pBASEX Abel Inversion

Elio G. Champenois

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1. The Abel Transform:

For a given physical process leading to the emission of charged particles, the probability distribution of these particles can be described as a function of particle kinetic energy (E) and direction, specified by the polar (θ) and azimuthal (ϕ) angles:

$$F(E,\theta,\phi), \text{ such that } \int_0^\infty \int_0^\pi \int_0^{2\pi} F(E,\theta,\phi) E^2 \sin\theta d\phi d\theta dE = N \tag{1}$$

Given some time of evolution t, this distribution in kinetic energy space becomes a Newton sphere which can be represented as a spatial distribution:

$$r = vt \tag{2}$$

$$E = \frac{m}{2} v^2 = \alpha r^2 \tag{3}$$

$$\alpha = \frac{m}{2t^2} \tag{4}$$

$$\frac{dE}{dr} = 2\alpha r = 2\sqrt{\alpha E} \tag{5}$$

$$f(r,\theta,\phi), \text{ such that } \int_0^\infty \int_0^\pi \int_0^{2\pi} f(r,\theta,\phi) r^2 \sin\theta d\phi d\theta dr = N \tag{6}$$

$$F(E,\theta,\phi) E^2 dE = f(r,\theta,\phi) r^2 dr \tag{7}$$

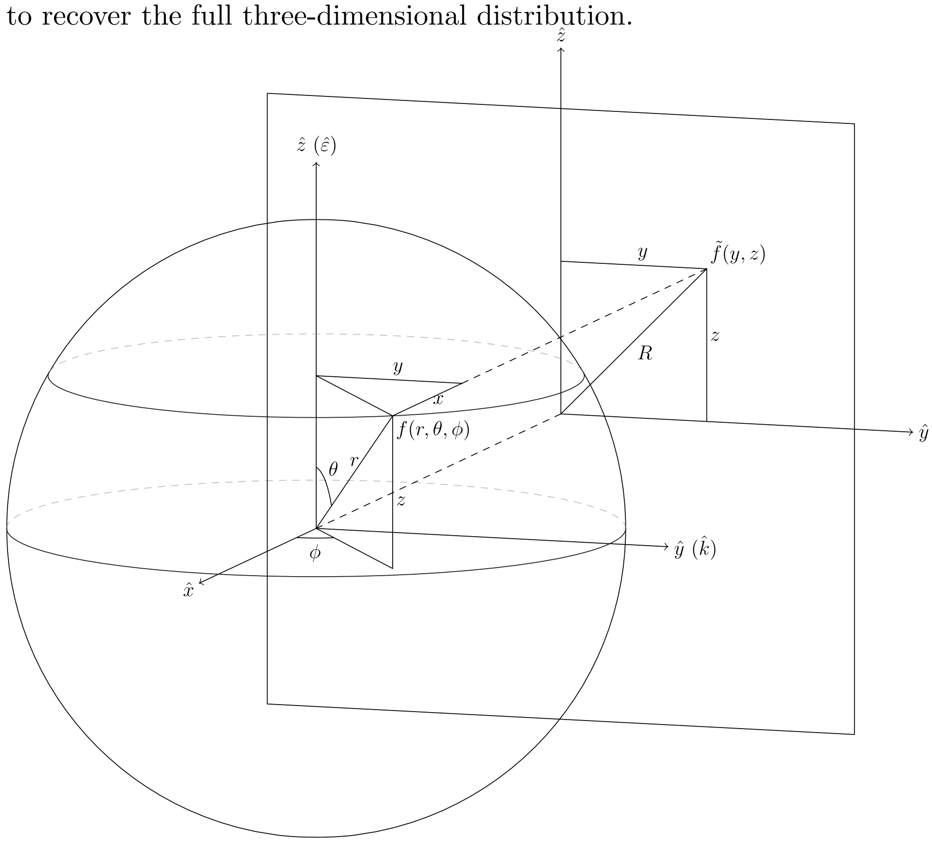
$$F(E,\theta,\phi) = \frac{f(r,\theta,\phi) r^2}{E^2} (\frac{dE}{dr})^{-1} \tag{8}$$

$$= \frac{f(r,\theta,\phi)}{2(\alpha E)^{3/2}} \tag{9}$$

A Velocity Map Imaging (VMI) spectrometer measures the projection of this three-dimensional distribution onto a two-dimensional plane. Mathematically, this projection is known as an Abel transform.

$$\tilde{f}(y,z) = \int_{-\infty}^{+\infty} dx f(r,\theta,\phi) \tag{10}$$

In general, the reduced dimensionality of this measurement would make it impossible to recover the full three-dimensional distribution.



2. Axial Symmetry:

For the case of photoionization of an isotropic target or an unaligned ensemble with linearly polarized light whose polarization vector lies parallel to the detection plane, axial symmetry is achieved, and we can describe the original distribution with only two planar coordinates:

$$f(r,\theta,\phi) \Rightarrow f(r,\theta) \tag{11}$$

$$\tilde{f}(y,z) = 2\int_0^\infty dx f(r,\theta) \tag{12}$$

With this axial symmetry, no information is lost in the projection. The challenge is now to perform an inverse Abel transform and recover the original distribution from its detected projection.

Conservation of angular momentum during the light-matter interaction further simplifies the task at hand, as the original distribution can be described with a general radial part multiplied by an angular part described as a sum of the Legendre polynomials. The highest order Legendre polynomial to include will be twice the order of the light-matter interaction.

$$l_{max} = 2N_{photons} \tag{13}$$

$$f(r,\theta) = \frac{\sigma(r)}{4\pi}[1 + \sum_{\substack{l=2 \\ l\ even}}^{l_{max}} \beta_l(r) P_l(\cos\theta)] \tag{14}$$

When dealing with an anistropic target or an aligned ensemble, this decomposition still works assuming axial symmetry still holds. However, it is no longer possible to truncate the sum of Legendre polynomials to get complete agreement. Still, partially due to the orthogonality of the Legendre polynomials, setting an arbitrary truncation can still be useful in approximating the angular distribution and extracting potentially relevant observables.

3. The pBASEX approach:

   Although it will no longer be possible to describe any arbitrary distribution, the use of radial basis functions to describe $\sigma(r)$ and $\beta_l(r)$ will allow for Abel inversion:

$$\sigma(r) \simeq \sum_k c_{k0} f_k(r) \tag{15}$$

$$f(r,\theta) = \frac{1}{4\pi} \sum_k c_{k0} f_k(r)[1 + \sum_{\substack{l=2 \\ l\ even}}^{l_{max}} \beta_l(r) P_l(\cos\theta)] \tag{16}$$

$$\beta_l(r) \simeq \frac{\sum_k c_{kl} f_k(r)}{\sum_k c_{k0} f_k(r)} \tag{17}$$

$$f(r,\theta) = \frac{1}{4\pi} \sum_k \sum_{\substack{l=0 \\ l\ even}}^{l_{max}} c_{kl} f_k(r) P_l(\cos\theta) \tag{18}$$

$$= \sum_k \sum_{\substack{l=0 \\ l\ even}}^{l_{max}} c_{kl} f_{kl}(r,\theta) \tag{19}$$

These basis functions can now be Abel transformed:

$$
\begin{aligned}
R &= \sqrt{y^2+z^2} && (20)\\
r &= \sqrt{R^2+x^2} && (21)\\
\cos\theta &= \frac{z}{\sqrt{R^2+x^2}} && (22)\\
\tilde{f}(y,z) &= 2\int_0^\infty dx f(r,\theta) && (23)\\
&= 2\sum_k \sum_{\substack{l=0\\ l\ even}}^{l_{max}} c_{kl} \int_0^\infty dx f_{kl}(\sqrt{R^2+x^2}, \cos^{-1}\frac{z}{\sqrt{R^2+x^2}}) && (24)\\
&= \frac{1}{2\pi}\sum_k \sum_{\substack{l=0\\ l\ even}}^{l_{max}} c_{kl} \int_0^\infty dx f_k(\sqrt{R^2+x^2}) P_l(\frac{z}{\sqrt{R^2+x^2}}) && (25)\\
&= \sum_k \sum_{\substack{l=0\\ l\ even}}^{l_{max}} c_{kl}\tilde{f}_{kl}(y,z) && (26)
\end{aligned}
$$

In practice, the measured distribution must be represented as a discrete function, whether this discretization is explicit due to detector pixelization or achieved through binning. Due to the finite measurement domain, the data can then be represented as a vector $\vec{b} \in \mathbb{R}^{n_p}$, where n_p is the number of pixels. In a similar way, the Abel transformed basis functions can be represented as a matrix $G \in \mathbb{R}^{n_p \times n_b}$, where n_b is the number of basis functions, and the coefficients of the basis functions as a vector $\vec{c} \in \mathbb{R}^{n_p}$. It is now possible to find the coefficients by fitting the data using:

$$G\vec{c} = \vec{b} \tag{27}$$

Assuming a square and euclidean pixel grid, there will be $\sqrt{n_p}$ points sampled in each axis. This number is an appropriate upper limit on the amount of radial basis functions to use to avoid overfitting on $\sigma(r)$. In most applications, the sum over Legendre polynomials will be truncated such that:

$$
\begin{aligned}
l_{max} &\ll \sqrt{n_p}\\
n_b \leq l_{max}\sqrt{n_p} &\ll n_p
\end{aligned}
$$

This leads to an underdetermined system when solving for the coefficients, which makes least squares linear regression an appropriate tool. We find the optimal coefficient vector $\vec{c}_*$ such that:

$$\vec{c}_* = \underset{\vec{c}}{\operatorname{argmin}} \|G\vec{c} - \vec{b}\|^2 \tag{28}$$

This problem has an analytical solution. Using the singular value decomposition of G, we can obtain the optimal coefficients and recover the original distribution:

$$G = U\Sigma V^T \tag{29}$$

$$\vec{c}_* = V\Sigma^{-1}U^T\vec{b} \tag{30}$$

$$\sigma(r) = \sum_k c_{k0} f_k(r) \tag{31}$$

$$\beta_l(r) = \frac{\sum_k c_{kl} f_k(r)}{\sum_k c_{k0} f_k(r)} \tag{32}$$

We also note that use of the singular value decomposition allows for both a regularized fit with regularization values λ_i as the diagonal elements of $\lambda \in \mathbb{R}^{n_b \times n_b}$:

$$\vec{c}_* = \underset{\vec{c}}{\operatorname{argmin}} \|G\vec{c} - \vec{b}\|^2 + \|\lambda^{1/2}\vec{c}\|^2 \tag{33}$$

$$= V\tilde{\Sigma^{-1}}U^T\vec{b} \tag{34}$$

$$\tilde{\Sigma^{-1}}_{ij} = \delta_{ij}\frac{\Sigma_{ii}}{\Sigma_{ii}^2 + \lambda_i} \tag{35}$$

or a weighted fit with pixel weights w_i as the diagonal elements of $W \in \mathbb{R}^{n_p \times n_p}$:

$$\vec{c}_* = \underset{\vec{c}}{\operatorname{argmin}} \|W^{1/2}(G\vec{c} - \vec{b})\|^2 \tag{36}$$

$$= V\Sigma^{-1}(U^TWU)^{-1}U^TW\vec{b}. \tag{37}$$

The particle kinetic energy spectrum and angular distribution are the two outputs. The angular distribution follows trivially from $\beta_l(r)$, while a bit more work is needed for the kinetic energy spectrum:

$$\beta_l(E) = \frac{\sum_k c_{kl} f_k(\sqrt{\frac{E}{\alpha}})}{\sum_k c_{k0} f_k(\sqrt{\frac{E}{\alpha}})} \tag{38}$$

$$F(E,\theta,\phi) = \frac{f(\sqrt{\frac{E}{\alpha}},\theta)}{2(\alpha E)^{3/2}} \tag{39}$$

$$= \frac{1}{8\pi(\alpha E)^{3/2}} \sum_k \sum_{\substack{l=0 \\ l\ even}}^{l_{max}} c_{kl} f_k(\sqrt{\frac{E}{\alpha}}) P_l(\cos\theta) \tag{40}$$

Working towards a more useful representation of the kinetic energy spectrum:

$$N = \int_0^\infty \int_0^\pi \int_0^{2\pi} F(E,\theta,\phi) E^2 \mathrm{sin}\theta d\phi d\theta dE \tag{41}$$

$$= \frac{1}{8\pi\alpha^{3/2}} \sum_k \sum_{\substack{l=0 \\ l\ even}}^{l_{max}} c_{kl} \int_0^\infty \int_0^\pi \int_0^{2\pi} f_k(\sqrt{\frac{E}{\alpha}}) P_l(\mathrm{cos}\theta)\sqrt{E}\mathrm{sin}\theta d\phi d\theta dE \tag{42}$$

$$= \frac{1}{2\alpha^{3/2}} \sum_k c_{k0} \int_0^\infty f_k(\sqrt{\frac{E}{\alpha}})\sqrt{E} dE \tag{43}$$

$$= \int_0^\infty I(E) dE \tag{44}$$

$$I(E) = \frac{1}{2\alpha^{3/2}} \sum_k c_{k0} f_k(\sqrt{\frac{E}{\alpha}})\sqrt{E} \tag{45}$$

4. Choice of basis functions:

The standard choice for basis functions are Gaussian functions:

$$f_k(r) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}(\frac{r-r_k}{\sigma_k})^2} \tag{46}$$

Typically, these functions will be evenly spaced and have constant width:

$$r_k = r_0 + k\Delta r \tag{47}$$

$$\sigma_k = \sigma \tag{48}$$

A range of values for σ will work decently, but we can choose one that allows to generate a relatively flat function:

$$f(r) = \frac{1}{2}[f_k(r) + f_{k+1}(r)] \tag{49}$$

$$f(\frac{r_k + r_{k+1}}{2}) = f(r_k + \Delta r/2) = f(r_k) = f(r_{k+1}) \tag{50}$$

$$e^{-\frac{(\Delta r/2)^2}{2\sigma^2}} = \frac{1}{2}[1 - e^{-\frac{\Delta r^2}{2\sigma^2}}] \tag{51}$$

$$\sigma = (0.45291...)\Delta r \approx 0.5\Delta r \tag{52}$$

The integrals that need to be calculated are then of the form:

$$\tilde{f}_{kl}(x,y) = \frac{1}{(2\pi)^{3/2}\sigma} \int_0^\infty dz e^{-\frac{1}{2}(\frac{\sqrt{R^2+z^2}-r_k}{\sigma})^2} P_l(\frac{x}{\sqrt{R^2+z^2}}) \tag{53}$$

We can write the Legendre polynomials as a sum over monomials:

$$\tilde{f}_{kl}(x,y) = \frac{2^l}{(2\pi)^{3/2}\sigma} \sum_{n=0}^{l/2} x^{2n} \binom{l}{2n} \binom{\frac{l+2n-1}{2}}{l} \int_0^\infty dz \frac{e^{-\frac{1}{2}(\frac{\sqrt{R^2+z^2}-r_k}{\sigma})^2}}{(R^2+z^2)^n} \tag{54}$$

$$= \frac{2^l}{(2\pi)^{3/2}\sigma} \sum_{n=0}^{l/2} x^{2n} \binom{l}{2n} \binom{\frac{l+2n-1}{2}}{l} I_{kn}(x,y) \tag{55}$$

An analytic solution is possible by using a truncated Taylor expansion rather than the Gaussian radial basis function. The Taylor expansion must be truncated at an odd M for the function to have zeroes. Numerical methods or lower bounds can be used to find the domain of this new radial basis function, delimited by these zeroes.

$$e^{-\frac{1}{2}(\frac{r-r_k}{\sigma})^2} \simeq \begin{cases} \sum_{m=0}^{M}(-\frac{1}{2\sigma^2})^m \frac{(r-r_k)^{2m}}{m!}, & r_k - r_M \le r \le r_k + r_M \\ 0, \text{ elsewhere} \end{cases} \tag{56}$$

$$\sum_{m=0}^{M} \frac{1}{m!}(-\frac{r_M^2}{2\sigma^2})^m = 0 \tag{57}$$

$$\sqrt{R^2 + z_\pm^2} = r_k \pm r_M \tag{58}$$

$$z_\pm = \sqrt{\max(0, (r_k \pm r_M)^2 - R^2)} \tag{59}$$

$$I_{kn}(x,y) = \sum_{m=0}^{M} \frac{1}{m!}(-\frac{1}{2\sigma^2})^m \int_{z_-}^{z_+} dz \frac{(\sqrt{R^2+z^2} - r_k)^{2m}}{(R^2+z^2)^n} \tag{60}$$

$$= \sum_{m=0}^{M} \sum_{j=0}^{2m} \frac{1}{m!}(-\frac{1}{2\sigma^2})^m \binom{2m}{j} (-r_k)^{2m-j} \int_{z_-}^{z_+} dz (R^2+z^2)^{\frac{j}{2}-n} \tag{61}$$

$$= \sum_{m=0}^{M} \frac{1}{m!}(-\frac{r_k}{2\sigma^2})^m \sum_{j=0}^{2m} \binom{2m}{j} (-\frac{R}{r_k})^j R^{-2n} [z\,{}_2F_1(\frac{1}{2}, n-\frac{j}{2}; \frac{3}{2}; -\frac{z^2}{R^2})] \Big|_{z_-}^{z_+} \tag{62}$$

There are no more numerical integrals, but samplings of the hypergeometric function are needed:

$$\tilde{f}_{kl}(x,y) = \frac{2^l}{(2\pi)^{3/2}\sigma} \sum_{n=0}^{l/2} (\frac{x}{R})^{2n} \binom{l}{2n} \binom{\frac{l+2n-1}{2}}{l} \times \tag{63}$$

$$\sum_{m=0}^{M} \frac{1}{m!}(-\frac{r_k}{2\sigma^2})^m \sum_{j=0}^{2m} \binom{2m}{j} (-\frac{R}{r_k})^j [{}_2F_1(\frac{1}{2}, n-\frac{j}{2}; \frac{3}{2}; -\frac{z^2}{R^2}) z] \Big|_{z_-}^{z_+} \tag{64}$$

5. Implementation:

To summarize, the pBASEX algorithm is implemented in the following steps:

(a) Sampling of the Abel transformed basis functions using equations (25-26, 29).

(b) Fitting of data to these sampled functions using equation (30).

(c) Reconstruction of the inverted data using equations (38, 45).