Statistics of X-ray polarimetry

Dura lex, sed lex

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Frontiers in X-ray Polarimetry (FiXP) Academy

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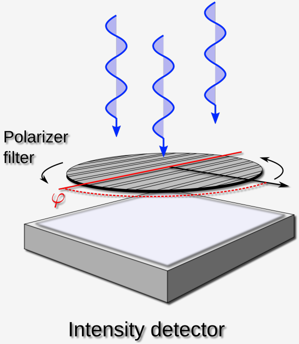
Outline

1. **Introduction**
2. **Measuring (linear) polarization**
   - Modulation curve analysis
   - Stokes parameters
3. **The IXPE's way**
   - Event-by-event Stokes parameters
   - Statistical uncertainty on polarization
   - Polarization detection (and the MDP)
   - Bias for low signal-to-noise measurements
4. **Towards data analysis of astronomical sources**
   - Model and model-independent analysis
   - Forward fitting
   - Final suggestions
5. **Conclusions**

Introduction

(X-ray) polarimeters convert (linear) polarization in a ($\cos^2$) modulation of their response

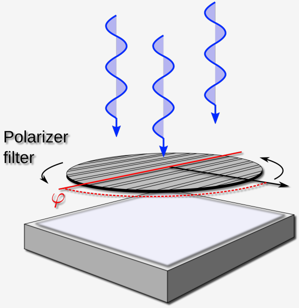
Optical polarimeters



Response is the intensity as a function of filter rotation

(X-ray) polarimeters convert (linear) polarization in a ($\cos^2$) modulation of their response

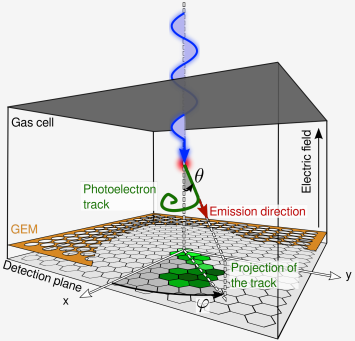
Optical polarimeters



Intensity detector

Response is the intensity as a function of filter rotation

Photoelectric polarimeters

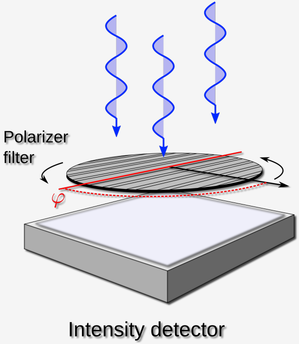


Response is the azimthual distribution of photoelectrons

$$\frac{d\sigma}{d\Omega} \propto \cos^2\phi \, \frac{\sin^2\theta}{(1-\beta\cos\theta)^4}$$

(X-ray) polarimeters convert (linear) polarization in a ($\cos^2$) modulation of their response

Optical polarimeters



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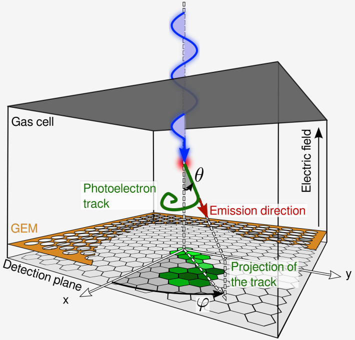
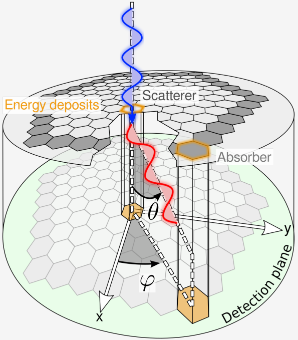
Photoelectric polarimeters



Response is the azimthual distribution of photoelectrons

$$\frac{d\sigma}{d\Omega} \propto \cos^2\phi \, \frac{\sin^2\theta}{(1-\beta\cos\theta)^4}$$

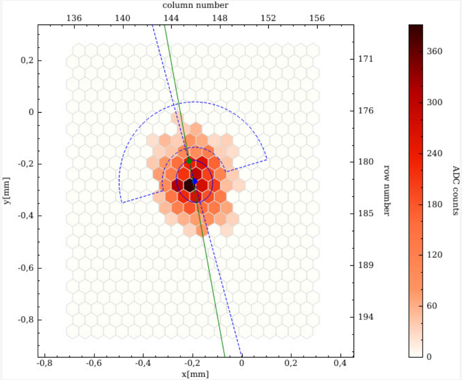
Compton polarimeters



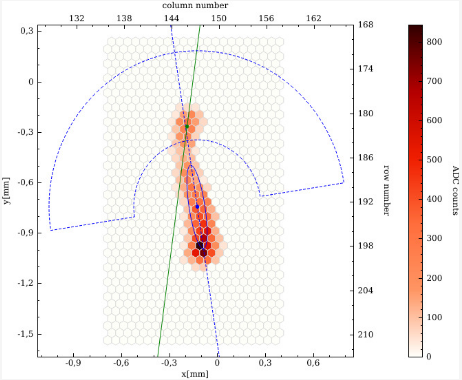
Response is the azimuthal distribution of scattered photons

$$\frac{d\sigma}{d\Omega} \propto \left[\frac{E}{E'} + \frac{E'}{E} - 2\sin^2\theta\,\cos^2\phi\right]$$

Response of the Gas Pixel Detector on-board IXPE



(a) 2.3 keV

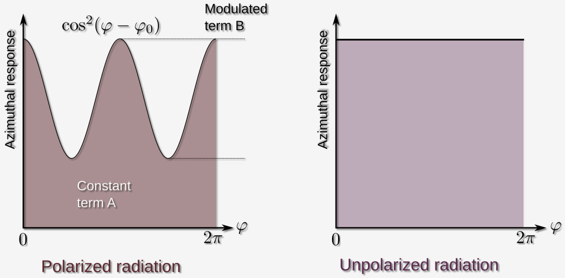


(b) 6.4 keV

- Photoelectron “track” need to be reconstructed with an appropriate algorithm
- All characteristics of the photon are measured
- Quality of tracks (and then accuracy in the reconstruction) varies

Measuring (linear) polarization

The **modulation curve** is the histogram of the azimuthal distribution of the event



Angle of polarization ϕ_0: related to the phase of the measured modulation curve φ_0

➥ $\varphi_0 = \phi_0$ for, e.g., photoelectric polarimeters

➥ $\varphi_0 = \phi_0 + \pi/2$ for, e.g., Compton polarimeters

Degree of polarization $\mathcal{P}$: proportional to the modulation amplitude

➥ the constant of proportionality is the **modulation factor** μ

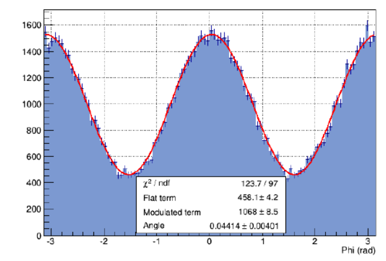
1. Fit the modulation curve with the function:
   $\mathcal{M}(\phi) = A + B\cos^2(\phi - \phi_0)$ (or $= C + M\cos[2(\varphi - \varphi_0)]$)
   - ϕ_0 is the angle of polarization
2. Calculate the amplitude modulation:

$$M = \frac{\mathcal{M}_{\max} - \mathcal{M}_{\min}}{\mathcal{M}_{\max} + \mathcal{M}_{\min}} = \frac{B}{B + 2A}$$

3. Rescale the measured modulation by the modulation factor:

$$\mathcal{P} = \frac{M}{\mu} = \frac{1}{\mu}\frac{B}{B + 2A}$$

This is equivalent to rescale by μ and say $\mathcal{P} = I_{\rm pol}/I_{\rm tot}$



Stokes parameters

- Modulation curve approach to extract polarization from data has limitations:
  - ➥ Modulation and phase are treated as independent parameters - but they are not
  - ➥ Assume ideal detector - no calibration can be applied
- Use of Stokes parameters offers many practical advantages:
  - ➥ Independent, normal-distributed variables, at least when modulation is small and for sufficiently-large set of data - true for all astronomical observations
  - ➥ They are additive - straightforward to apply calibration
  - ➥ Can be handled as fluxes with an appropriate response matrix
  - ➥ Common approach to other wavelengths
- Stokes parameters do not substitute polarization degree and phase
  - ➥ Latter remain relevant physical quantities in most of the cases

Why Stokes parameters? It may seem that the Stokes parameters, rather than following naturally from our physical concept of polarized radiation, are pulled out of a hat; the author sympathizes with this view, but notes that this holds to some extent for each of the alternative forms presented in section 4.3.

Tinbergen [2005]

- A 4-D vector fully describing the polarization of radiation, (I, Q, U, V) or (S_1, S_2, S_3, S_4)...
- Definitions adapt to instrumental approach
- Flux quantities derived by radiation components

$$\begin{cases} I = I_0 + I_{90} \\ Q = I_0 - I_{90} \\ U = I_{45} - I_{-45} \\ V = I_{\mathrm{rc}} - I_{\mathrm{lc}} \end{cases}$$

- ➥ I is the total intensity
- ➥ Q and U are related to linear polarization (degree and angle)
- ➥ V is the circular polarization (can be ignored at high energy)

Stokes parameters in X-rays I

- Polarization degree and angle

$$\mathcal{P} = \frac{1}{\mu}\sqrt{\left(\frac{Q}{I}\right)^2 + \left(\frac{U}{I}\right)^2} = \frac{1}{\mu}\sqrt{q^2 + u^2} \qquad \phi_0 = \frac{1}{2}\arctan\frac{U}{Q} = \frac{1}{2}\arctan\frac{u}{q}$$

- q and u are the normalized Stokes parameters
- arctan has to consider the sign!
- μ normalization for the PD, **unless** Q and U are already normalized!

Stokes parameters in X-rays II

- Can be derived from data with different (yet equivalent) approaches
  - **Fit of the modulation curve** with a function depending explicitly on Stokes parameters, Strohmayer and Kallman [2013]

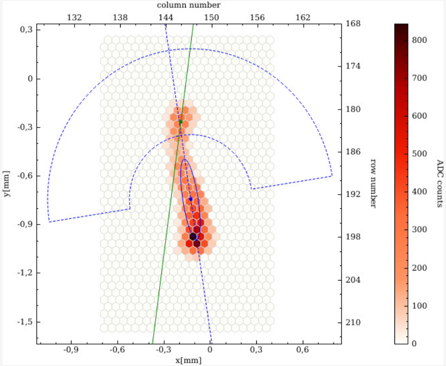
$$\mathcal{M}(\phi) = I + Q\cos(2\phi) + U\sin(2\phi) = I[1 + q\cos(2\phi) + u\sin(2\phi)]$$

    [In the paper q and u are inverted with respect to the common definition that we are using here]

  - **Estimate photon-by-photon**, Kislat et al. [2015]
    The approach that used (also) for **IXPE**, simplifies application of energy and space-resolved calibrations

The IXPE's way

Event-by-event Stokes parameters I



- X-ray polarimeters provide for each detected event its azimuthal direction φ_k
  - ➥ In case of the GPD, this is the direction of emission of the photoelectron
- For each of them, we can derive an estimate of these event quantities ("event" Stokes parameter):

$$i_k = 1 \qquad q_k = 2\cos 2\varphi_k \qquad u_k = 2\sin 2\varphi_k$$

- ➥ "Practical" definition accounting for peculiarities of X-ray polarimeters
- ➥ The factor 2 is just moved with respect to the original formulae in Kislat et al. [2015]

- Calibration is applied event-by-event

$$i_{\mathrm{cal}} = i_k \qquad q_{\mathrm{cal}} = q_k - q_{\mathrm{sm}} \qquad u_{\mathrm{cal}} = u_k - u_{\mathrm{sm}}$$

- q_{sm} and u_{sm} are the Stokes parameters measured for unpolarized radiation
  - Depend on photon energy and absorption position on the detector
  - Measured during calibrations
- Normal users will handle only **calibrated Stokes parameters**
  - Data can be treated as affected by statistical uncertainties only
  - Quantities in the LV2 (processed) data files provided by the HEASARC

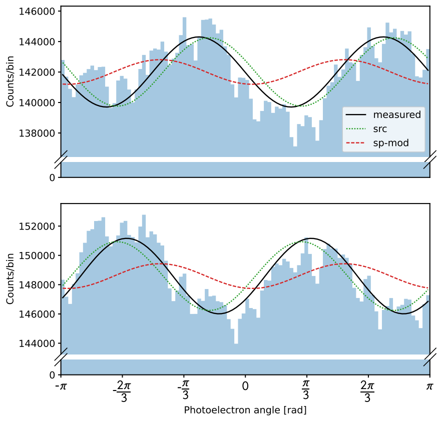


Figure: Decoupling source signal and spurious modulation

Event-by-event Stokes parameters III

- Stokes parameters for an observation of N events:

$$I = \sum_N i_{\rm cal} = N$$

$$Q = \frac{\sum_N q_{\rm cal}}{\langle\mu\rangle} \quad \text{or} \quad q = \frac{\sum_N q_{\rm cal}}{\langle\mu\rangle N} \quad \text{with} \quad \sigma_q = \sqrt{\frac{1}{N-1}\left(\frac{2}{\langle\mu\rangle^2} - q^2\right)} \approx \sqrt{\frac{2}{\langle\mu\rangle^2(N-1)}}$$

$$U = \frac{\sum_N u_{\rm cal}}{\langle\mu\rangle} \qquad u = \frac{\sum_N u_{\rm cal}}{\langle\mu\rangle N} \quad \text{with} \quad \sigma_u = \sqrt{\frac{1}{N-1}\left(\frac{2}{\langle\mu\rangle^2} - u^2\right)} \approx \sigma_q$$

- μ must be averaged in the energy range of interest and weighted by the effective area

⚠ Estimate on the single event (or on a few...) are **not** statistically significative

➥ To have $\sigma_q = \sigma_u = 0.1$, $N > 600$ for $\mu = 0.3$

Event-by-event Stokes parameters IV

⚠ Taken singularly, calibrated event Stokes parameters are **NOT** proper quantities

- ➥ No possible to derive a $\varphi_{k,\mathrm{cal}}$
- ➥ However: $\langle Q \rangle = \sum_N q_{\mathrm{cal}} = Q_{\mathrm{src}}$ and $\langle U \rangle = \sum_N u_{\mathrm{cal}} = U_{\mathrm{src}}$.

- Stokes parameters are fluxes: background subtraction must be carried out on **unnormalized** parameters:

$$\begin{cases} I = I_{\mathrm{src}} + \eta\ I_{\mathrm{bkg}} \\ Q = Q_{\mathrm{src}} + \eta\ Q_{\mathrm{bkg}} \\ U = U_{\mathrm{src}} + \eta\ U_{\mathrm{bkg}} \end{cases} \Rightarrow \begin{cases} I_{\mathrm{src}} = I - \eta\ I_{\mathrm{bkg}} \\ Q_{\mathrm{src}} = Q - \eta\ Q_{\mathrm{bkg}} \\ U_{\mathrm{src}} = U - \eta\ U_{\mathrm{bkg}} \end{cases} \quad \text{with } \eta = \frac{T_{\mathrm{obs}}}{T_{\mathrm{bkg}}} \times \frac{A_{\mathrm{obs}}}{A_{\mathrm{bkg}}}$$

with (because Q and U are normal variables!):

$$\sigma_{Q\_\mathrm{src}} = \sqrt{\sigma_Q^2 + \left(\frac{T_{\mathrm{obs}}}{T_{\mathrm{bkg}}}\right)^2 \sigma^2_{Q\_\mathrm{bkg}}} \quad \text{with} \quad \sigma_{Q_i} = \sqrt{\frac{2N_i}{\langle \mu \rangle}^2}$$

$$\sigma_{U\_\mathrm{src}} = \ldots$$

Statistical uncertainty on polarization

- Q and U or PD and PA encode the same information
  - Q and U are normal and independent variables, PD follows a Rice distribution
- Uncertainties on polarization are usually calculated assuming that q and u are normally distributed and **independent** variables
  - Adequate when $\mu\mathcal{P} < 0.3$
  - For other cases, the full treatment is in Kislat et al. [2015]

- Uncertainties are different when we treat separately polarization degree and angle or we combined the two:
  - **Separate (or 1D) treatment**: I have a confidence of 68.3% that polarization degree (**or** angle) is in the interval $\mathcal{P}_0 \pm \sigma_{1D}$ (**or** $\phi_0 \pm \sigma_{1D}$), ignoring the other parameter
    - Returned by FTOOLS/IXPEPOLARIZATION or IXPEOBSSIM
    - Reasonable only for high signal-to-noise measurement
  - **Combined (or 2D) treatment**: I have a confidence of 68.3% that polarization degree is in the interval $\mathcal{P}_0 \pm \sigma_{2D}$ **and simultaneously** polarization angle is in the interval $\phi_0 \pm \sigma_{2D}$
    - This is the typical case to consider

- $\mathcal{P}$ and ϕ are treated separately [Kislat et al., 2015]:

$$\sigma_{\mathcal{P}} \approx \sigma_q \approx \sigma_u \approx \sqrt{\frac{2}{N\mu^2}} \qquad \sigma_\phi \approx \frac{\sigma_{\mathcal{P}}}{2\mathcal{P}}$$

- σ_ϕ depends on $\mathcal{P}$
- Both depends on μ

- Appropriate, e.g., for evaluating the modulation factor measured for calibrations

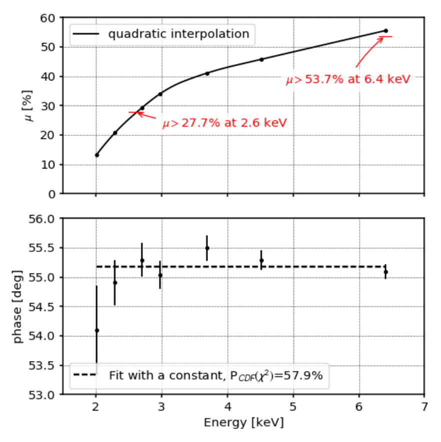


Figure: Calibration of modulation factor for DU2

Statistical uncertainty - 2D case

- The uncertainty at a confidence level C is defined by the region in the $(\mathcal{P},\phi_0)$ plane [Muleri, 2022]:

$$\begin{cases} \mathcal{P} = \sqrt{\bar{\mathcal{P}} + \Delta_C^2 + 2\bar{\mathcal{P}}\Delta_C \cos\left[2(\psi - \bar{\phi}_0)\right]} \\ \phi = \frac{1}{2}\arctan\frac{\bar{\mathcal{P}}\sin 2\phi_0 + \Delta_C \sin 2\psi}{\bar{\mathcal{P}}\cos 2\bar{\phi}_0 + \Delta_C \cos 2\psi} \end{cases} \quad \text{with} \quad \psi \in [0,\pi]$$

where

$\bar{\mathcal{P}}, \bar{\phi}_0$: measured polarization degree and angle

$$\Delta_C = \frac{1}{\mu}\sqrt{\frac{-4\ln(1-C)}{N}}$$

- Equivalently, drawn with XSPEC/steppar for 2 interesting parameters

confidence level	$\Delta\chi^2$
68.3% (1σ)	2.296
90%	4.605
99%	9.210

1D or 2D uncertainties?

- Evolution of the uncertainty contour in the $(\mathcal{P},\phi_0)$ plane for **decreasing** Signal-to-Noise (S/N)
- When the significance is low, contours are no symmetric
- Contours are closed as long the measurement is significant at the specified statistical confidence
- 1D uncertainties (bars) $\sim$40% smaller than the extreme values of the 2D region
- **IXPE** team usual practice:
  - Use 1D for written text or table
  - Show 2D in a figure
  - Always specify what one is doing
- Normalized (by I and μ) Stokes parameters are another possibility

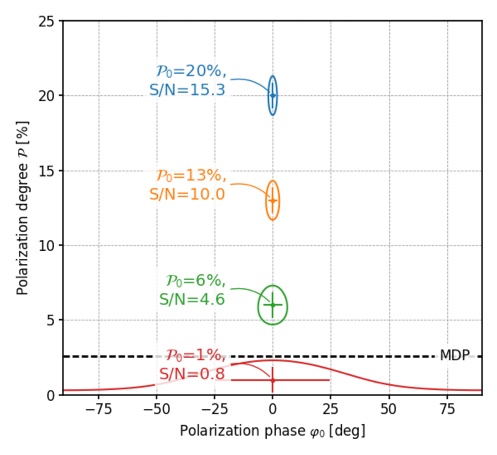


Figure: $N = 3 \times 10^5$, $\phi_0 = 0$, $\mu = 0.3$, C=68.3%

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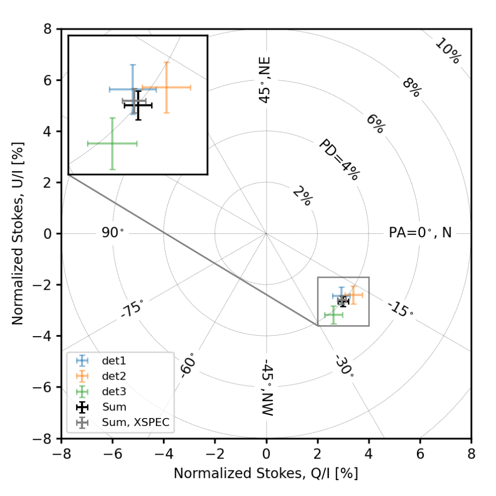


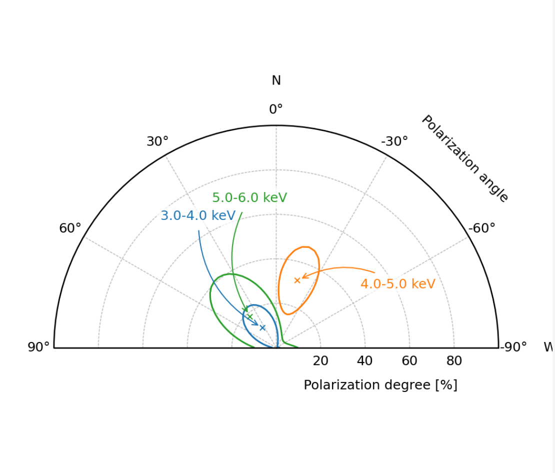
Polarization detection

- When do we say that there is detection?
- N bins gives you N chance that a statistical fluctuations give you a signal
- Test the null hypothesis that the quantity:

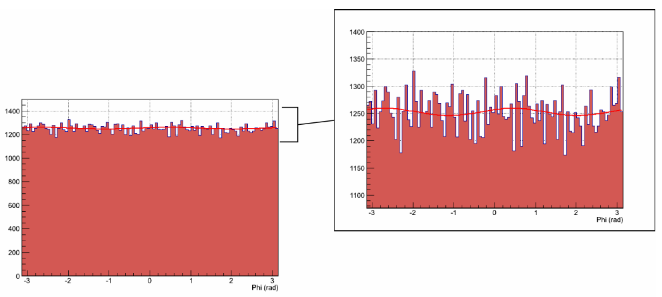
$$\sum_N (P/\sigma_{p,1D})^2$$

is a χ^2 variabile with $2\times$N degrees of freedom

Null prob	Detection description
$>$99%	probable
$>$99.9%	highly probable
$>$99.99%	secure



Is 4-5 keV a detection?



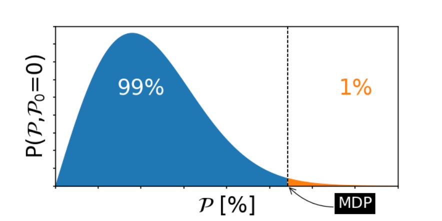
Real data from the Gas Pixel Detector

- A modulation of a certain amplitude is always detected because of statistical fluctuations on the content of each bin of the modulation curve.
- The MDP is the maximum polarization which can be produced by statistical fluctuations only in absence of true source polarization, at a certain confidence level $C = 99\%$
- Test the hypothesis that observed signal is obtained because of statistical fluctuations for an unpolarized source

- Probability density function: probability of measuring $(\mathcal{P},\phi)$ in case of true values $(\mathcal{P}_0,\phi_0)$

$$P(\mathcal{P},\mathcal{P}_0,\phi,\phi_0)=\frac{N\mathcal{P}\mu^2}{4\pi}\exp\left[-\frac{N\mu^2}{4}\left(\mathcal{P}^2+\mathcal{P}_0^2-2\mathcal{P}\mathcal{P}_0\cos 2(\phi-\phi_0)\right)\right] \quad (1)$$

  - ➥ in the usual assumptions that Stokes parameters are uncorrelated and normally distributed
  - ➥ ... and no background



- The MDP is the maximum polarization which we expect to measure with a probability of 99% when the true polarization is zero
- In other words, the MDP is the polarization upper boundary when the cumulative function is 0.99

Deriving the MDP II

- To derive MDP we must solve [Weisskopf et al., 2010; Strohmayer and Kallman, 2013]

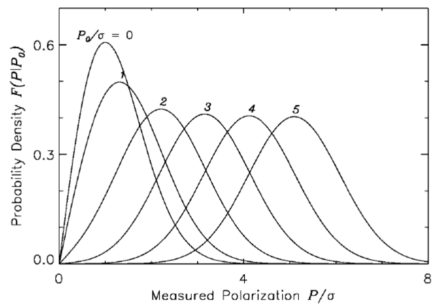
$$0.99 = \int_0^{2\pi}\int_0^{\mathrm{MDP}} P(\mathcal{P},\mathcal{P}_0=0)\mathrm{d}\mathcal{P}\mathrm{d}\phi \int_0^{2\pi}\int_0^{\mathrm{MDP}} \frac{N\mathcal{P}\mu^2}{4\pi}\exp\left[-\frac{N\mathcal{P}^2\mu^2}{4}\right]\mathrm{d}\mathcal{P}\mathrm{d}\phi 0$$

- Result with no background is: $\mathrm{MDP} = \frac{4.29}{\mu\sqrt{N}}$
  - .... that is, N$> 2\times 10^6$ to have MDP $= 1\%$ when $\mu = 0.3$
- Result with background is [Elsner et al., 2012]:

$$\mathrm{MDP} = \frac{4.29}{\mu}\frac{\sqrt{N_{\mathrm{source}}+N_{\mathrm{bkg}}}}{N_{\mathrm{source}}}$$

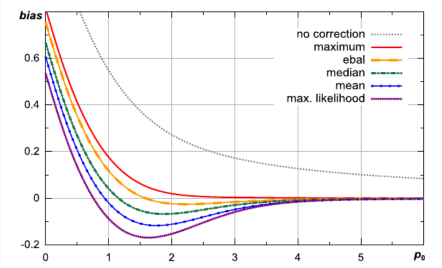
- **Personal suggestion**: Do not abuse of the MDP!
  - No equivalent outside X-ray polarimetry

- There is a known (positive) bias on measured polarization degree when $S/N \lesssim 6$ [Simmons and Stewart, 1985; Vaillancourt, 2006]



$$F(P|P_0) \equiv P(\mathcal{P},\mathcal{P}_0) = \int_\phi P(\mathcal{P},\mathcal{P}_0,\phi,\phi_0)\mathrm{d}(\phi-\phi_0)$$

- Alternative estimators for the measured polarization proposed by Simmons and Stewart [1985], e.g.
  - ➥ Maximum, median, mean, ...
  - ➥ Reduces, but do not eliminate the bias
  - ➥ All based on true value, not the measured one

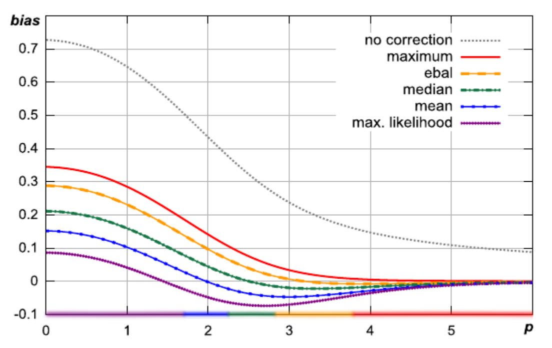


Maier et al. [2014]

- In Bayesian approach the true polarization is treated as the stocastic variable

$$P(\mathcal{P}_0, \mathcal{P}) = \frac{P(\mathcal{P}_0) \cdot P(\mathcal{P}|\mathcal{P}_0)}{\int_0^\infty P(\mathcal{P}_0) \cdot P(\mathcal{P}|\mathcal{P}_0) d\mathcal{P}_0}$$

- The best estimator is now derived by the S/N
- For S/N>2.8, $\mathcal{P}_0 = \sqrt{\mathcal{P}^2 - \sigma_\mathcal{P}}$ [Maier et al., 2014]
- Confidence intervals derived by parametric functions



p_0 is now the S/N

Towards data analysis of astronomical sources

Polarization analysis

Two possible questions:

- What is the polarization in this energy range
  - ➥ Use the PCUBE algoritm of IXPEOBSSIM (or FTOOLS/IXPEPOLARIZATION)
- If the spectrum can be decomposed in these components, which polarization can be associated to each of them?
  - ➥ As in spectral decomposition, the deconvolution may **not** be unique!
  - ➥ Use XSPEC(also inside IXPEOBSSIM), or other forward-folding software

Deconvolution of instrumental response with forward fitting I

- Measured signal has to be deconvolved for the instrumental response to derive the true one from the source
- Common approach with spectrometers is **forward fitting** procedure

$$O(E) = \int_{E'} I(E') \times \underbrace{\epsilon(E') \times R(E', E)}_{\text{response function } \mathcal{I}(E', E)} \, \mathrm{d}E'$$

$$\begin{aligned} E', E &: \text{true and measured energy} \\ I(E'), O(E) &: \text{true and observed source spectrum} \\ \epsilon(E') &: \text{effective area as a function of energy} \\ R(E', E) &: \text{energy redistribution matrix} \end{aligned}$$

- Forward fitting procedure:
  1. assumes a model parametrization $I_0(E')$;
  2. convolves it with the instrumental response to obtain an expected "observed" spectrum in such a parametrization;
  3. compare the expected and actual observed spectra to constrain model's parameters

Generalization for X-ray polarimetry I

- Forward fitting can be extended to X-ray polarimetry [Strohmayer, 2017]
- Model parametrization include a model for source polarization
  - Stokes $I(E')$, $Q(E')$ and $U(E')$
  - or Flux $I(E')$, polarization degree $\mathcal{P}(E')$ and phase $\phi(E')$
- Instrumental response is:

$$\mathcal{I}(E', E, \phi', \phi) = \underbrace{\epsilon(E') \times R(E', E)}_{\dagger} \times V(E', E, \underbrace{\phi' - \phi}_{\ddagger})$$

† No dependence on ϕ' of effective area or energy dispersion
‡ No azimuthal systematic effects

- Here V represent the probability that a photon with energy E' and polarization ϕ' is reconstructed to have energy E and polarization ϕ

Generalization for X-ray polarimetry II

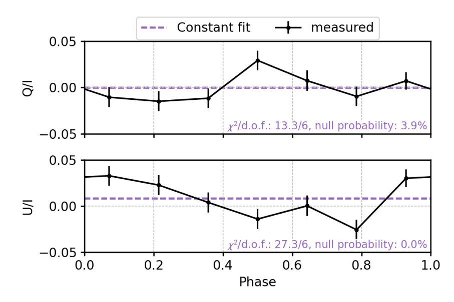
- Forward fitting simultaneously on the three Stokes parameters, convolved with the appropriate Instrument response function:

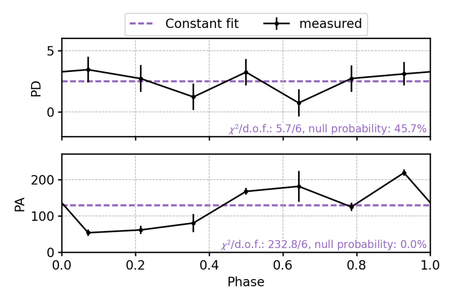
$$
\begin{aligned}
O_I(E) &= \int_{E'} I(E') \times \epsilon(E') \times R(E', E)\mathrm{d}E' \\
O_Q(E) &= \int_{E'} Q(E') \times \mu(E') \times \epsilon(E') \times R(E', E)\mathrm{d}E' \\
O_U(E) &= \int_{E'} U(E') \times \mu(E') \times \epsilon(E') \times R(E', E)\mathrm{d}E'
\end{aligned}
$$

- Analogous to apply three times the classical approach, with the addition of the modulation factor $\mu(E')$ in the Instrument response function
- XSPEC can accomodate such a procedure with minimum addictions
  - Q and U can be obtained with simple multiplicative models from I
  - $\mu(E)$ is a generalization of the effective area
- Needed tools are already available in FTOOLS and IXPEOBSSIM

Polarization variation

- Hypothesis that polarization (both PD **and** PA) is not changed best tested with Stokes parameters
- Answering if either PD or PA is changing is more tricky
  - ➥ Assumption on the other parameter has to be done
  - ➥ Caution is necessary





Same data from LMC X-1

Weighted vs Unweighted analysis

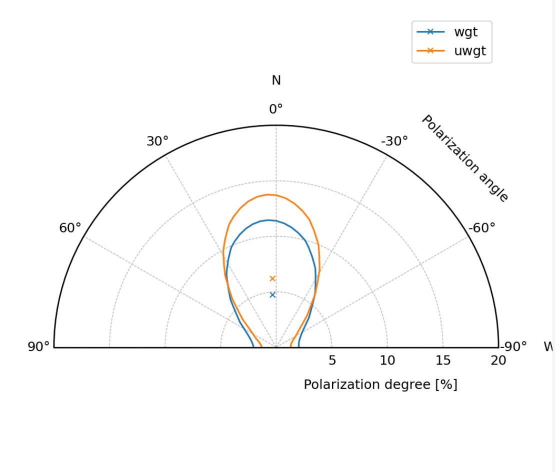
Long story: Di Marco et al. [2022]

Short story:

- Improve the significance of "better" events for polarimetry
  - ➥ Increases μ at the expense of quantum efficiency
- Event Stokes parameters are calculated as:

$$\begin{cases} i_k = w_k \\ q_k = w_k \cdot 2\cos 2\varphi_k \\ u_k = w_k \cdot 2\sin 2\varphi_k \end{cases}$$

- Requires different response matrices
- Overall sensitivity gain $\sqrt{20\%}$
  - ➥ Almost like having a forth telescope...



Conclusions

Summary & Conclusions

- X-ray polarimetry is a young science - and so it is the data analysis!
- Fundamental quantities for general users:
  - Stokes parameters: I, Q and U
  - Physical quantites: polarization degree and phase, and relative uncertainties
  - (Minimum Detectable Polarization)
- Each has its own meaning and usefulness
- Measurements with low statistical significance should be treated with particular care
- Spectro-polarimetric modelling a (simple for the user) extension of traditional spectral modelling with forward folding technique

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