Mathematical Representations

Sune N. Jespersen

Chantal M.W. Tax

Declaration of Financial Interests or Relationships

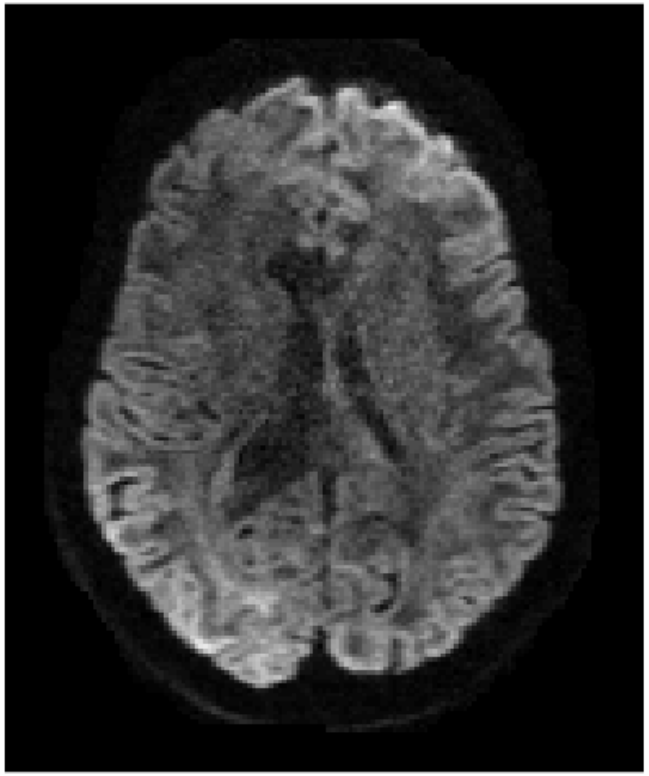
Speaker Name: Chantal M.W. Tax

I have no financial interests or relationships to disclose with regard to the subject matter of this presentation.

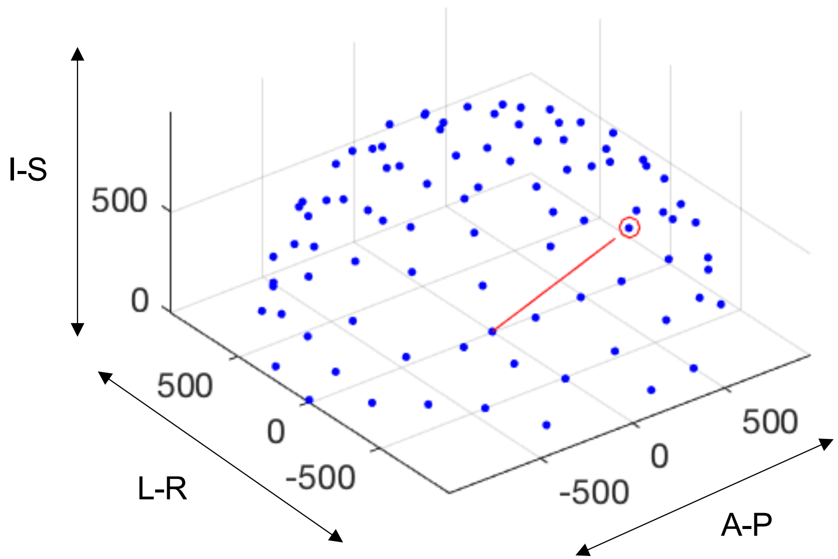
Mathematical Representations

- Cumulant Expansion
- DTI/DKI
- Multiple Gaussian Compartments
- Spherical Harmonics
- Rotational Invariants
- Propagator Imaging

Spherical Harmonics (SH)

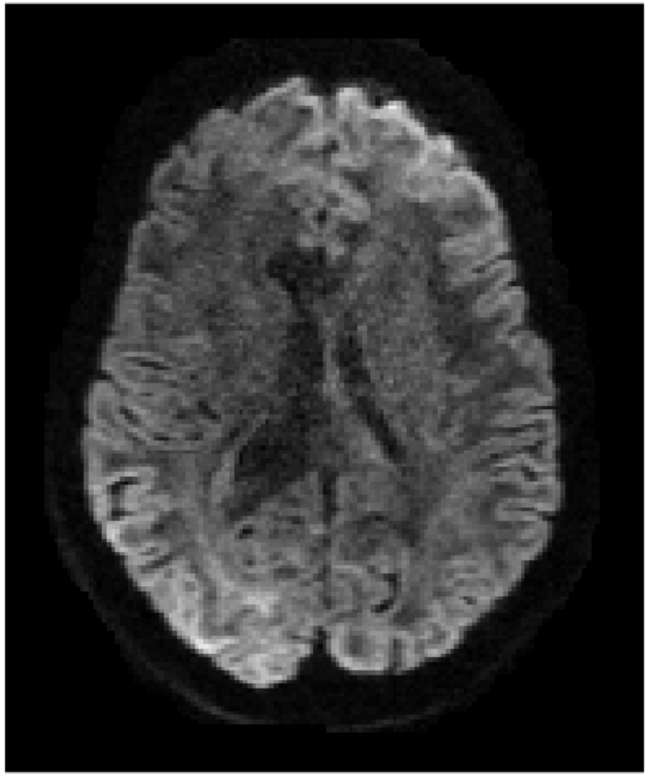


$b = 1000\ s/mm^2$



$\hat{\boldsymbol{g}}$

Spherical Harmonics (SH)



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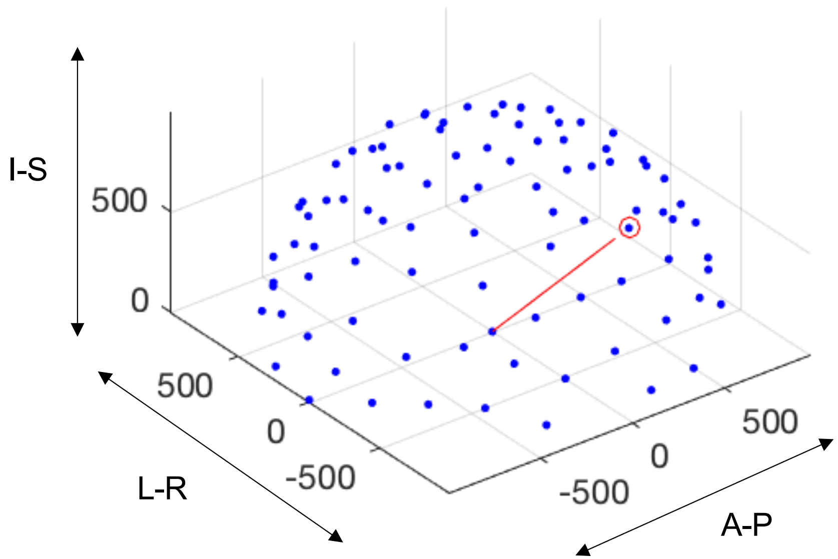
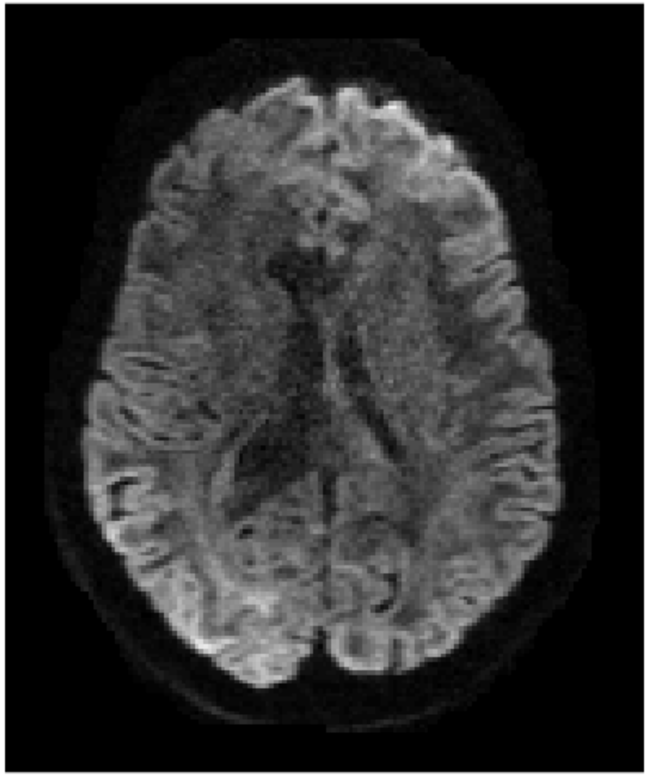


$\hat{\boldsymbol{g}} = \hat{\boldsymbol{g}}(\theta, \phi) \in S^2$

Spherical Harmonics (SH)



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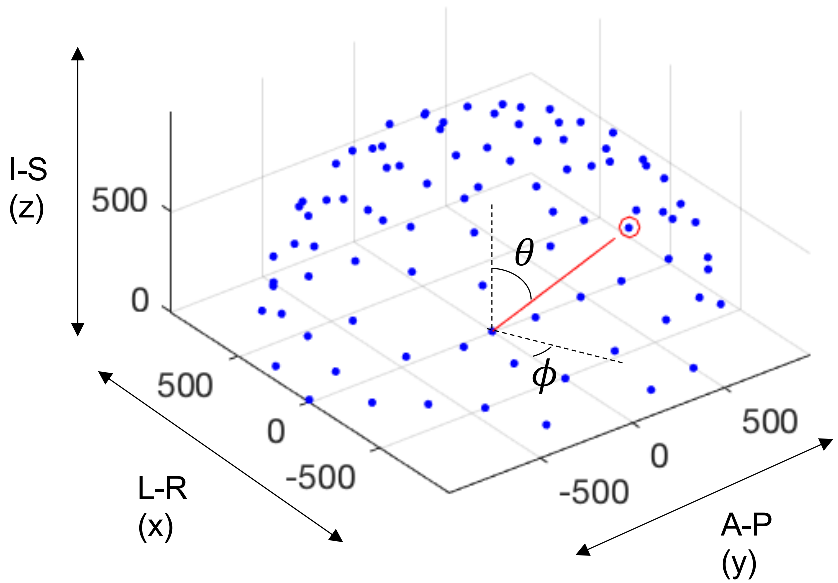
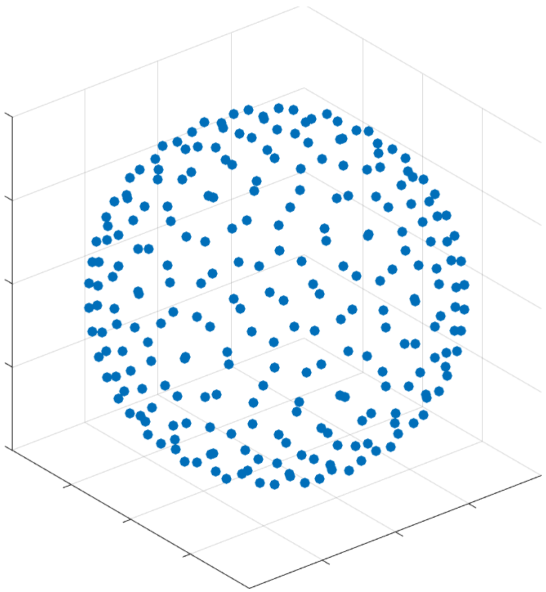


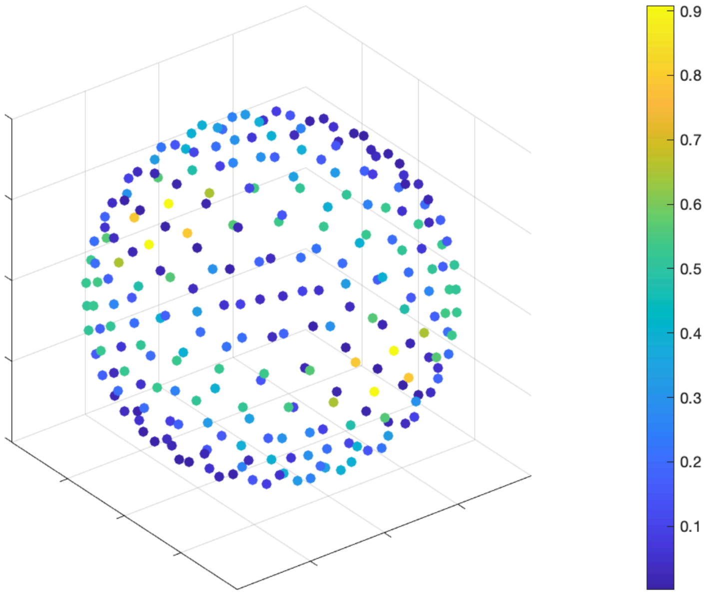
$$\widehat{\boldsymbol{g}} = \widehat{\boldsymbol{g}}(\theta, \phi)$$
$$= (\sin\theta\cos\phi, \sin\theta\sin\phi, \sin\theta)$$

Spherical Harmonics (SH): functions on a sphere

$\boldsymbol{g} = \boldsymbol{g}(\theta, \phi)$



$f\big(\boldsymbol{g}(\theta, \phi)\big)$



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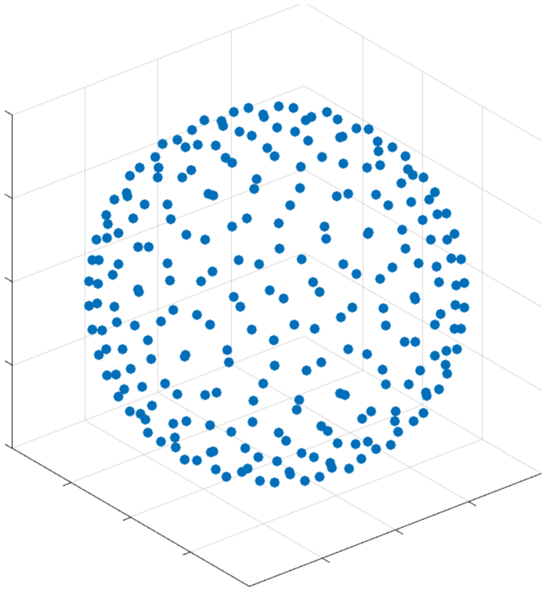
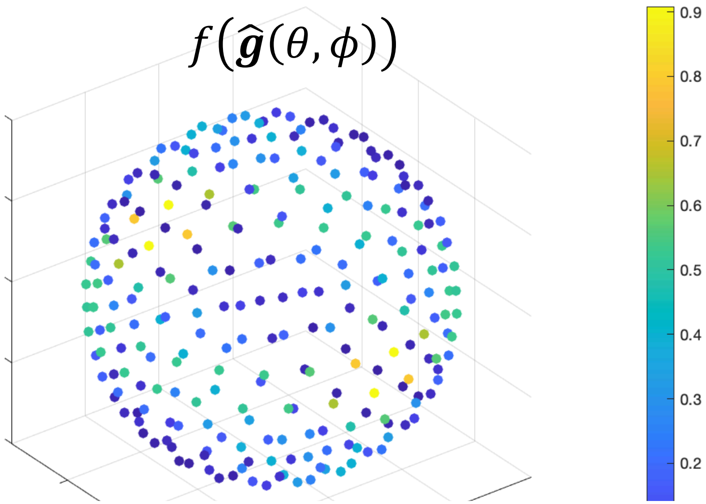
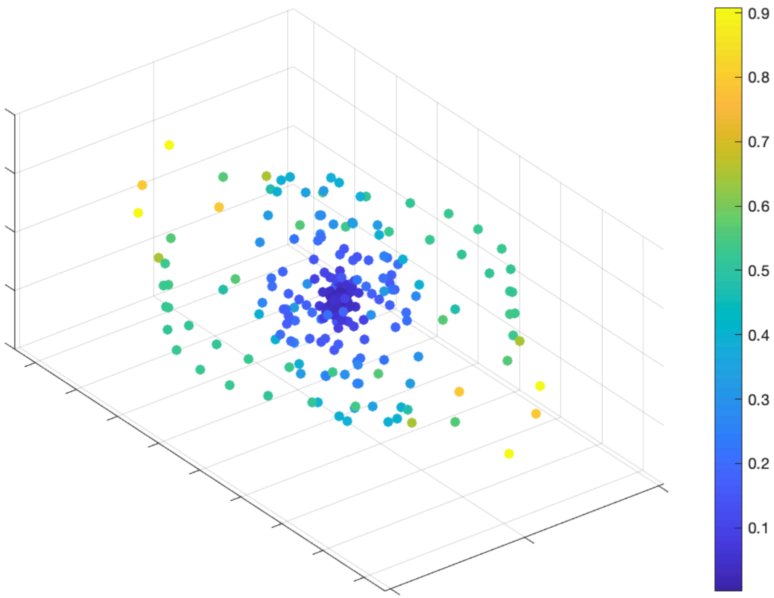


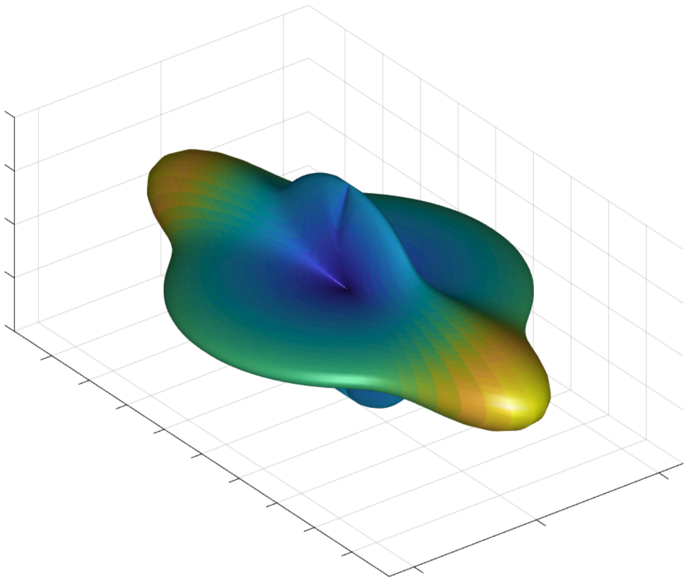
$$f\big(\hat{\boldsymbol{g}}(\theta, \phi)\big)$$





$$f\big(\hat{\boldsymbol{g}}(\theta, \phi)\big) = \sum_{l,m} p_{lm}\, Y_{lm}(\theta, \phi)$$

continuous functions



Spherical Harmonics (SH)

$$f(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} p_{lm} \, Y_{lm}(\theta,\phi)$$

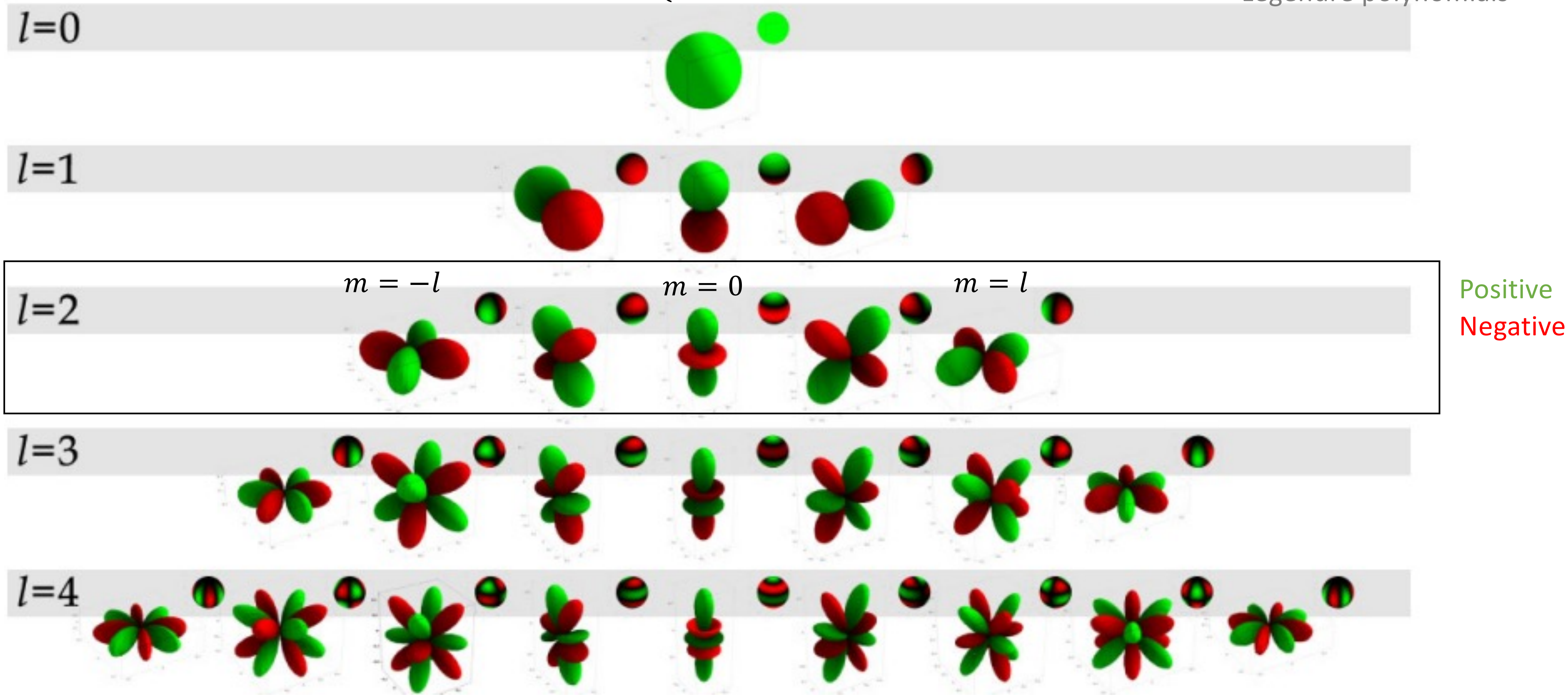
Real SH

$$Y_{lm}(\theta,\phi) = \begin{cases} \sqrt{2}\,\mathrm{Im}[Y_l^{-m}] & \text{if } m < 0 \\ Y_l^0 & \text{if } m = 0 \\ \sqrt{2}\,\mathrm{Re}[Y_l^m] & \text{if } m > 0 \end{cases}$$

Complex SH

$$Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} \, P_l^m(\cos\theta) e^{im\phi}$$

Legendre polynomials



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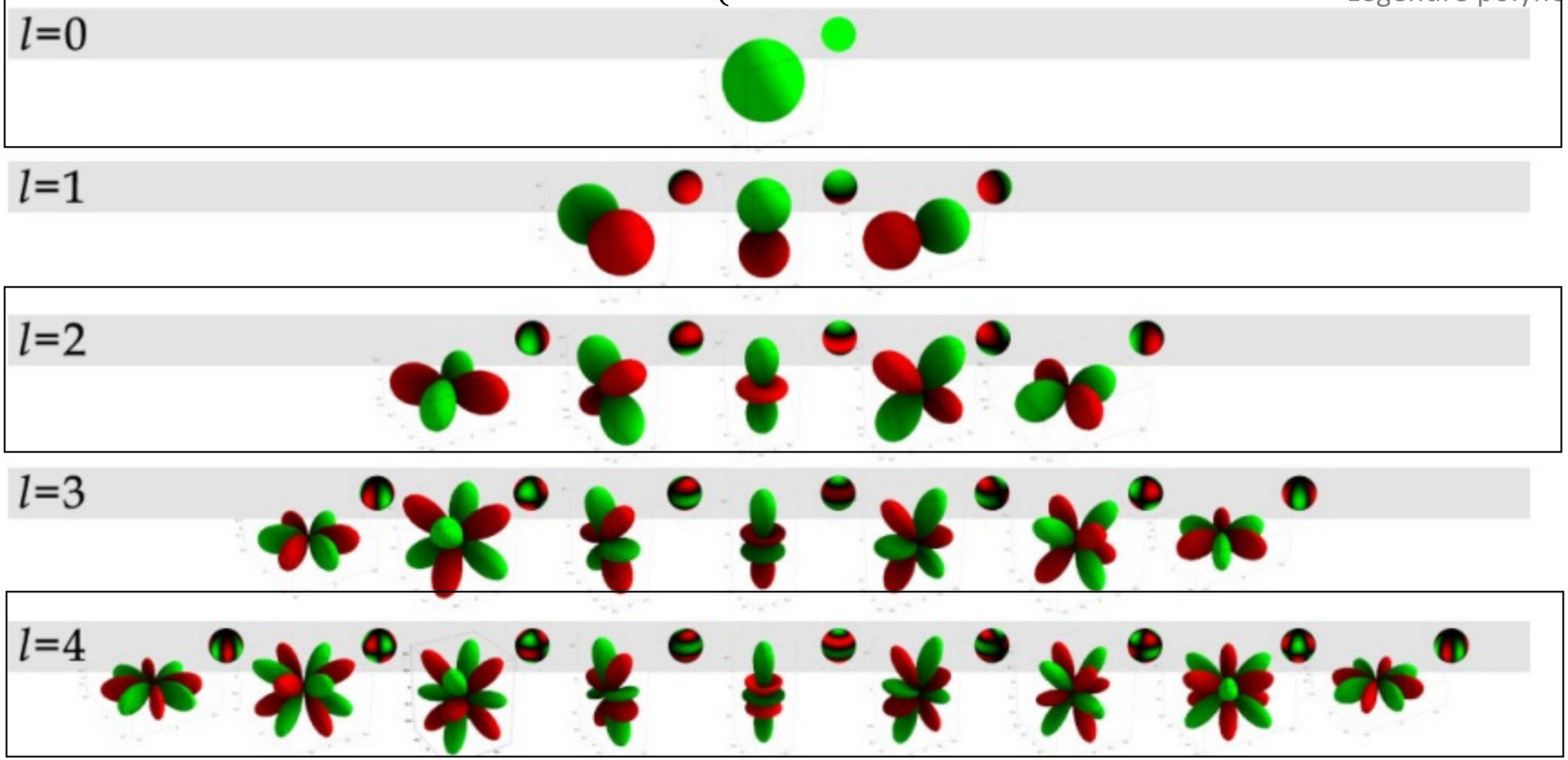
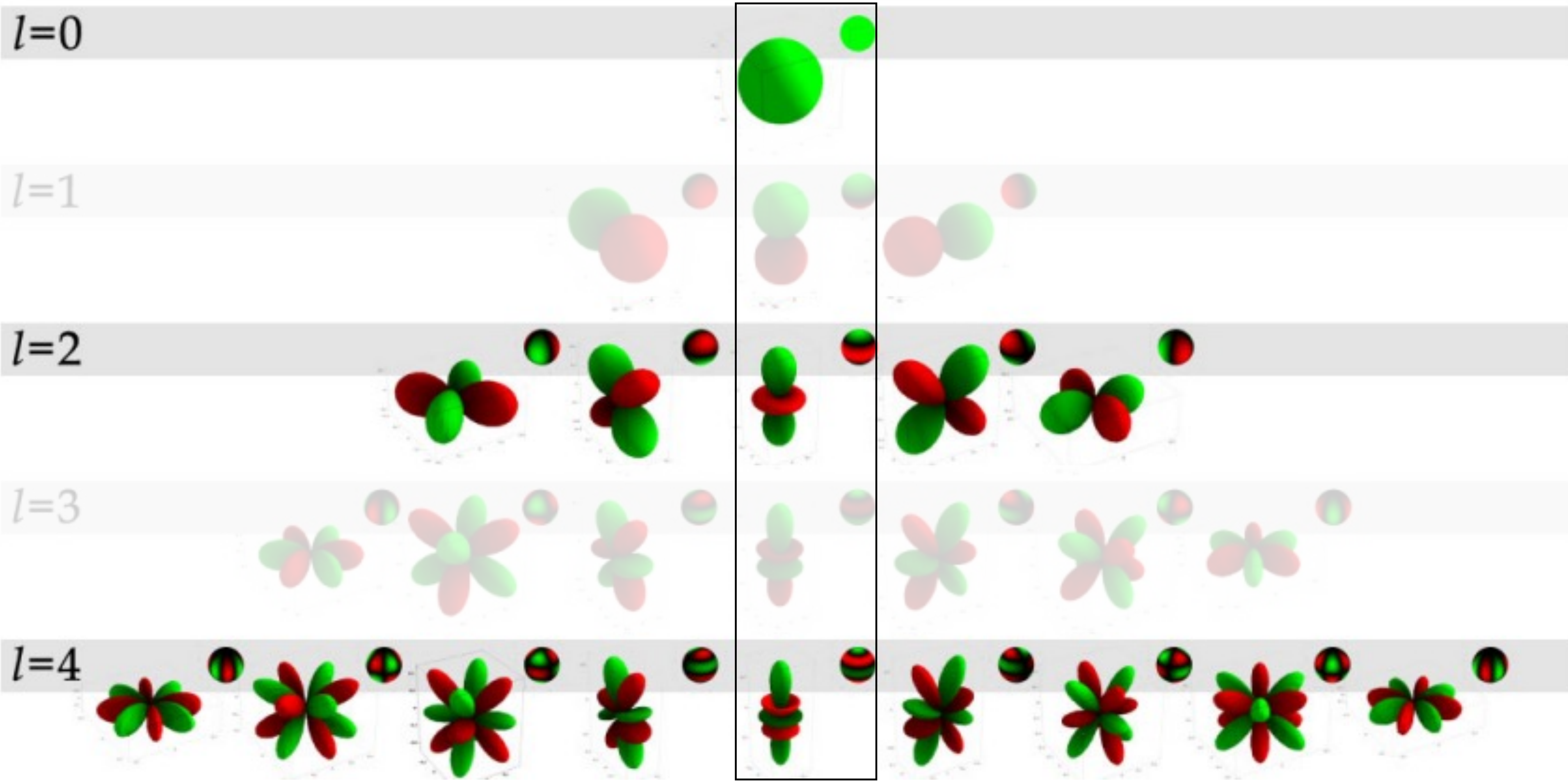


Positive

Negative

Exercise 6

What is roughly the angular resolution of $Y_{l0}(\theta, \phi) \propto P_l(\cos\theta)$? (Hint: determine the width of the lobes)



Exercise 7

$$f\big(\boldsymbol{g}(\theta,\phi)\big) = \sum_{l=0}^{L_{\max}} \sum_{m=-l}^{l} p_{lm}\, Y_{lm}(\theta,\phi)$$

Plot the signal $S(\boldsymbol{g}) = 0.4\exp(-12g_z^2) + 0.6\exp(-12g_x^2)$ over the sphere and compare to the spherical harmonics expansions with $L_{\max} = 2, 4, 6, 8$

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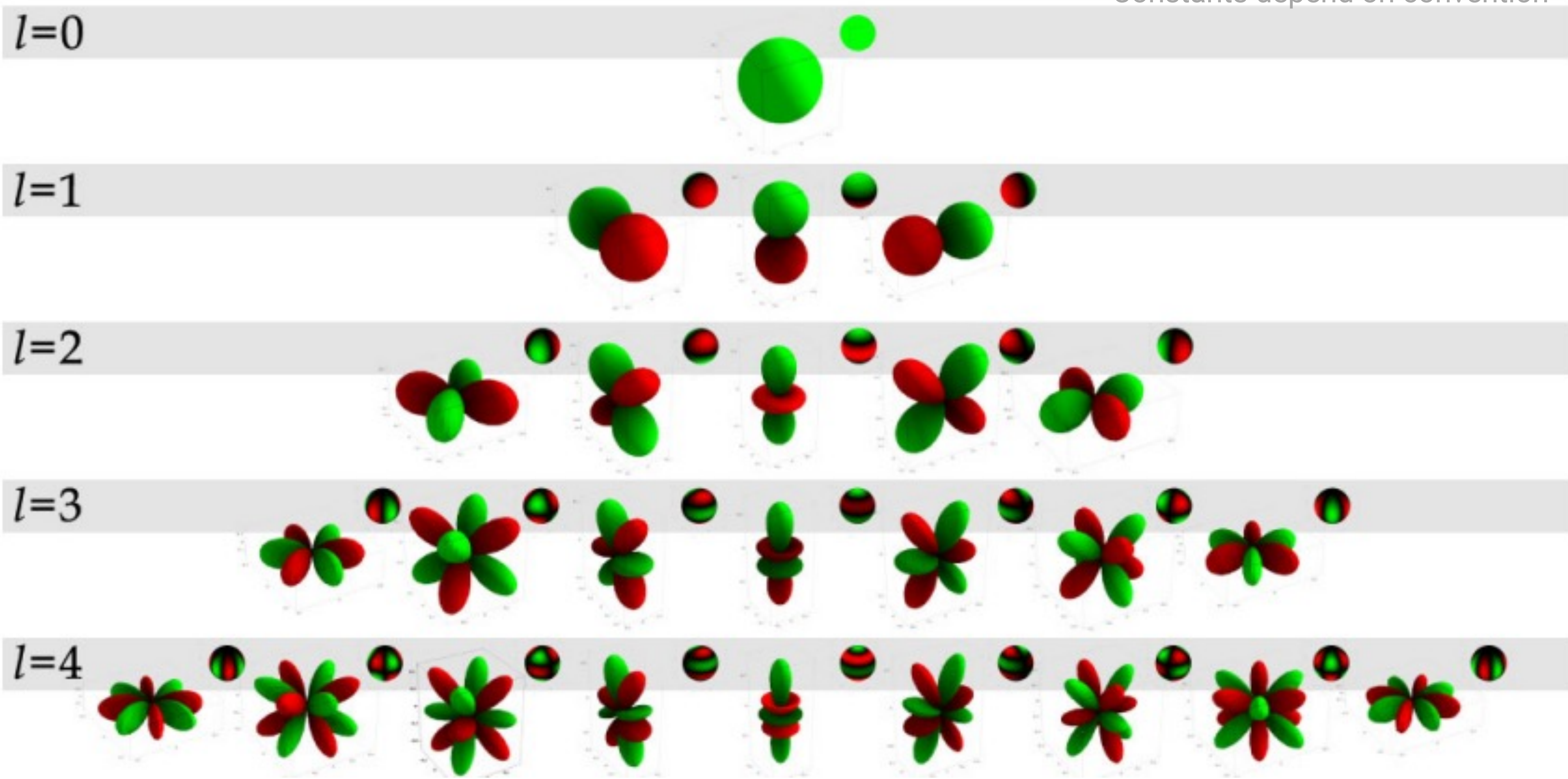
- Rotational Invariants
- Propagator Imaging

Rotational invariants

$$p_l = \left(\frac{4\pi}{(2l+1)} \sum_{m=-l}^{l} |p_{lm}|^2 \right)^{1/2}$$

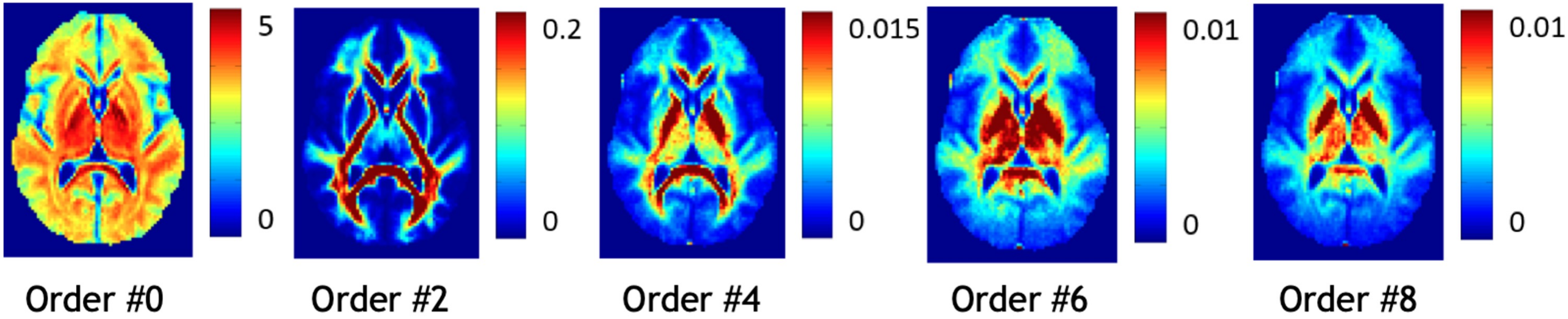
Constants depend on convention



Rotational invariants

$$p_l = \left(\frac{4\pi}{(2l+1)} \sum_{m=-l}^{l} |p_{lm}|^2 \right)^{1/2}$$

Rotationally Invariant Spherical Harmonic (RISH) features

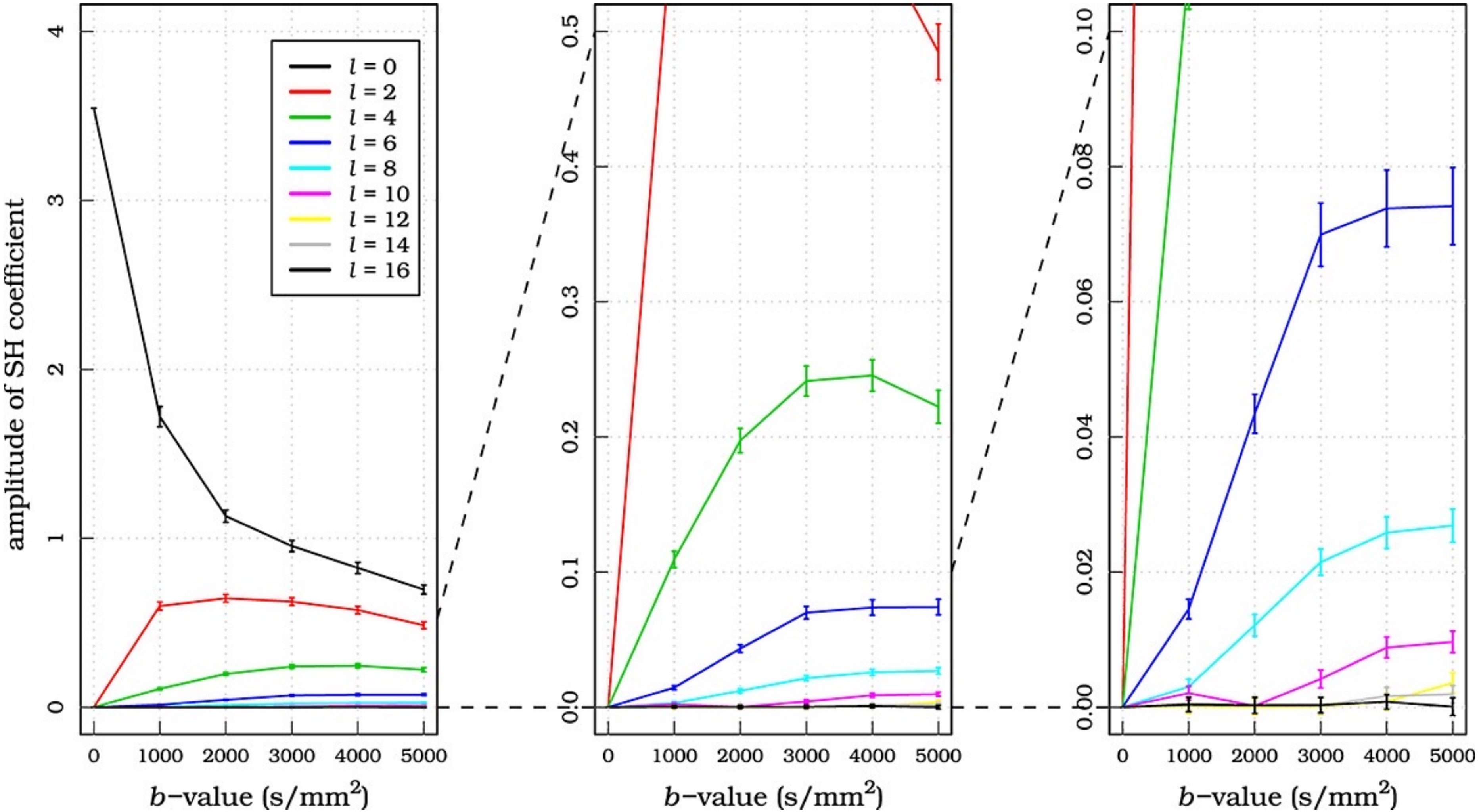


Tax et al., Handbook of Diffusion MR Tractography, p 669-688, 2025

Exercise 8

Plot $p_l(b)$ vs b for $S(b, \boldsymbol{g}) = 0.5\exp(-3bg_z^2) + 0.5\exp(-2bg_x^2)$ and formulate the connection between diffusion weighting and angular resolution based on your results.

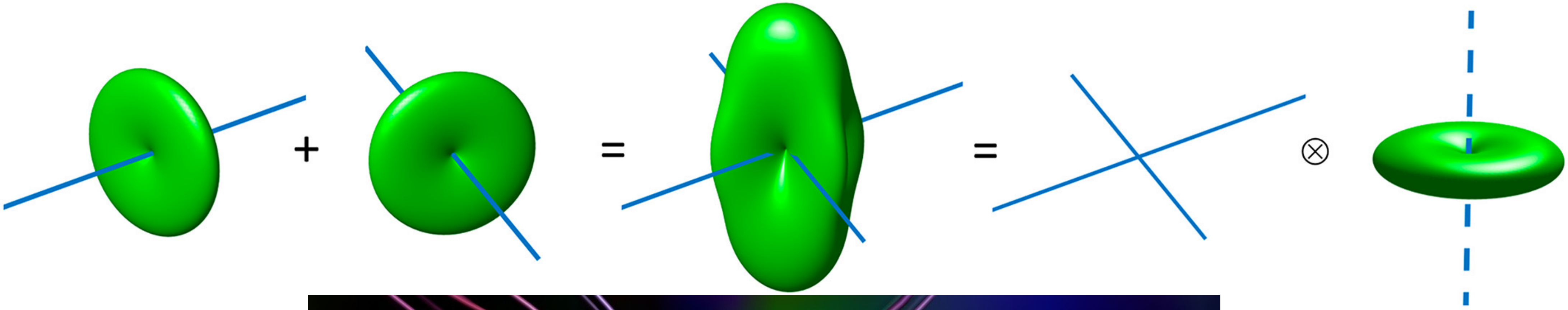
Spherical Harmonics (SH): Angular resolution and b-value

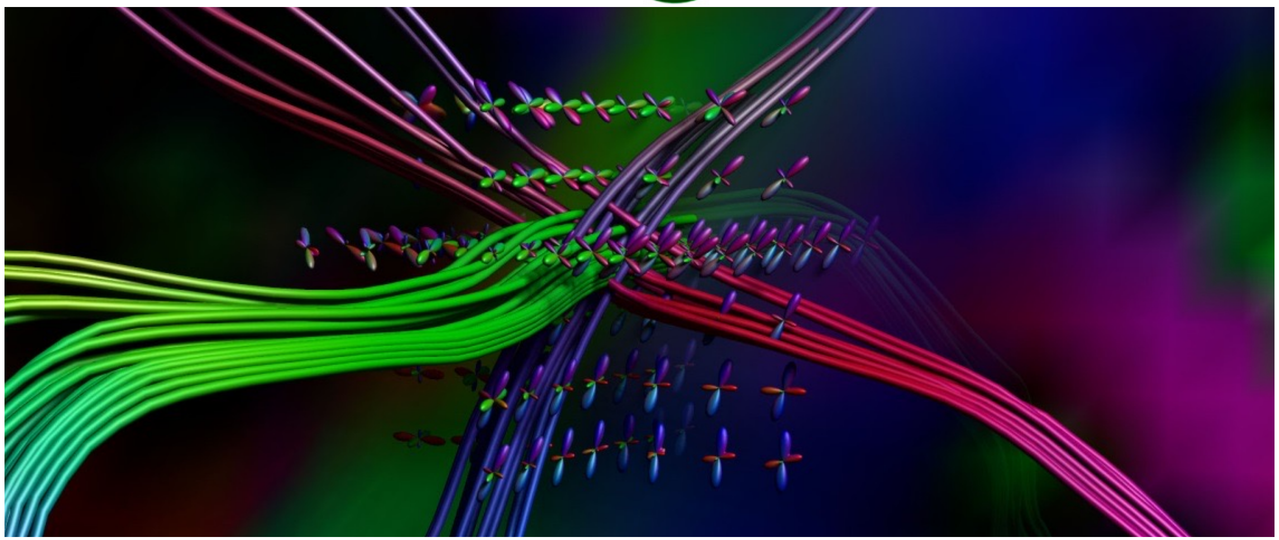


Tournier et al. NMR Biomed 2013

Spherical Harmonics (SH): fiber Orientation Distribution Function (fODF)

$S_1(b, \hat{\boldsymbol{g}})$ $S_2(b, \hat{\boldsymbol{g}})$ $S(b, \hat{\boldsymbol{g}})$ $\mathcal{P}(\hat{\boldsymbol{n}})$ (fODF) $K(b, \hat{\boldsymbol{g}} \cdot \hat{\boldsymbol{n}})$ (kernel)





Dell'Acqua and Tournier, NMR Biomed 2018; Image courtesy Alexander Leemans

Exercise 9

The most anisotropic fODF has the form $\mathcal{P}(\theta,\phi)=\frac{1}{2\pi}\delta(1-\cos^2\theta)$. Derive the corresponding spherical harmonic coefficients p_{lm} and rotational invariants p_l. (Hints: $\mathcal{P}$ is independent on ϕ, $\delta(1-x^2)=\frac{1}{2}\delta(1-x)$ for $x\in[0\ 1]$, and $P_l(1)=1$).

$$f(\theta,\phi)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} p_{lm}\,Y_{lm}(\theta,\phi)$$

Real SH

$$Y_{lm}(\theta,\phi)=\begin{cases}\sqrt{2}\,\mathrm{Im}[Y_l^{-m}] & \text{if } m<0\\ Y_l^0 & \text{if } m=0\\ \sqrt{2}\,\mathrm{Re}[Y_l^{m}] & \text{if } m>0\end{cases}$$

Complex SH

$$Y_l^m(\theta,\phi)\ =\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\,P_l^m(\cos\theta)e^{im\phi}$$

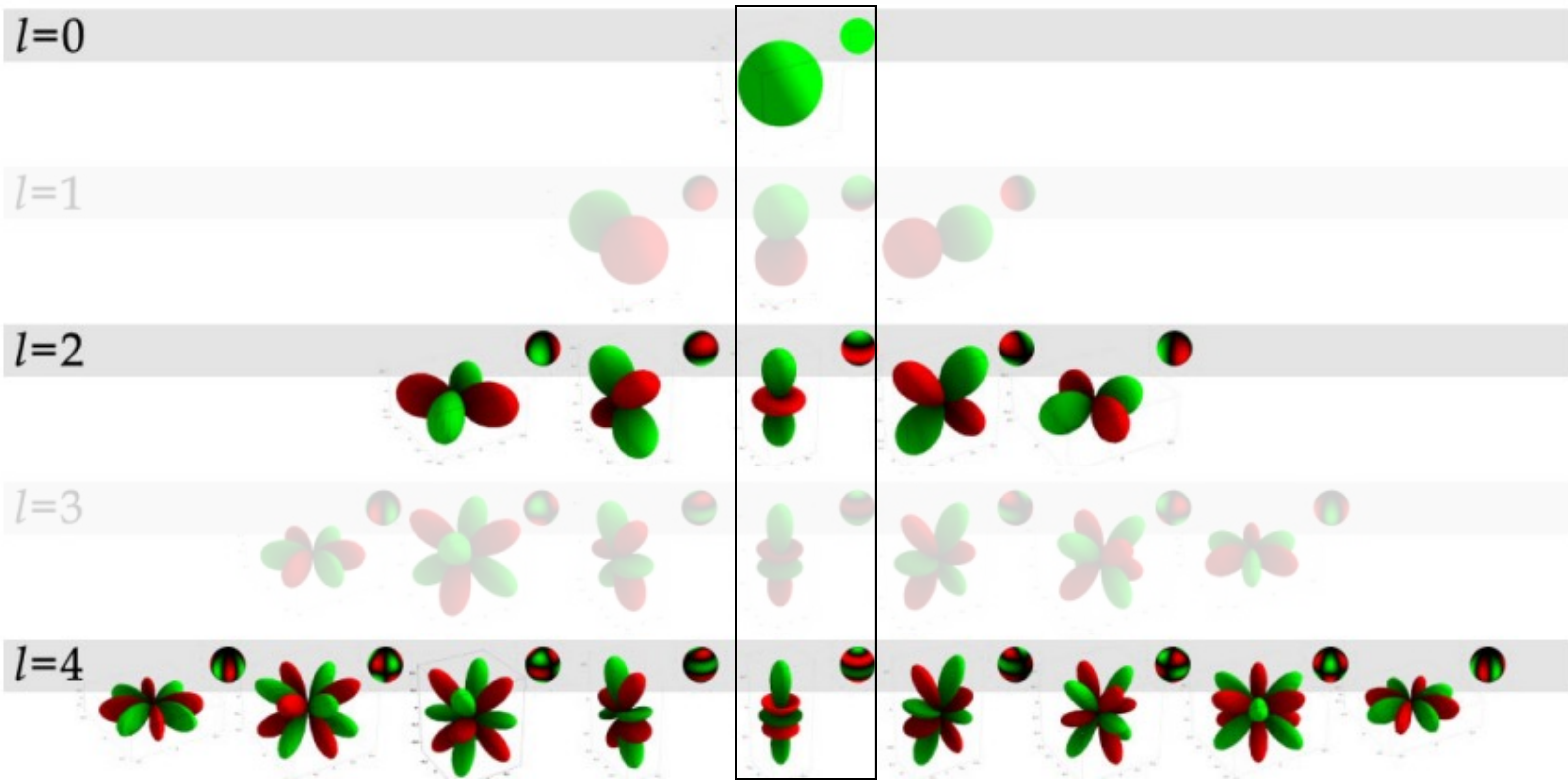
Legendre polynomials

$$p_{lm}=\int_0^{2\pi}\int_0^{\pi} f(\theta,\phi)Y_l^{m*}(\theta,\phi)\sin\theta\,d\theta d\phi$$

$$p_l=\left(\frac{4\pi}{(2l+1)}\sum_{m=-l}^{l}|p_{lm}|^2\right)^{1/2}$$

Exercise 9: Solution

The most anisotropic fODF has the form $\mathcal{P}(\theta, \phi) = \frac{1}{2\pi}\delta(1 - \cos^2\theta)$. Derive the corresponding spherical harmonic coefficients p_{lm} and rotational invariants p_l. (Hints: $\mathcal{P}$ is independent on ϕ, $\delta(1 - x^2) = \frac{1}{2}\delta(1 - x)$ for $x \in [0\ 1]$, and $P_l(1) = 1$).



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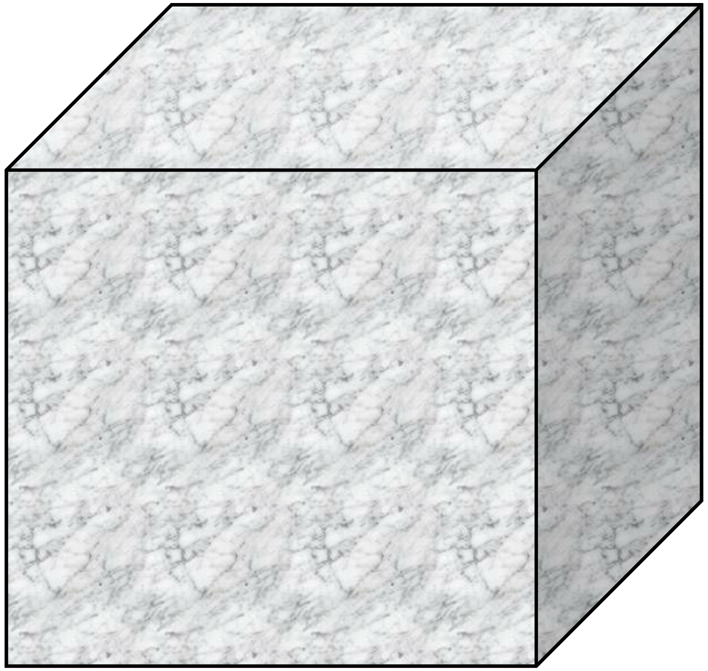
Propagator Imaging

Diffusion propagator

$$P(\boldsymbol{x}(0), \boldsymbol{x}(t), t)$$

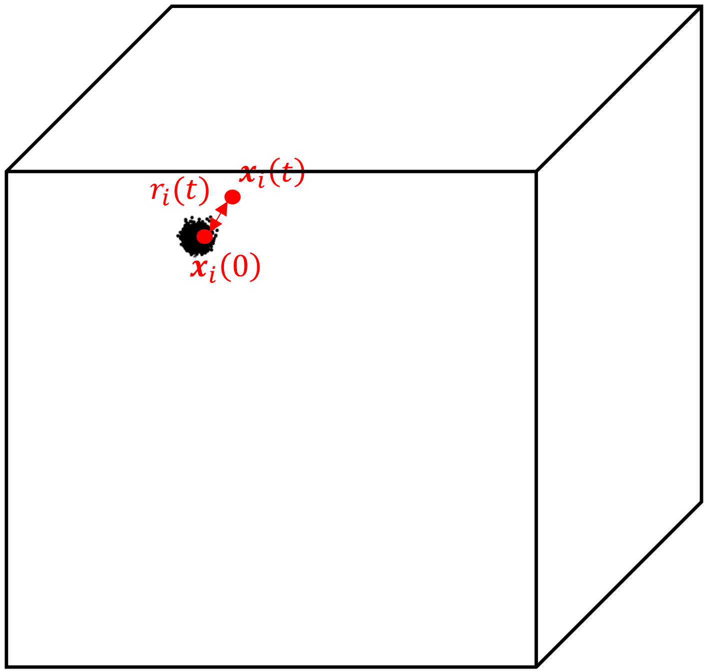


$$\boldsymbol{r}(t) = \boldsymbol{x}(t) - \boldsymbol{x}(0)$$

Propagator Imaging

Diffusion propagator

$$P(\boldsymbol{x}(0), \boldsymbol{x}(t), t)$$



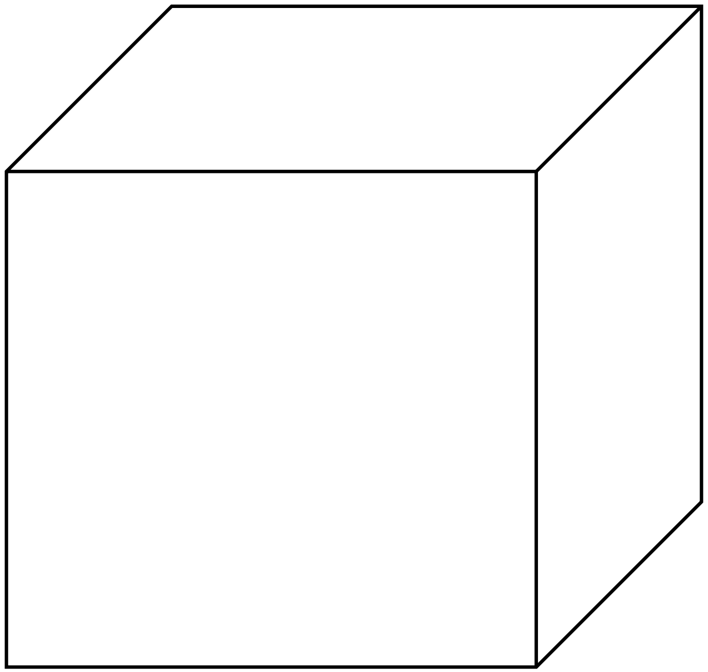
$$\boldsymbol{r}(t) = \boldsymbol{x}(t) - \boldsymbol{x}(0)$$

Propagator Imaging

Voxel-averaged diffusion propagator

Diffusion MRI signal

$$P(\boldsymbol{r}(t), t) = \langle P(\boldsymbol{x}_0, \boldsymbol{x}(t), t)\rangle_{\boldsymbol{x_0}} = \frac{1}{V}\int P(\boldsymbol{x}_0, \boldsymbol{x}(t), t)\, d\boldsymbol{x}_0$$



$$\boldsymbol{r}(t) = \boldsymbol{x}(t) - \boldsymbol{x}(0)$$

Propagator Imaging: Narrow Pulse Approximation (very small δ)

$$\boldsymbol{q} = \gamma\delta\boldsymbol{G}\ [1/\mu m]$$

Voxel-averaged diffusion propagator

$$P(\boldsymbol{r},t) = \int \frac{S(\boldsymbol{q})}{S(0)} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} d\boldsymbol{r}$$

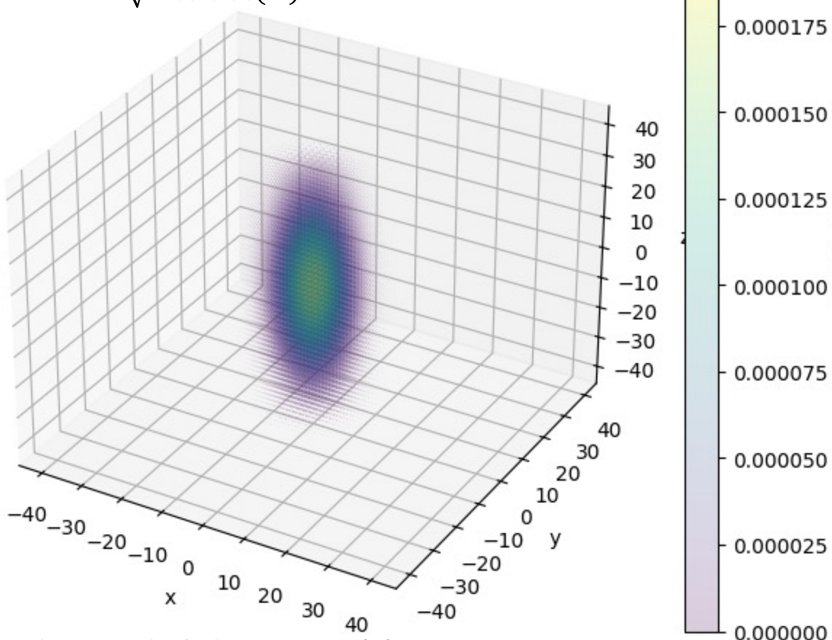
Diffusion MRI signal

$$\frac{S(q)}{S(0)} = \int P(\boldsymbol{r},t) e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} d\boldsymbol{q}$$

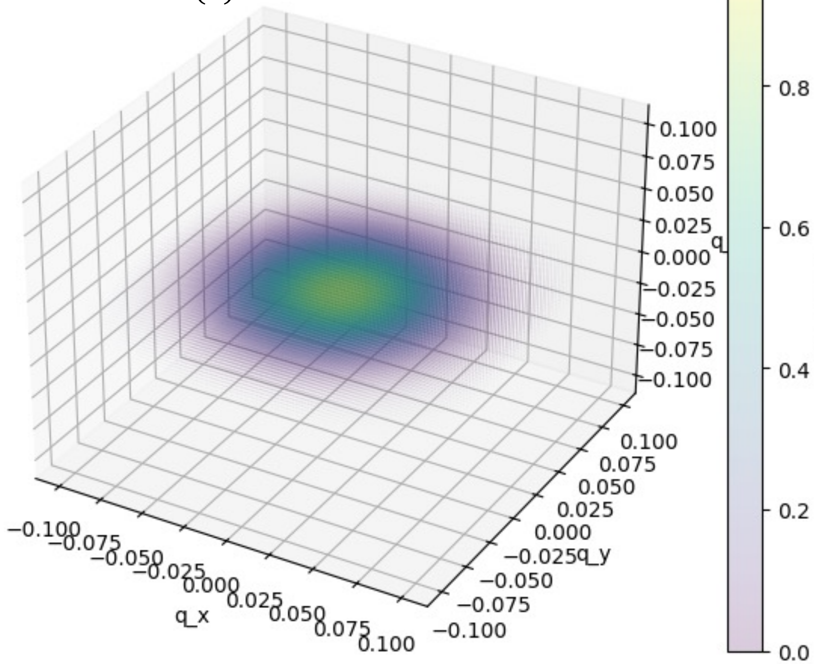
Fourier Transform →

← Inverse Fourier Transform

$$P(\boldsymbol{r},t) = \frac{1}{\sqrt{4\pi t\ \det(\boldsymbol{D})}} \exp\left(-\frac{1}{4t}\boldsymbol{r}^T\boldsymbol{D}^{-1}\boldsymbol{r}\right)$$



$$\frac{S(q)}{S(0)} = \exp(-t\boldsymbol{q}^T\boldsymbol{D}\boldsymbol{q})$$

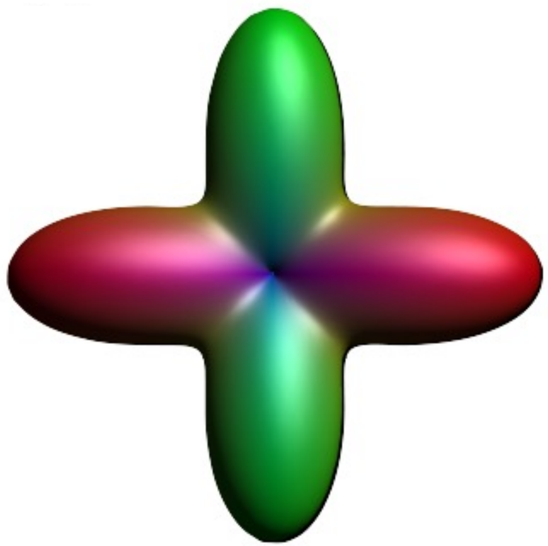


Callaghan et al. Journal of Physics E, 21(8), 820.

Diffusion ODF vs fiber ODF

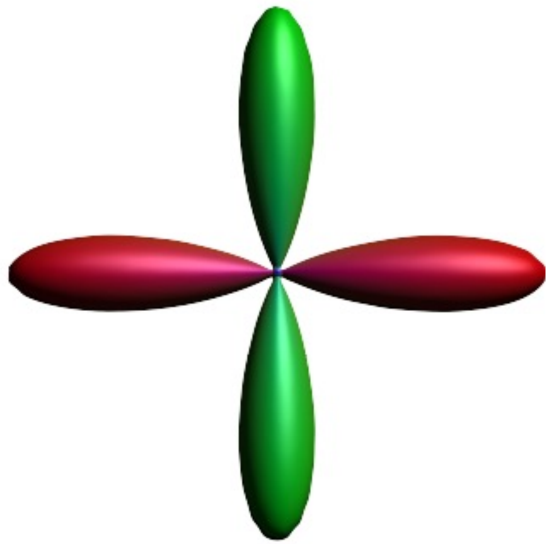
Voxel-averaged propagator

$P(\boldsymbol{r}, t)$



Diffusion ODF

$\int_0^\infty P(r\hat{\boldsymbol{n}}, t) r^2 dr$



Fiber ODF
(Deconvolution with a kernel)