be finalised

- Fortran $\rightarrow$ C++ $\rightarrow$ private G4EmModel
    - G4 experts expertise will be welcome.

- Donation to the Geant4 Collaboration if agreeable by the G4 Coll.

Conclusion

- Presently available physical models on the market inapropriate:
    - for simulation of high-resolution γ telescopes with pairs
    - for simulation of γ polarimeters with pairs

- VEGAS-based exact, 5D, polarized event photon conversion event generator built, validated, published.

  validation already extended to $E = 1\,\mathrm{PeV}$

- De-VEGAS-ification almost completed: single-shot single-photon generation possible.

- Geant4 Physics Model later this year.

Back-up slides

Form Factors

- Form factors must be taken into account as the fraction of the total cross section lost increase with energy:

$$\frac{\sigma_{\mathrm{noFF}}}{\sigma_{\mathrm{FF}}} = \frac{41\log\left(2E/m\right) - 109}{41\log\left(183Z^{-1/3}\right) - 1} \tag{1}$$

- for 2 elements Z_1 and Z_2;

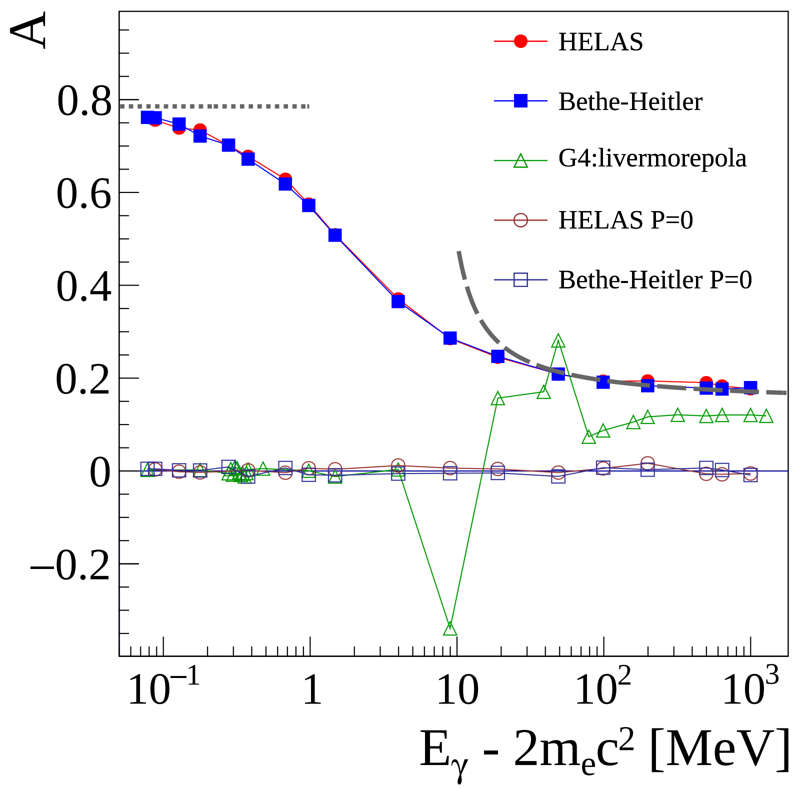
  noting that $(1 - F(q^2, Z_1)) < (1 - F(q^2, Z_2))$ for $Z_1 > Z_2$,

  - use Z_2 mock-up to shoot Z_1
  - The efficiency loss would be asymptotically

$$\frac{\sigma_{\mathrm{FF},Z_1}}{\sigma_{\mathrm{FF},Z_2}} = \frac{41\log\left(183Z_1^{-1/3}\right) - 1}{41\log\left(183Z_2^{-1/3}\right) - 1}, \tag{2}$$

For example, $\frac{\sigma_{\mathrm{FF},Ar}}{\sigma_{\mathrm{FF},Xe}} \approx 1.095.$ (after Z^2 dependence rescaled).

Polarisation asymmetry: asymptotic expressions



- Low energy

$$A = \frac{\pi}{4}.$$

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- High energy

$$A \approx \frac{\frac{4}{9}\ln 2E - \frac{20}{28}}{\frac{28}{9}\ln 2E - \frac{218}{27}}$$

V. F. Boldyshev et al., Yad. Fiz. 14 (1971) 1027, (Sov.J.Nucl.Phys. 14 (1972) 576).