E_{recoil}-Q-Distribution

Daniel Wegner

August 12, 2011

Contents

1 Derivation

The aim of this paper is to derive the propability density of the quantity

$$\vec{q} = \begin{pmatrix} E_{recoil} \\ Q \end{pmatrix} \tag{1}$$

The quantity $\vec{q}$ depends from

$$\vec{r} = \begin{pmatrix} E_{ion} \\ E_{heat} \end{pmatrix} \tag{2}$$

The dependency is given by

$$T : \vec{r} \to \vec{q}, \begin{pmatrix} E_{ion} \\ E_{heat} \end{pmatrix} \to \begin{pmatrix} E_{recoil} \\ Q \end{pmatrix} = \begin{pmatrix} \left(1 + \frac{V}{\epsilon_\gamma}\right) E_{heat} - \frac{V}{\epsilon_\gamma} E_{ion} \\ \frac{E_{ion}}{\left(1 + \frac{V}{\epsilon_\gamma}\right) E_{heat} - \frac{V}{\epsilon_\gamma} E_{ion}} \end{pmatrix} \tag{3}$$

Then the inverse transformation is given by

$$T^{-1} : \vec{q} \to \vec{r}, \begin{pmatrix} E_{recoil} \\ Q \end{pmatrix} \to \begin{pmatrix} E_{ion} \\ E_{heat} \end{pmatrix} = \begin{pmatrix} Q E_{recoil} \\ \frac{1 + Q \frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} E_{recoil} \end{pmatrix} \tag{4}$$

The derivative then is given by

$$T'(\vec{r}) = \begin{pmatrix} \frac{\partial E_{recoil}}{\partial E_{ion}} & \frac{\partial E_{recoil}}{\partial E_{heat}} \\ \frac{\partial Q}{\partial E_{ion}} & \frac{\partial Q}{\partial E_{heat}} \end{pmatrix} = \begin{pmatrix} -\frac{V}{\epsilon_\gamma} & 1 + \frac{V}{\epsilon_\gamma} \\ \frac{1}{E_{recoil}} + \frac{V}{\epsilon_\gamma} \frac{E_{ion}}{E_{recoil}^2} & -\left(1 + \frac{V}{\epsilon_\gamma}\right) \frac{E_{ion}}{E_{recoil}^2} \end{pmatrix} \tag{5}$$

and thus the determinant of it is

$$\det T'(\vec{r}) = \frac{V}{\epsilon_\gamma}\left(1 + \frac{V}{\epsilon_\gamma}\right) \frac{E_{ion}}{E_{recoil}^2} - \left(1 + \frac{V}{\epsilon_\gamma}\right)\left(\frac{1}{E_{recoil}} + \frac{V}{\epsilon_\gamma} \frac{E_{ion}}{E_{recoil}^2}\right) = -\frac{1 + \frac{V}{\epsilon_\gamma}}{E_{recoil}} \tag{6}$$

Obviously for all values for E_{recoil} the determinant doesn't vanish and thus the transformation is invertible in the whole domain according to the inverse function theorem.

If we assume that $\vec{r}$ is a multivariate normal-distributed quantity, that means it follows the propability density function

$$f(\vec{r}) = \frac{1}{2\pi\sqrt{\det C}} \exp\left(-\frac{1}{2}(\vec{r} - \vec{r}_0)^T C^{-1} (\vec{r} - \vec{r}_0)\right) \tag{7}$$

with the covariance matrix

$$C = \begin{pmatrix} \sigma_{ion}^2 & \sigma_{ion-heat}^2 \\ \sigma_{ion-heat}^2 & \sigma_{heat}^2 \end{pmatrix} \tag{8}$$

, we get the propability density function $g(\vec{q})$ [1][p. 246]

$$g(\vec{q}) = \frac{f(T^{-1}(\vec{q}))}{|\det T'(T^{-1}(\vec{q}))|} \tag{9}$$

$$= \exp\left(-\frac{1}{2} \begin{pmatrix} Q E_{recoil} - \overline{E_{ion}} \\ \frac{1 + Q \frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} E_{recoil} - \overline{E_{heat}} \end{pmatrix}^T \begin{pmatrix} \sigma_{ion}^2 & \sigma_{ion-heat}^2 \\ \sigma_{ion-heat}^2 & \sigma_{heat}^2 \end{pmatrix}^{-1} \begin{pmatrix} Q E_{recoil} - \overline{E_{ion}} \\ \frac{1 + Q \frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} E_{recoil} - \overline{E_{heat}} \end{pmatrix}\right) \tag{10}$$

$$\times \frac{|E_{recoil}|}{2\pi\sqrt{\sigma_{ion}^2 \sigma_{heat}^2 - \sigma_{ion-heat}^4}\left(1 + \frac{V}{\epsilon_\gamma}\right)} \tag{11}$$

2 Marginal Distributions

2.1 $g_{E_{recoil}}(Q)$

In order to determine the marginal distribution

$$g_{E_{recoil}}(Q) = \int_{-\infty}^{\infty} dE_{recoil}\, g(E_{recoil}, Q) \tag{12}$$

which is the projection of $g(E_{recoil}, Q)$ on the Q axis, all terms in the exponent of (11) are ordered with respect to powers of E_{recoil}:

$$g(E_{recoil}, Q) = k_E \cdot |E_{recoil}| \exp(a_E E_{recoil}^2 + b_E E_{recoil} + c_E) \tag{13}$$

with

$$k_E = \frac{1}{2\pi \sqrt{\sigma_{ion}^2 \sigma_{heat}^2 - \sigma_{ion-heat}^4} \left(1 + \frac{V}{\epsilon_\gamma}\right)} \tag{14}$$

$$a_E = -\frac{g_{11}}{2}Q^2 - g_{12}Q \cdot \frac{1 + Q\frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} - \frac{g_{22}}{2}\left(\frac{1 + Q\frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}}\right)^2 \tag{15}$$

$$b_E = g_{11}Q\overline{E_{ion}} + g_{12}Q\overline{E_{heat}} + g_{12}\overline{E_{ion}}\frac{1 + Q\frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{1 + Q\frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} \tag{16}$$

$$c_E = -\frac{g_{11}}{2}\overline{E_{ion}}^2 - g_{12}\overline{E_{ion}} \cdot \overline{E_{heat}} - \frac{g_{22}}{2}\overline{E_{heat}}^2 \tag{17}$$

with the inverse covariance matrix

$$G = \begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix} = C^{-1} = \frac{1}{\sigma_{ion}^2 \sigma_{heat}^2 - \sigma_{ion-heat}^4} \begin{pmatrix} \sigma_{heat}^2 & -\sigma_{ion-heat}^2 \\ -\sigma_{ion-heat}^2 & \sigma_{ion}^2 \end{pmatrix} \tag{18}$$

In order to integrate (13) over E_{recoil}, we can simplify it by completing the square:

$$\int_{-\infty}^{\infty} dE_{recoil}\, g(E_{recoil}, Q) = \tag{19}$$

$$\int_{-\infty}^{\infty} dE_{recoil}\, k_E |E_{recoil}| \exp\left(a_E \cdot \left(E_{recoil} + \frac{b_E}{2a_E}\right)^2\right) \exp\left(c_E - \frac{b_E^2}{4a_E}\right) \tag{20}$$

$$= \exp\left(c_E - \frac{b_E^2}{4a_E}\right) \int_{-\infty}^{\infty} dE_{recoil}\, k_E |E_{recoil}| \exp\left(a_E \cdot \left(E_{recoil} + \frac{b_E}{2a_E}\right)^2\right) \tag{21}$$

$$\overset{x=E_{recoil}+\frac{b_E}{2a_E}}{=} k_E \exp\left(c_E - \frac{b_E^2}{4a_E}\right) \int_{-\infty}^{\infty} dx \left(\left|x - \frac{b_E}{2a_E}\right| \exp\left(a_E x^2\right)\right) \tag{22}$$

$$= k_E \exp\left(c_E - \frac{b_E^2}{4a_E}\right) \cdot \left[\int_{\frac{b_E}{2a_E}}^{\infty} dx \left(\left(x - \frac{b_E}{2a_E}\right)\exp\left(a_E x^2\right)\right) - \int_{-\infty}^{\frac{b_E}{2a_E}} dx \left(\left(x - \frac{b_E}{2a_E}\right)\exp\left(a_E x^2\right)\right)\right] \tag{23}$$

(23) then becomes:

$$\int_{-\infty}^{\infty} dE_{recoil}\, g(E_{recoil}, Q) = \tag{24}$$

$$= k_E \exp\left(c_E - \frac{b_E^2}{4a_E}\right) \cdot \left[\left[\frac{1}{2a_E}\exp(a_E x^2)\right]_{\frac{b_E}{2a_E}}^{\infty} - \left[\frac{1}{2a_E}\exp(a_E x^2)\right]_{-\infty}^{\frac{b_E}{2a_E}}\right. \tag{25}$$

$$\left. - \int_{\frac{b_E}{2a_E}}^{\infty} dx \frac{b_E}{2a_E}\exp(a_E x^2) + \int_{-\infty}^{\frac{b_E}{2a_E}} dx \frac{b_E}{2a_E}\exp(a_E x^2)\right] \tag{26}$$

Substituting $\tilde{a}_E = -a_E$ and $y = \sqrt{\tilde{a}_E}x$ leads to

$$\int_{-\infty}^{\infty} dE_{recoil}\, g(E_{recoil}, Q) \tag{27}$$

$$= k_E \exp\left(c_E + \frac{b_E^2}{4\tilde{a}_E}\right) \cdot \left[\frac{1}{\tilde{a}_E}\exp\left(-\frac{b_E^2}{4\tilde{a}_E}\right) + \int_{-\frac{b_E}{2\sqrt{\tilde{a}_E}}}^{\infty} dy \frac{b_E}{2\tilde{a}_E\sqrt{\tilde{a}_E}}\exp(-y^2) - \int_{-\infty}^{-\frac{b_E}{2\sqrt{\tilde{a}_E}}} dy \frac{b_E}{2\tilde{a}_E\sqrt{\tilde{a}_E}}\exp(-y^2)\right] \tag{28}$$

$$= \frac{k_E}{\tilde{a}_E}\exp(c_E) + k_E \exp\left(c_E + \frac{b_E^2}{4\tilde{a}_E}\right) \cdot \frac{b_E}{2\tilde{a}_E\sqrt{\tilde{a}_E}} \cdot \int_{-\frac{b_E}{2\sqrt{\tilde{a}_E}}}^{\frac{b_E}{2\sqrt{\tilde{a}_E}}} dy \exp(-y^2) \tag{29}$$

$$\boxed{= \frac{k_E}{\tilde{a}_E}\exp(c_E) + k_E \exp\left(c_E + \frac{b_E^2}{4\tilde{a}_E}\right) \cdot \frac{b_E}{2\tilde{a}_E\sqrt{\tilde{a}_E}} \cdot \sqrt{\pi}\,\mathrm{erf}\left(\frac{b_E}{2\sqrt{\tilde{a}_E}}\right)} \tag{30}$$

2.2 $g_Q(E_{recoil})$

In order to determine the marginal distribution

$$g_Q(E_{recoil}) = \int_{-\infty}^{\infty} dE_{recoil}\, g(E_{recoil}, Q) \tag{31}$$

which is the projection of $g(E_{recoil}, Q)$ on the E_{recoil} axis, all terms in the exponent of (11) are ordered with respect to powers of Q:

$$g(E_{recoil}, Q) = k_Q \exp(a_Q Q^2 + b_Q Q + c_Q) \tag{32}$$

with

$$k_Q = \frac{|E_{recoil}|}{2\pi\sqrt{\sigma_{ion}^2 \sigma_{heat}^2 - \sigma_{ion-heat}^4}\left(1 + \frac{V}{\epsilon_\gamma}\right)} \tag{33}$$

$$a_Q = -\left(\frac{g_{11}}{2} + g_{12}\frac{\frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}} + \frac{g_{22}}{2}\frac{\left(\frac{V}{\epsilon_\gamma}\right)^2}{\left(1 + \frac{V}{\epsilon_\gamma}\right)^2}\right) E_{recoil}^2 \tag{34}$$

$$b_Q = -\left(g_{12}\frac{1}{1 + \frac{V}{\epsilon_\gamma}} + g_{22}\frac{\frac{V}{\epsilon_\gamma}}{\left(1 + \frac{V}{\epsilon_\gamma}\right)^2}\right) E_{recoil}^2 \tag{35}$$

$$+ \left(g_{11}\overline{E_{ion}} + g_{12}\overline{E_{heat}} + g_{12}\overline{E_{ion}}\frac{\frac{V}{\epsilon}}{1 + \frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{\frac{V}{\epsilon_\gamma}}{1 + \frac{V}{\epsilon_\gamma}}\right) E_{recoil} \tag{36}$$

$$c_Q = -\frac{g_{11}}{2}\overline{E_{ion}}^2 - g_{12}\overline{E_{ion}} \cdot \overline{E_{heat}} - \frac{g_{22}}{2}\overline{E_{heat}}^2 - \frac{g_{22}}{2}\frac{1}{\left(1 + \frac{V}{\epsilon_\gamma}\right)^2}E_{recoil}^2 \tag{37}$$

$$+ \left(g_{12}\overline{E_{ion}}\frac{1}{1 + \frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{1}{1 + \frac{V}{\epsilon_\gamma}}\right) E_{recoil} \tag{38}$$

Again completing the square in the exponent of (32) results in

$$g_Q(E_{recoil}) = \int_{-\infty}^{\infty} dQ\, g(E_{recoil}, Q) \tag{39}$$

$$= k_Q \exp\left(c_Q - \frac{b_Q^2}{4a_Q}\right) \int_{-\infty}^{\infty} dQ \exp\left(a_Q\left(Q + \frac{b_Q}{2a_Q}\right)^2\right) \tag{40}$$

$$= k_Q \exp\left(c_Q - \frac{b_Q^2}{4a_Q}\right) \frac{\sqrt{\pi}}{\sqrt{-a_Q}} \tag{41}$$

$$= \frac{|E_{recoil}|}{2\pi\sqrt{\sigma_{ion}^2\,\sigma_{heat}^2 - \sigma_{ion-heat}^4}}\left(1 + \frac{V}{\epsilon_\gamma}\right) \times \tag{42}$$

$$\exp\left(-\frac{g_{11}}{2}\overline{E_{ion}}^2 - g_{12}\overline{E_{ion}}\cdot\overline{E_{heat}} - \frac{g_{22}}{2}\overline{E_{heat}}^2 - \frac{g_{22}}{2}\frac{1}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}E_{recoil}^2 \right. \tag{43}$$

$$+ \left(g_{12}\overline{E_{ion}}\frac{1}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{1}{1+\frac{V}{\epsilon_\gamma}}\right)E_{recoil} - \left(g_{12}\frac{1}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\frac{\frac{V}{\epsilon_\gamma}}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)E_{recoil}^2$$

$$\left. - \frac{\left(\left(g_{11}\overline{E_{ion}} + g_{12}\overline{E_{heat}} + g_{12}\overline{E_{ion}}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}}\right)E_{recoil}\right)^2}{-4\left(\frac{g_{11}}{2} + g_{12}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + \frac{g_{22}}{2}\frac{\left(\frac{V}{\epsilon_\gamma}\right)^2}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)E_{recoil}^2}\right) \times \tag{44}$$

$$\frac{\sqrt{\pi}}{\sqrt{\left(\frac{g_{11}}{2} + g_{12}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + \frac{g_{22}}{2}\frac{\left(\frac{V}{\epsilon_\gamma}\right)^2}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)E_{recoil}^2}} \tag{45}$$

$$= \frac{1}{\sqrt{2\pi}\sqrt{\sigma_{ion}^2\sigma_{heat}^2 - \sigma_{ion-heat}^4}\sqrt{g_{11}\left(1+\frac{V}{\epsilon_\gamma}\right)^2 + 2g_{12}\frac{V}{\epsilon_\gamma}\left(1+\frac{V}{\epsilon_\gamma}\right) + g_{22}\left(\frac{V}{\epsilon_\gamma}\right)^2}} \times \tag{46}$$

$$\exp\left(-\frac{g_{22}}{2}\frac{1}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2} + \frac{\left(g_{12}\frac{1}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}}\right)^2\left(\frac{\frac{V}{\epsilon_\gamma}}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)}{4\left(\frac{g_{11}}{2} + g_{12}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + \frac{g_{22}}{2}\frac{\left(\frac{V}{\epsilon_\gamma}\right)^2}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)}E_{recoil}^2\right. \tag{47}$$

$$+ g_{12}\overline{E_{ion}}\frac{1}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{1}{1+\frac{V}{\epsilon_\gamma}} - 2\frac{\left(g_{12}\frac{1}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}}\right)\left(g_{11}\overline{E_{ion}} + g_{12}\overline{E_{heat}} + g_{12}\overline{E_{ion}}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}}\right)}{4\left(\frac{g_{11}}{2} + g_{12}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + \frac{g_{22}}{2}\frac{\left(\frac{V}{\epsilon_\gamma}\right)^2}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)}E_{recoil} \tag{48}$$

$$+ -\frac{g_{11}}{2}\overline{E_{ion}}^2 - g_{12}\overline{E_{ion}}\cdot\overline{E_{heat}} - \frac{g_{22}}{2}\overline{E_{heat}}^2 + \frac{\left(g_{11}\overline{E_{ion}} + g_{12}\overline{E_{heat}} + g_{12}\overline{E_{ion}}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + g_{22}\overline{E_{heat}}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}}\right)^2}{4\left(\frac{g_{11}}{2} + g_{12}\frac{\frac{V}{\epsilon_\gamma}}{1+\frac{V}{\epsilon_\gamma}} + \frac{g_{22}}{2}\frac{\left(\frac{V}{\epsilon_\gamma}\right)^2}{\left(1+\frac{V}{\epsilon_\gamma}\right)^2}\right)}\right) \tag{49}$$

$$= \frac{1}{\sqrt{2\pi}\sqrt{\sigma_{heat}^2\left(1+\frac{V}{\epsilon_\gamma}\right)^2 - 2\sigma_{ion-heat}^2\frac{V}{\epsilon_\gamma}\left(1+\frac{V}{\epsilon_\gamma}\right) + \sigma_{ion}^2\left(\frac{V}{\epsilon_\gamma}\right)^2}}\exp\left(-\frac{1}{2}\frac{\left(E_{recoil} - \left(\overline{E_{heat}}\left(1+\frac{V}{\epsilon_\gamma}\right) - \overline{E_{ion}}\frac{V}{\epsilon_\gamma}\right)\right)^2}{\sigma_{heat}^2\left(1+\frac{V}{\epsilon_\gamma}\right)^2 - 2\sigma_{ion-heat}^2\frac{V}{\epsilon_\gamma}\left(1+\frac{V}{\epsilon_\gamma}\right) + \sigma_{ion}^2\left(\frac{V}{\epsilon_\gamma}\right)^2}\right) \tag{50}$$

Obviously this is a normal distribution, which is not surprising since E_{recoil} is a weighted sum of two normal distributed quantities, E_{ion} and E_{heat}:

$$E_{recoil} = \left(1+\frac{V}{\epsilon_\gamma}\right)E_{heat} - \frac{V}{\epsilon_\gamma}E_{ion} \tag{51}$$

3 Statistical moments

In order to determine the means $\langle Q \rangle$ and $\langle E_{recoil} \rangle$ we have to calculate

$$\langle Q^n \rangle = \int_{-\infty}^{\infty} dQ \, Q^n \cdot \int_{-\infty}^{\infty} dE_{recoil} \, g(E_{recoil}, Q) = \int_{-\infty}^{\infty} dQ \, Q^n \cdot g_{E_{recoil}}(Q) \tag{52}$$

$$\langle E_{recoil}^n \rangle = \int_{-\infty}^{\infty} dQ \int_{-\infty}^{\infty} dE_{recoil} E_{recoil}^n g(E_{recoil}, Q) = \int_{-\infty}^{\infty} dE_{recoil} \, E_{recoil}^n \cdot g_Q(E_{recoil}) \tag{53}$$

As $g_Q(E_{recoil})$ from (50) is normal distributed, the central moments are trivial. We directly obtain from (50):

$$\overline{E_{recoil}} = \left(1 + \frac{V}{\epsilon_\gamma}\right) \overline{E_{heat}} - \frac{V}{\epsilon_\gamma} \overline{E_{ion}} \tag{54}$$

$$\sigma_{E_{recoil}} = \sqrt{\sigma_{heat}^2 \left(1 + \frac{V}{\epsilon_\gamma}\right)^2 - 2\sigma_{ion-heat}^2 \frac{V}{\epsilon_\gamma} \left(1 + \frac{V}{\epsilon_\gamma}\right) + \sigma_{ion}^2 \left(\frac{V}{\epsilon_\gamma}\right)^2} \tag{55}$$

4 Interpretation

What does this probability density function $g(E_{recoil}, Q)$ now describe?
The multivariate normaldistribution in (7) describes, how an experimental value

$$\vec{r} = \vec{r}_{exp} = \begin{pmatrix} E_{ion} \\ E_{heat} \end{pmatrix}_{exp} \tag{56}$$

is scattered under the assumption that a certain true value

$$\vec{r}_0 = \vec{r}_{true} = \begin{pmatrix} E_{ion} \\ E_{heat} \end{pmatrix}_{true} \tag{57}$$

is given. Thus we obtain the conditional probability density

$$f(\vec{r}_{exp} | \vec{r}_{true}) = \frac{1}{2\pi \det C} \exp\left(-\frac{1}{2}(\vec{r}_{exp} - \vec{r}_{true})^T C^{-1}(\vec{r}_{exp} - \vec{r}_{true})\right) \tag{58}$$

where the covariance matrix is given by

$$C = \begin{pmatrix} \sigma_{ion}^2 & \sigma_{ion-heat}^2 \\ \sigma_{ion-heat}^2 & \sigma_{heat}^2 \end{pmatrix} \tag{59}$$

with true uncertainties σ_{ion}, σ_{heat} and covariance $\sigma_{ion-heat}$. The more interesting question now is, what statements can be done about the true value $\vec{r}_{true}$, when a certain value $\vec{r}_{exp}$ is measured. The reverse conditional probabiltiy density can be obtained by using Bayes' theorem:

$$h(\vec{r}_{true} | \vec{r}_{exp}) = \frac{f(\vec{r}_{exp} | \vec{r}_{true}) f_{true}(\vec{r}_{true})}{f_{exp}(\vec{r}_{exp})} \tag{60}$$

If a flat prior

$$f_{true}(\vec{r}_{true}) = \text{const} \tag{61}$$

is assumed for all $\vec{r}_{true}$, we have

$$h(\vec{r}_{true} | \vec{r}_{exp}) = f(\vec{r}_{exp} | \vec{r}_{exp}) \tag{62}$$

, since the posterior

$$f_{exp}(\vec{r}_{exp}) = \text{const} \tag{63}$$

is a fixed parameter in $h(\vec{r}_{true} | \vec{r}_{exp})$, which only leads to normalization

$$\int_{-\infty}^{\infty} h(\vec{r}_{true} | \vec{r}_{exp}) d\vec{r}_{true} = 1 \tag{64}$$

Obviously $h(\vec{r}_{true}|\vec{r}_{exp}) = f(\vec{r}_{exp}|\vec{r}_{true})$ is symmetric in the arguments, and the true value $\vec{r}_{true}$ is normal-distributed with mean of the measured value $\vec{r}_{exp}$. Now a coordinate transformation

$$\vec{r}_{true} = \begin{pmatrix} E_{ion} \\ E_{heat} \end{pmatrix}_{true} \rightarrow \vec{q}_{true} = \begin{pmatrix} E_{recoil} \\ Q \end{pmatrix}_{true} \tag{65}$$

$$h(\vec{r}_{true}|\vec{r}_{exp}) \rightarrow g(\vec{q}_{true}|\vec{r}_{exp}) = g(E_{recoil}, Q) \tag{66}$$

can be done which is derived in section 1.

The probability that the true value $\vec{q}_{true}$ which lead to the measured value $\vec{r}_{exp}$, lies in an area Ω in the E_{recoil}-Q-plane, is:

$$P(\vec{q}_{true} \in \Omega) = \iint_\Omega g(E_{recoil}, Q)d\Omega \tag{67}$$

Annotations

- The true covariance matrix C_{true} is not available and can only be estimated by C_{exp}. If the uncertainties $\sigma_{ion,exp}$ and $\sigma_{heat,exp}$ are estimated by linear interpolation between uncertainties $\sigma_{ion,heat,0}$ with $E = 0$ and $\sigma_{ion,heat,calib}$ with $E = E_{calib}$, we have for heat and ion channels:

$$\sigma(E) = \sqrt{\sigma_0^2 + \frac{E^2}{E_{calib}^2}(\sigma_{calib}^2 - \sigma_0^2)} \tag{68}$$

and we obtain by error propagation

$$\sigma_{\sigma(E)} = \sqrt{\left(2\sigma_0^2\left(1 - \frac{E^2}{E_{calib}^2}\right)\right)^2 \frac{\sigma_{\sigma_0}^2}{\sigma(E)^2} + \left(\sigma_{calib}\frac{E^2}{E_{calib}^2}\right)^2 \frac{\sigma_{\sigma_{calib}}^2}{\sigma(E)^2} + \left(\frac{E}{E_{calib}^2}(\sigma_{calib}^2 - \sigma_0^2)\right)^2} \tag{69}$$

$$\approx \frac{E}{E_{calib}^2}\left(\sigma_{calib}^2 - \sigma_0^2\right) \tag{70}$$

With typical values $E_{calib} = 356.0 keV$ for ^{133}Ba gamma calibration and $\sigma_{calib}^2 - \sigma_0 = 1..100 keV$, we obtain:

$$\sigma_{\sigma(E)} = 0.(00)0008E \tag{71}$$

There might be additional systematic errors due to the interpolation itself, since the uncertainties for arbitrary energies might not be exactly linear interpolable (extrapolable). Calibration with multiple known peaks, could provide more clarification about this dependancy $\sigma(E)$. Therefore confidence regions for single events depending on $\sigma_{ion,heat}(E)$ might be larger or smaller than estimated.

5 Toy experiments

In order to test the goodness of this density function, one can do monte carlo simulation.This can be done in ROOT by creating many events (E_{Recoil}, Q) from Gaussian distributed quantities E_{Ion} with uncertainty $\sigma_{E_{Ion}}$ and E_{Heat} with uncertainty $\sigma_{E_{Heat}}$ and fixed parameters V, ϵ, where

$$E_{Recoil} = \left(1 + \frac{V}{\epsilon}\right)E_{Heat} - \frac{V}{\epsilon}E_{Ion} \tag{72}$$

$$Q = \frac{E_{Ion}}{E_{Recoil}} \tag{73}$$

Then by filling a TH2D histogram with these events and compare it to another TH2D histogram created from the propability density function (pdf) $g(E_{Recoil}, Q)$ by the TH2D::FillRandom() method, one can do a χ^2 test to test the null hypothesis H_0, that both samples origin from the same distribution. For each bin the quantity

$$z_i = \frac{n_{pdf,i} - n_{mc,i}}{\sqrt{n_{pdf,i} + n_{mc,i}}} \tag{74}$$

can be determined which should be standard normally distributed for high numbers of events $n_{pdf,i}$ and $n_{mc,i}$. The test then is applied on

$$\chi^2 = \sum_i z_i^2 \tag{75}$$

where the sum goes over all bins with more than a certain number of events, which should be high enough to be normally distributed in good approximation.

5.1 Integral error estimation

The exact way to determine the expected bin contents would be to integrate $g(E_{recoil,Q}$ over the ranges of the bin and multiply with the total number of entries $n_{entries}$:

$$n_{i,pdf} = n_{entries} \cdot \int_{E_{recoil,i,min}}^{E_{recoil,i,max}} dE_{recoil} \int_{Q_{i,min}}^{Q_{i,max}} dQ \, g(E_{recoil}, Q) \tag{76}$$

As these integrations are very time-consuming the effort can be reduced by taylor-expanding $g(E_{recoil}, Q$ at the centers of the bins. Then with $\vec{a}_i = \begin{pmatrix} E_{recoil,i,min} \\ Q_{i,min} \end{pmatrix}$ and $\vec{b}_i = \begin{pmatrix} E_{recoil,i,max} \\ Q_{i,max} \end{pmatrix}$ we have

$$n_{i,pdf} = n_{entries} \cdot \int_{E_{recoil,i,min}}^{E_{recoil,i,max}} dE_{recoil} \int_{Q_{i,min}}^{Q_{i,max}} dQ \, g(E_{recoil}, Q) \tag{77}$$

$$= n_{entries} \cdot \int_{E_{recoil,i,min}}^{E_{recoil,i,max}} dE_{recoil} \int_{Q_{i,min}}^{Q_{i,max}} dQ \sum_{n_{E_{recoil}}=0}^{\infty} \sum_{n_Q=0}^{\infty} \frac{\left(\vec{x} - \frac{\vec{b}_i + \vec{a}_i}{2}\right)^{n_{E_{recoil}}} \left(\vec{x} - \frac{\vec{b}_i + \vec{a}_i}{2}\right)^{n_Q}}{n_{E_{recoil}}! n_Q!} \cdot \frac{\partial^{n_{E_{recoil}}}}{\partial E_{recoil}^{n_{E_{recoil}}}} \frac{\partial^{n_Q}}{\partial Q^{n_Q}} g(E_{re} \tag{78}$$

In the double for all terms where $n_{E_{recoil}}$ and n_Q are even the integral vanish as the indefinite integrals are odd with respect to the center of the bin:

$$n_{i,pdf} = n_{entries} \cdot \left(\left| \vec{b}_i - \vec{a}_i \right| g(E_{recoil,i}, Q) \right. \tag{79}$$

$$+ \frac{1}{6} \frac{\partial^2}{\partial E_{recoil}^2} g(E_{recoil,i}, Q_i) \cdot \left(\frac{E_{recoil,i,max} - E_{recoil,i,min}}{2} \right)^3 + \frac{1}{6} \frac{\partial^2}{\partial Q^2} g(E_{recoil,i}, Q_i) \cdot \left(\frac{Q_{i,max} - Q_{i,min}}{2} \right)^3 \tag{80}$$

$$+ \mathcal{O}\left(\left(\frac{E_{recoil,i,max} - E_{recoil,i,min}}{2} \right)^3 \left(\frac{Q_{i,max} - Q_{i,min}}{2} \right)^3 \right) \right) \tag{81}$$

This procedure is applied for some examples in the following:

Figure 1: Histograms with Monte Carlo events for some parameter combinations of $\bar{E_{Ion}}, \bar{E_{Heat}}, \sigma_{E_{Ion}}$, and $\sigma_{E_{Heat}}$ fitted with the pdf $f(E_{Recoil}, Q) = c \cdot g(E_{Recoil}, Q)$ and distribution of z_i for minimal number of pdf events $n_{min} > 400$

Table 1: χ^2 values for the corresponding parameter combinations and acceptance of the null hypothesis H_0

$\bar{E_{Ion}}$	$\bar{E_{heat}}$	$\sigma_{E_{Ion}}$	$\sigma_{E_{Heat}}$	χ^2 value	ndf	n_{min}	TMath::Prop(χ^2,ndf)	CL of pdf	H_0
100	100	1	1	57179	57110	400	0.418	90.1%	yes
100	100	5	1	34762.5	34576	400	0.239	95.3%	yes
100	100	1	5	29530	29038	400	0.020	96.2%	yes
100	50	1	1	65629	64877	400	0.019	87.4%	yes
100	50	5	1	51710	51732	400	0.526	91.2%	yes
100	50	1	5	29035	29322	400	0.882	96.4%	yes
50	100	1	1	90959	90805	400	0.358	68.7%	yes
50	100	1	5	73109	73203	400	0.597	83.8%	yes
50	100	5	1	61415	61112	400	0.193	88.7%	yes
20	20	5	5	58015	58449	400	0.898	84.7%	yes
20	20	1	5	31008	30129	400	0.0002	89.3%	no
20	20	5	1	34082	33851	400	0.188	86.5%	yes

The confidence level of the propability density function (CL of pdf) gives the percentage of the events in the χ^2 sum to the total sum of all monte carlo events. For the acceptance of the null hypothesis H_0, a significance level of 1% is assumed. That means it is accepted if TMath::Prob(χ^2,ndf)>0.01. So in one case out of 12 the null hypothesis H_0 has to be rejected.

5.2 script

The plots have been created by the script on in the scripts directory:

`$KDATA_ROOT/kqpa/scripts/ERecoilQDist_v30.C`

This file offers some methods:

a)
```
ERecoilQDist_v30(Double_t anEIonMean = 100,
                 Double_t anEHeatMean = 100,
                 Double_t anEIonSigma = 1,
                 Double_t anEHeatSigma = 1,
                 Double_t aNumBinsX = 2000,
                 Double_t aNumBinsY = 2000,
                 Long_t aNumEntries = 1E9,
                 Double_t aV = 3,
                 Double_t anEpsilon = 1,
                 Option_t* aFitOption = "'0LI"')
```

This methods creates two histograms "'mchist"' from creating random numbers distributed according the given parameters The histograms have the dimensions (aNumBinsX,aNumBinsY) and the boundaries are chosen, so that it covers $\pm$ aNumSigmas standard deviations calculated from error propagation around the center value.

$$\overline{E_{Recoil}} = \left(1 + \frac{V}{\epsilon_\gamma}\right)\overline{E_{Heat}} - \frac{V}{\epsilon_\gamma}\overline{E_{Ion}} \tag{82}$$

$$\overline{Q} = \frac{\overline{E_{Ion}}}{\overline{E_{Recoil}}} \tag{83}$$

In the case of E_{Recoil} this is the expectation value

$$\langle E_{Recoil}\rangle = \overline{E_{recoil}} \tag{84}$$

$$\langle E_{Ion}\rangle = \overline{E_{Ion}} \tag{85}$$

$$\langle E_{Heat}\rangle = \overline{E_{Heat}} \tag{86}$$

, as E_{Heat} and E_{Ion} are Gaussian distributed, but in the case of Q there is bias between $\overline{Q}$ and $\langle Q\rangle$:

$$\langle Q(E_{EIon}, E_{Recoil})\rangle = \left\langle \exp\left(\begin{pmatrix} E_{Ion} - \langle E_{Ion}\rangle \\ E_{Heat} - \langle E_{Heat}\rangle \end{pmatrix}\nabla\right) Q(E_{Ion}, E_{Recoil})\right\rangle \tag{87}$$

$$= \left\langle Q(\langle E_{Ion}\rangle, \langle E_{Heat}\rangle) + \frac{\partial Q}{\partial E_{Ion}}(E_{Ion} - \langle E_{Ion}\rangle) + \frac{\partial Q}{\partial E_{Heat}}(E_{Heat} - \langle E_{Heat}\rangle)\right. \tag{88}$$

$$+ \frac{\partial Q}{\partial E_{Ion}}\frac{\partial Q}{E_{Heat}}(E_{Ion} - \langle E_{Ion}\rangle)(E_{Heat} - \langle E_{Heat}\rangle) + \frac{1}{2}\frac{\partial^2 Q}{\partial E_{Ion}^2}(E_{Ion} - \langle E_{Ion}\rangle)^2 \tag{89}$$

$$+ \frac{1}{2}\frac{\partial^2 Q}{\partial E_{Heat}^2}(E_{Heat} - \langle E_{Heat}\rangle)^2 + \mathcal{O}\left(\left.\begin{pmatrix} E_{Ion} - \langle E_{Ion}\rangle \\ E_{Heat} - \langle E_{Heat}\rangle \end{pmatrix}^3\right)\right\rangle \tag{90}$$

$$= \overline{Q} + \left(\frac{1}{\langle E_{Recoil}\rangle} + \frac{V}{\epsilon_\gamma}\frac{\langle E_{Ion}\rangle}{\langle E_{Recoil}\rangle^2}\right)\left(1 + \frac{V}{\epsilon_\gamma}\right)\frac{\langle E_{Ion}\rangle}{\langle E_{Recoil}\rangle^2}\sigma_{Ion-Heat}^2 \tag{91}$$

$$+ \left(\frac{V}{\epsilon_\gamma}\frac{1}{\langle E_{Recoil}\rangle^2}\right)\left(1 + \frac{V}{\epsilon_\gamma}\frac{\langle E_{Ion}\rangle}{\langle E_{Recoil}\rangle}\right)\sigma_{Ion}^2 + \left(1 + \frac{V}{\epsilon_\gamma}\right)^2\frac{\langle E_{Ion}\rangle}{\langle E_{Recoil}\rangle^3}\sigma_{Heat}^2 \tag{92}$$

$$+ \mathcal{O}\left(\left\langle\left(\begin{pmatrix} E_{Ion} - \langle E_{Ion}\rangle \\ E_{Heat} - \langle E_{Heat}\rangle \end{pmatrix}\nabla\right)^3 Q(E_{Ion}, E_{Recoil})\right\rangle\right) \tag{93}$$

If the covariance matrix of $\begin{pmatrix} E_{Ion} \\ E_{Heat} \end{pmatrix}$ has very small entries, the square terms can be neglected. Additionally "'mchist"' is fitted with the pdf "'fkt"' alias 'f' and "'aFitOption"' and the histogram is stored in a ROOT file:

$<E_{Ion}>\_<E_{Heat}>\_<\sigma_{E_{Ion}}>\_<\sigma_{E_{Heat}}>$.root

b)
```
void ShowBinGausDistribution(Int_t aMinNumEntries = 400,
                             Int_t aMaxNumEntries = 1E50)
```

This method builds the histogram "pdfhist" for the theoretical distribution, where the bin contents $n_{pdf,i}$ are determined by evaluating the fitting function of the monte carlo histogram at the bin center values and a histogram "histres" representing the differences for each bin between the the entries in the monte carlo histogram and the pdf histogram. Then it builds a TH1D "gaushist" and fills it with the z_i calculated from the entries of "mchist" and "'pdfhist"'. Only entries with bin content larger than "aMinNumEntries" and smaller than "aMaxNumEntries" in "pdfhist" are considered. As the histograms might have different numbers of effective entries in the histograms' ranges, the z_i need some correction:

$$z_i = \frac{n_{mc,i} - c \cdot n_{pdf,i}}{n_{mc,i} + c^2 \cdot n_{pdf,i}} \tag{94}$$

where $c = \frac{n_{entries,mc}}{n_{entries,pdf}}$ is the quotient of the effective entries of both histograms. Then with the number of z_i (number of degrees of freedom) and the sum

$$\chi^2 = \sum_i z_i \tag{95}$$

a χ^2 test can be applied. χ^2, the number of degrees of freedom, the percentage of collected entries are printed.

c)
```
void MakeGraphs(const Char_t* aFileFormat = "pdf",
                Double_t aSignificanceLevel = 0.01)
```

This method makes graphs for the monte carlo histograms, their projections on both axis (<parameter_list>_px.<aFileFormat>) and <parameter_list>_py.<aFileFormat>), the projections of the residual histograms on both axis, ((<parameter_list>_pxres.<aFileFormat>) and <parameter_list>_respy.<aFileFormat>) and the Gaus histograms (<parameter_list>_gaus.<aFileFormat>) filled with z_i for all ROOT files in the current working directory and saves them in the specified file format.
Additionally it makes a tex file "graphics.tex" with includegraphics-commands for all images and a tex file "table.tex" which contains a table showing the results of the chi^2 tests based on the specified significance level.

References

[1] Henze, Stochastik I, Einfuhrung in die Wahrscheinlichkeitstheorie und Statistik, 2004