Beyond the Spherical Cow

A New Approach to Modeling Physical Quantities for Objects of Arbitrary Shape

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Outline

- Introductory comments about shapes
- Applications to magnetostatics/electrostatics
  - Demagnetization factors
  - $BaTiO_3$ crystals
- Interactions between arbitrary shapes
- Gravitation
- Moment of Inertia Tensor/Quadrupole Tensor
- General Relations
- Conclusions

It’s all a matter of shape

- When asked how to increase the milk production of cows, a theoretical physicist might answer, after much head-scratching and pages of calculations, "First, you start with a spherical cow." A real cow is too complicated. Scientists often resort to assumptions that simplify a problem, making it solvable. But the downside is that the solution may not represent anything "real."
(paraphrased from http://archive.ncsa.uiuc.edu/Cyberia/NumRel/BuildingBlocks.html)

- Example: Nearly all computations in magnetism involve the assumption that everything behaves like a magnetic dipole. Even when the particle shape is not spherical, the dipole approach continues to be used. This is only appropriate if the particles are far apart!

- In this talk, we will show that shape does matter, and that actual shapes can be taken into account correctly, without assumptions.

Beyond the Spherical Cow ...

Shape dependent quantities

- demagnetization and depolarization tensors
- gravitational/electric field
- capacitance
- moment-of-inertia tensor
- solid angle
- acoustic radiation impedance
- various transport properties
- ...

Typical problems

- Typically, these quantities require 3D integrations over the volume of the object, or over the surface of the object.
- For interacting objects, the integral is often a 6D integral over both particle volumes.
- Shape usually enters through the integration boundaries, via parameterized expressions for the volume or the surface.
- So, is there a way to incorporate the shape of the object via a function, rather than via integration boundaries?

The Shape Function

- Each object has a binary nature, i.e., a randomly chosen point is either inside the body, or it is not.

- Hence, we define the shape function as:

$$D(\mathbf{r}) = \begin{cases} 1 & \text{inside} \\ 0 & \text{outside} \end{cases}$$

- Note that this function is also known as the indicator function or the characteristic function.

- In a technical sense, this is not a real function, since its derivatives do not exist in the traditional calculus context. The shape function is therefore a generalized function (distribution), i.e., a 3-D hat function.

The Shape Function

- The shape function can be used to extend the integration volume from the volume of an object to all of space:

$$\iiint_V f(\mathbf{r})d\mathbf{r} = \iiint_{\text{all space}} D(\mathbf{r})f(\mathbf{r})d\mathbf{r}$$

- The advantages of using shape functions become more apparent in Fourier space. The Fourier transform of the shape function is known as the shape amplitude:

$$D(\mathbf{k}) = \iiint_{\text{all space}} D(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r} = \iiint_V e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}$$

- This is the only place where the actual shape information is used as integration boundaries.

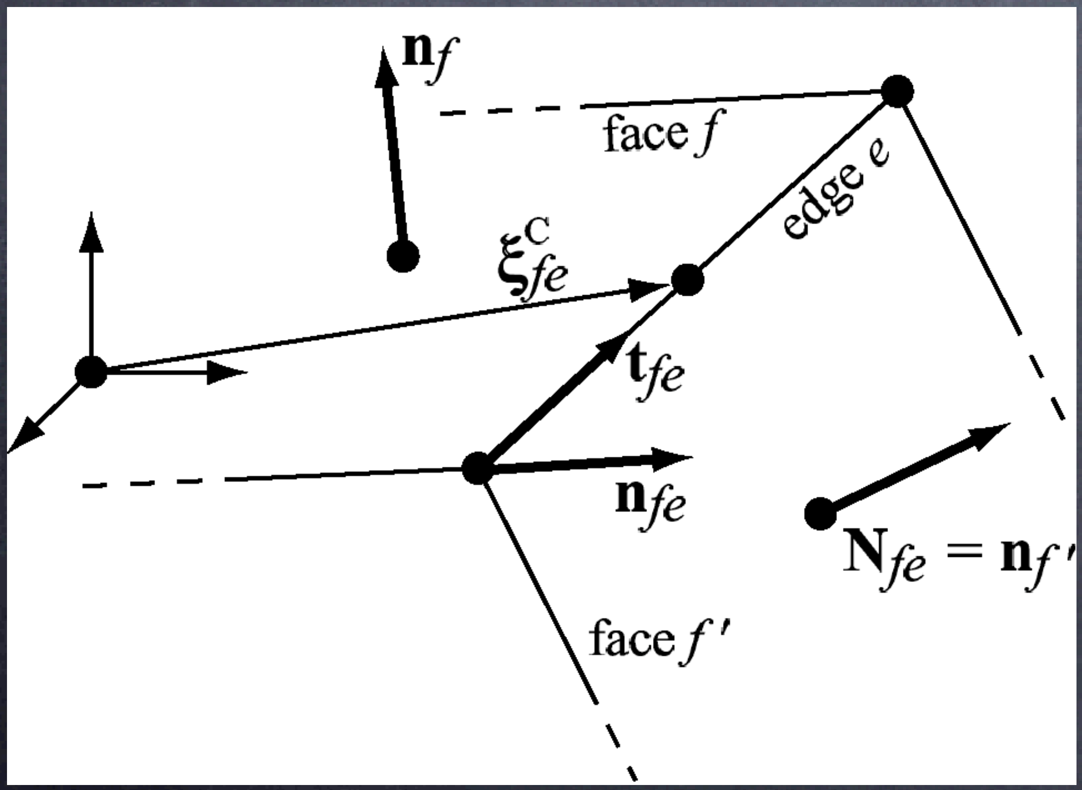
Example Shape Amplitudes

$$\text{Sphere:} \qquad D(\mathbf{k}) = \frac{4\pi R^2}{k} j_1(kR)$$

$$\text{Cylinder:} \qquad D(\mathbf{k}) = \frac{4\pi R}{k_\perp k_z} \sin(dk_z) J_1(k_\perp R)$$

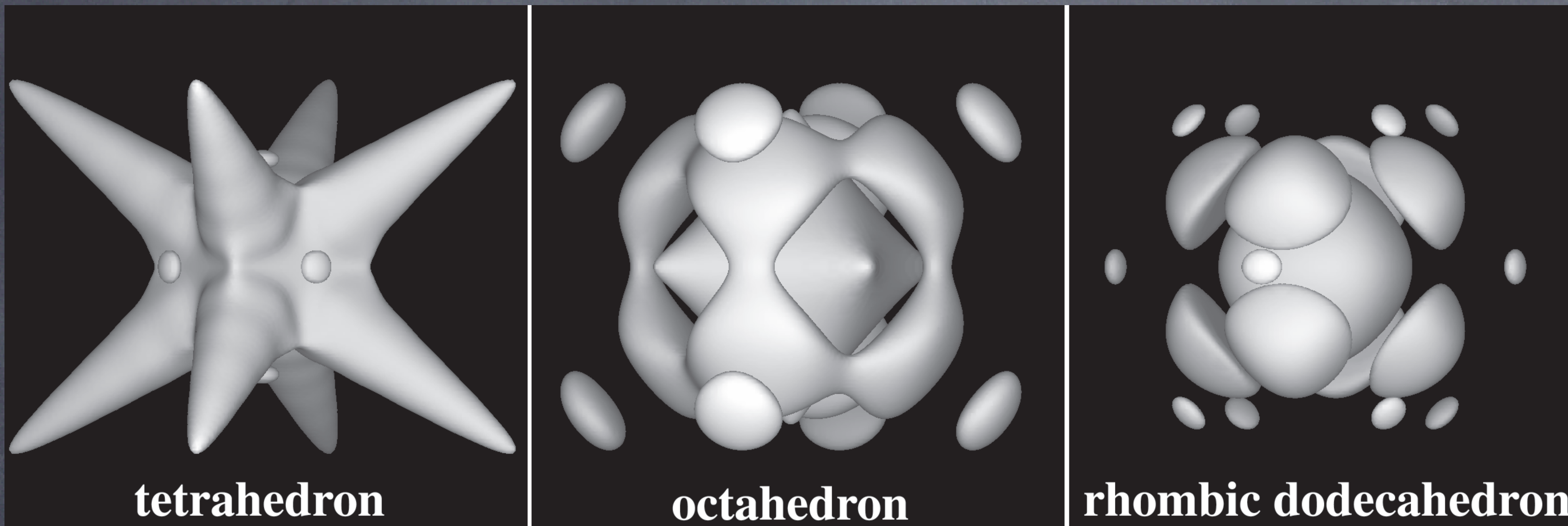
$$\text{Facetted Objects:} \qquad D(\mathbf{k}) = -\frac{1}{k^2} \sum_{f=1}^{F} \frac{\mathbf{k}\cdot\mathbf{n}_f}{k^2 - (\mathbf{k}\cdot\mathbf{n}_f)^2}$$

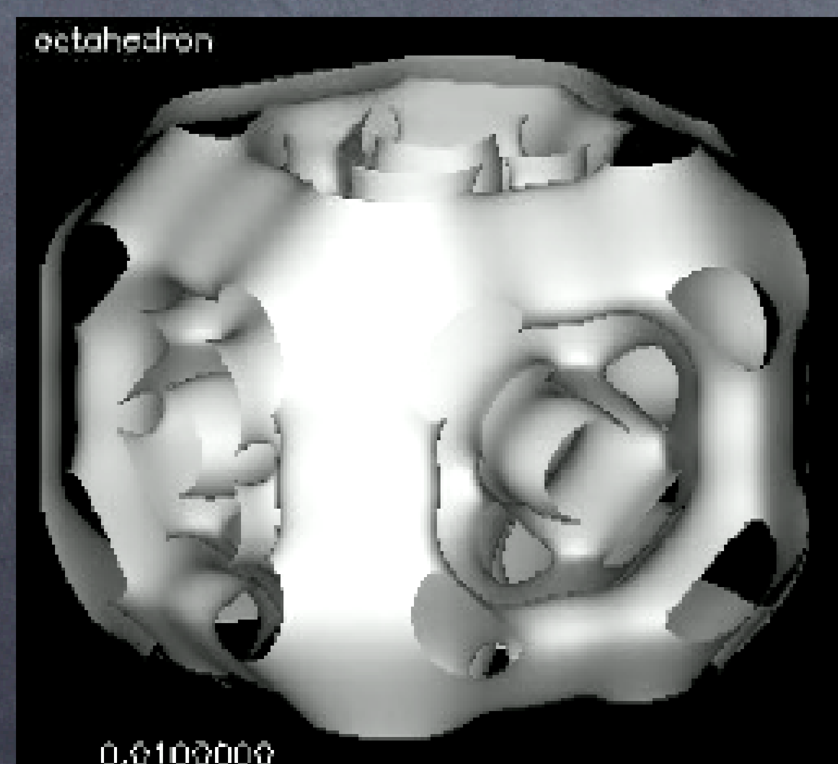
$$\times \sum_{e=1}^{E_f} L_{fe}\mathbf{k}\cdot\mathbf{n}_{fe}\mathrm{sinc}(\frac{L_{fe}}{2}\mathbf{k}\cdot\mathbf{t}_{fe}) e^{-\mathrm{i}\mathbf{k}\cdot\boldsymbol{\xi}_{fe}^{C}}$$



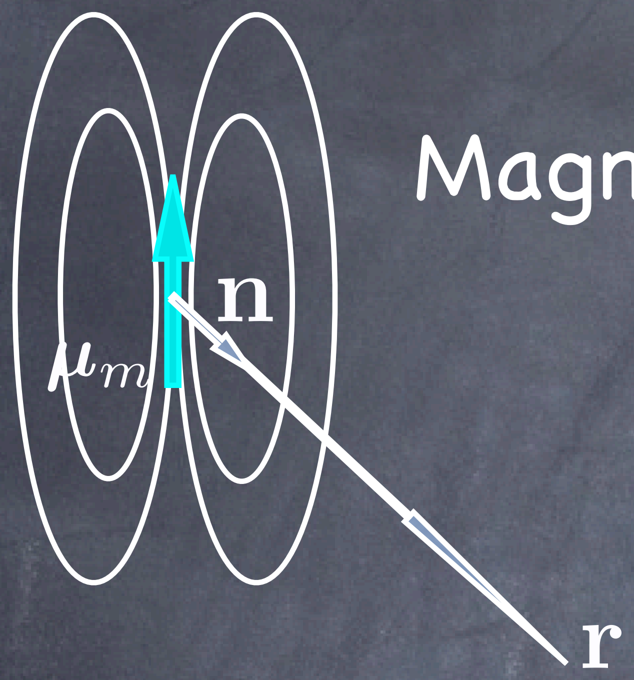
Shape amplitude is a real function for objects with a center of symmetry.

Example Shape Amplitudes





Magnetic Field and Energy of a dipole



Magnetic Induction: $\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi}\left[\frac{3\mathbf{n}(\mathbf{n}\cdot\boldsymbol{\mu}) - \boldsymbol{\mu}}{|\mathbf{r}|^3}\right]$

$= \mu_0 \mathbf{H}(\mathbf{r})$

$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$

Permeability of vacuum Magnetic Field

Magnetic Vector Potential: $\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi}\frac{\boldsymbol{\mu}\times\mathbf{r}}{|\mathbf{r}|^3}$

Magnetostatic Energy:

$$E(\mathbf{r}) = -\boldsymbol{\mu}\cdot\mathbf{B} = \frac{\mu_0}{4\pi}\left[\frac{\boldsymbol{\mu}_1\cdot\boldsymbol{\mu}_2}{|\mathbf{r}|^3} - 3\frac{(\mathbf{r}\cdot\boldsymbol{\mu}_1)(\mathbf{r}\cdot\boldsymbol{\mu}_2)}{|\mathbf{r}|^5}\right]$$

Tensors in Magnetism

$$E(\mathbf{r}) = \frac{\mu_0}{4\pi}\left[\frac{\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2}{r^3} - 3\frac{(\mathbf{r}\cdot\boldsymbol{\mu}_1)(\mathbf{r}\cdot\boldsymbol{\mu}_2)}{r^5}\right] = \mu_0 \boldsymbol{\mu}_1 : \boxed{\mathcal{D}(r)} : \boldsymbol{\mu}_2$$

Dipolar Tensor

$$\mathcal{D}^{\alpha\beta}(r) = \frac{1}{4\pi r^5}\left(r^2\delta^{\alpha\beta} - 3r^\alpha r^\beta\right)$$

Demagnetization tensor N describes the demagnetization field due to a given magnetization M.

$$\mathbf{B} = \mu_0(\mathbf{M} + \mathbf{H}) \quad \rightarrow \quad B_i = \mu_0(M_i - N_{ij}M_j)$$

Is there a relation between these two tensors and the shape amplitude ?

Dipolar tensor in Fourier Space

$$\mathcal{D}^{\alpha\beta}(r) = \frac{1}{4\pi r^5}\left(r^2\delta^{\alpha\beta} - 3r^\alpha r^\beta\right)$$

It is not too difficult to show that the dipolar tensor is the inverse Fourier transform of

$$\hat{k}^\alpha \hat{k}^\beta = \frac{k^\alpha k^\beta}{k^2}$$

direction cosines of frequency vector

$$\mathcal{D}^{\alpha\beta}(\mathbf{r}) = \frac{1}{8\pi^3}\iiint \mathrm{d}\mathbf{k}\, \frac{k^\alpha k^\beta}{k^2} e^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}}$$

Hint: use cylindrical coordinates to prove this relation; spherical coordinates result in diverging integrals...

The Fourier Space Formalism

- Consider an object with a given magnetization state $\mathbf{M}(\mathbf{r})$

Basic Equation: $$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi}\int \mathbf{M}(\mathbf{r}') \times \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\mathrm{d}\mathbf{r}'$$ "convolution"

Vector potential: $$\mathbf{A}(\mathbf{k}) = -\mathrm{i}\mu_0 \frac{\mathbf{M}(\mathbf{k}) \times \mathbf{k}}{k^2}$$ vector cross product

Fourier Transform of $\mathbf{M}(\mathbf{r})$: $$\mathbf{M}(\mathbf{k}) = \int \mathbf{M}(\mathbf{r}) e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$ Includes shape information

Magnetic Induction: $$\mathbf{B}(\mathbf{k}) = -\mathrm{i}\mathbf{k} \times \mathbf{A}(\mathbf{k})$$ Nabla operator in Fourier Space

$$\mathbf{B}(\mathbf{k}) = -\frac{\mu_0}{k^2}\mathbf{k} \times \mathbf{M}(\mathbf{k}) \times \mathbf{k} = \mu_0\left[\mathbf{M}(\mathbf{k}) - \mathbf{k}\frac{\mathbf{M}(\mathbf{k})\cdot\mathbf{k}}{k^2}\right] = \mu_0\left[\mathbf{M}(\mathbf{k}) + \mathbf{H}(\mathbf{k})\right]$$

Demagnetization Field

Analytical Expressions

For a uniformly magnetized object: $\boxed{\mathbf{M}(\mathbf{k}) = M_0 \hat{\mathbf{m}} D(\mathbf{k})}$

$$\mathbf{B} = \mu_0(\mathbf{M} + \mathbf{H}) \quad \rightarrow \quad B^\alpha = \mu_0(M^\alpha - N^{\alpha\beta} M^\beta)$$

Demagnetization Field $$\mathbf{H}(\mathbf{r}) = -\frac{M_0}{8\pi^3} \int \mathrm{d}^3\mathbf{k} \frac{D(\mathbf{k})}{k^2} \mathbf{k}(\hat{\mathbf{m}} \cdot \mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

Demagnetization Tensor (point function) $$N^{\alpha\beta}(\mathbf{r}) = \frac{1}{8\pi^3} \int \mathrm{d}^3\mathbf{k} \frac{k^\alpha k^\beta}{k^2} D(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

Demagnetization Tensor (ballistic) $$\langle N \rangle^{\alpha\beta}(\mathbf{r}) = \frac{1}{8\pi^3 V} \int \mathrm{d}^3\mathbf{k} \frac{k^\alpha k^\beta}{k^2} |D(\mathbf{k})|^2$$

Demagnetization Energy $$E = \frac{\mu_0 M_0^2}{16\pi^3} \int \mathrm{d}^3\mathbf{k} \frac{|D(\mathbf{k})|^2}{k^2} (\hat{\mathbf{m}} \cdot \mathbf{k})^2$$

Demagnetization Tensor

$$N^{\alpha\beta}(\mathbf{r}) = \frac{1}{8\pi^3}\int \mathrm{d}^3\mathbf{k}\,\frac{k^\alpha k^\beta}{k^2} D(\mathbf{k}) e^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}}$$

$$= \mathcal{F}^{-1}\left[\mathcal{F}[\mathcal{D}^{\alpha\beta}(\mathbf{r})]\,\mathcal{F}[D(\mathbf{r})]\right]$$

$$= D^{\alpha\beta}(\mathbf{r}) \otimes D(\mathbf{r})$$

- So, the demagnetization tensor is equal to the convolution of the dipolar tensor with the shape function, which is consistent with our intuitive understanding: all the possible magnetic fields are copied to each location in the object.
- The actual demag field is obtained by contracting w.r.t. to the magnetic moment direction. $H^\alpha = -N^{\alpha\beta}(\mathbf{r})M^\beta$

Properties of Demag Tensor

- Trace:

$$\mathrm{Tr}[N^{\alpha\beta}] = \frac{1}{8\pi^3}\int \mathrm{d}^3\mathbf{k}\frac{D(\mathbf{k})}{k^2}\sum_{\alpha=1}^{3} k^\alpha k^\alpha e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \frac{1}{8\pi^3}\int \mathrm{d}^3\mathbf{k} D(\mathbf{k}) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = D(\mathbf{r})$$

- Symmetry: Being a second rank tensor, N inherits the symmetry of the corresponding shape; in particular, if the shape has a rotational axis of order greater than 2, then the tensor is isotropic in the plane normal to that axis (Neumann principle)

- Computability (numerical): Numerical computation is relatively straightforward, thanks to FFT algorithms, BUT ...

Analytical vs. Numerical

- In an analytical computation, the shape amplitude has infinite support.
- In a numerical FFT-based computation, the support is finite (finite frequency range).
- An inverse numerical FFT of an analytical shape amplitude will give rise to Gibbs oscillations...
- This can be avoided by using a filter function:

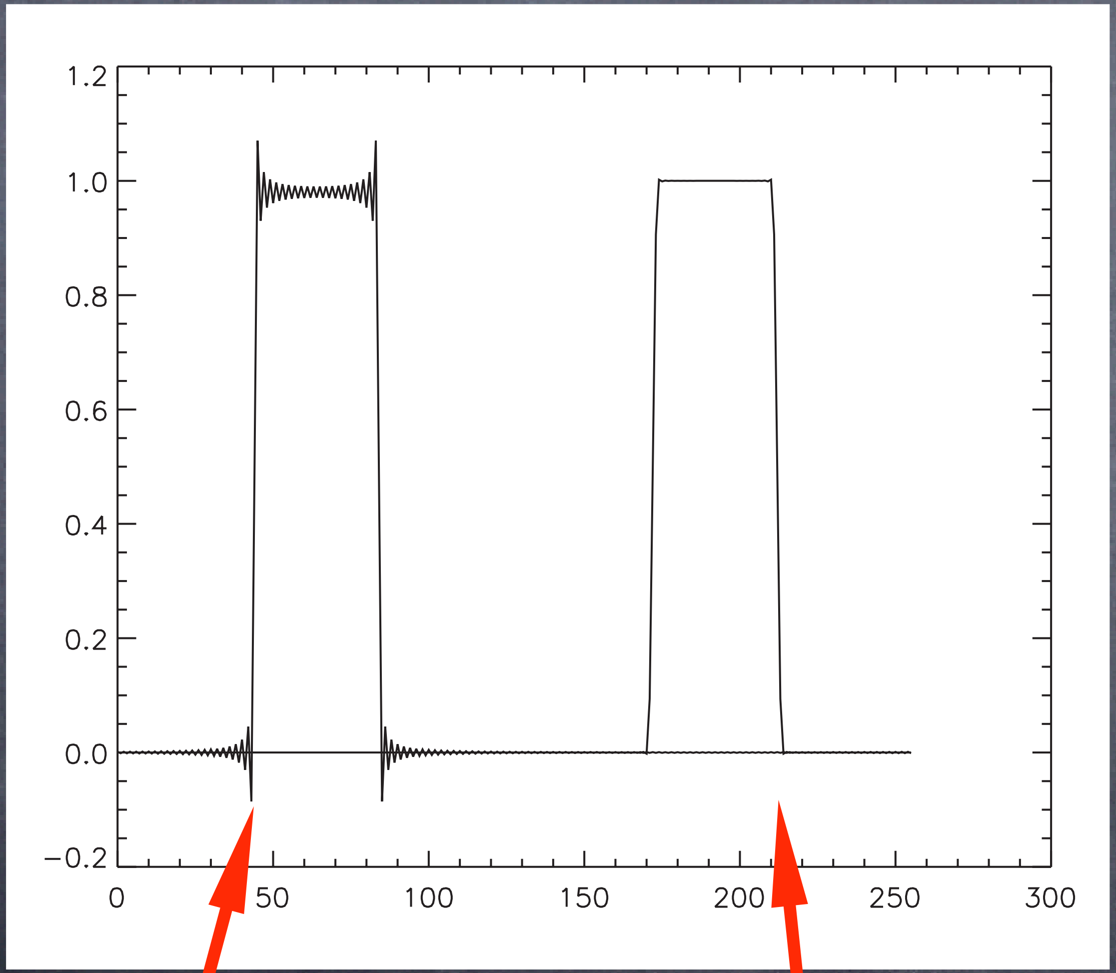
$$g(k) = \frac{3}{k^2}\left[\mathrm{sinc}^2(k) - \mathrm{sinc}(2k)\right]$$

$$g(r) = \begin{cases} (2|r|+1)(|r|-1)^2 & |r| < 1 \\ 0 & \text{elsewhere} \end{cases}$$

Example

Rectangular prism with dimensions $(2L_x, 2L_y, 2L_z)$

$$D(\mathbf{k}) = V \frac{\sin L_x k_x}{L_x k_x} \frac{\sin L_y k_y}{L_y k_y} \frac{\sin L_z k_z}{L_z k_z}$$



Deviation from true step function extends to only 1 pixel on either side of boundary.

Regular FFT

Filtered FFT

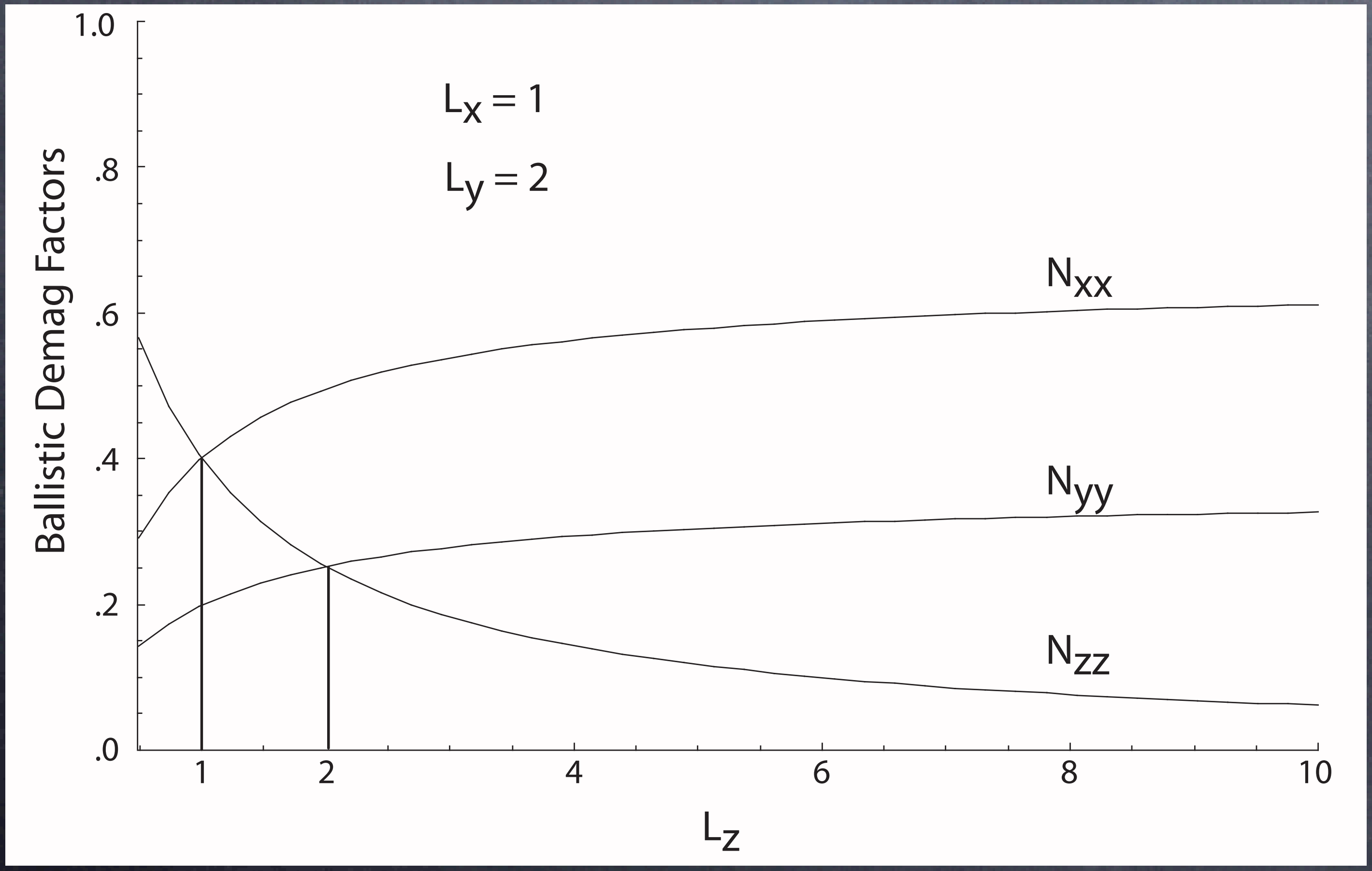
Example (continued)

- For numerical work, the demag tensor is given by:

$$N^{\alpha\beta}(\mathbf{r}) = \mathrm{FFT}^{-1}\left[\frac{k^\alpha k^\beta}{k^2} D(\mathbf{k}) g(|\mathbf{k}|)\right]$$

But: $$\langle N^{\alpha\beta}\rangle = \frac{1}{8\pi^3 V}\int \mathrm{d}\mathbf{k}\,\frac{k^\alpha k^\beta}{k^2}|D(\mathbf{k})|^2$$ (Ballistic)

No filter function needed!



Graphical Representation

A symmetric 3x3 matrix has 3 real eigenvalues and associated eigenvectors.

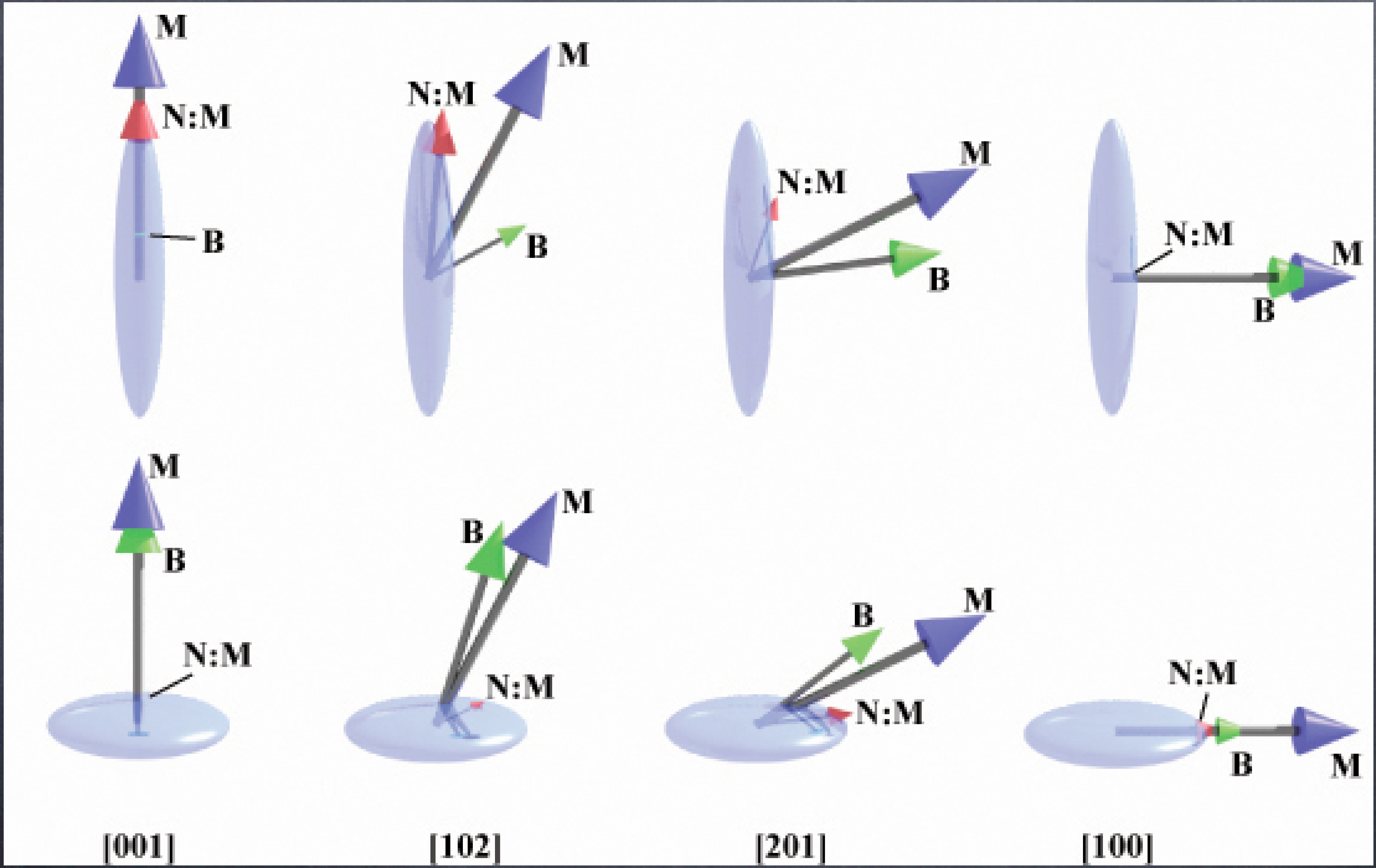
$$N_{ij} \quad \rightarrow \quad \tilde{\mathcal{O}} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \mathcal{O}$$

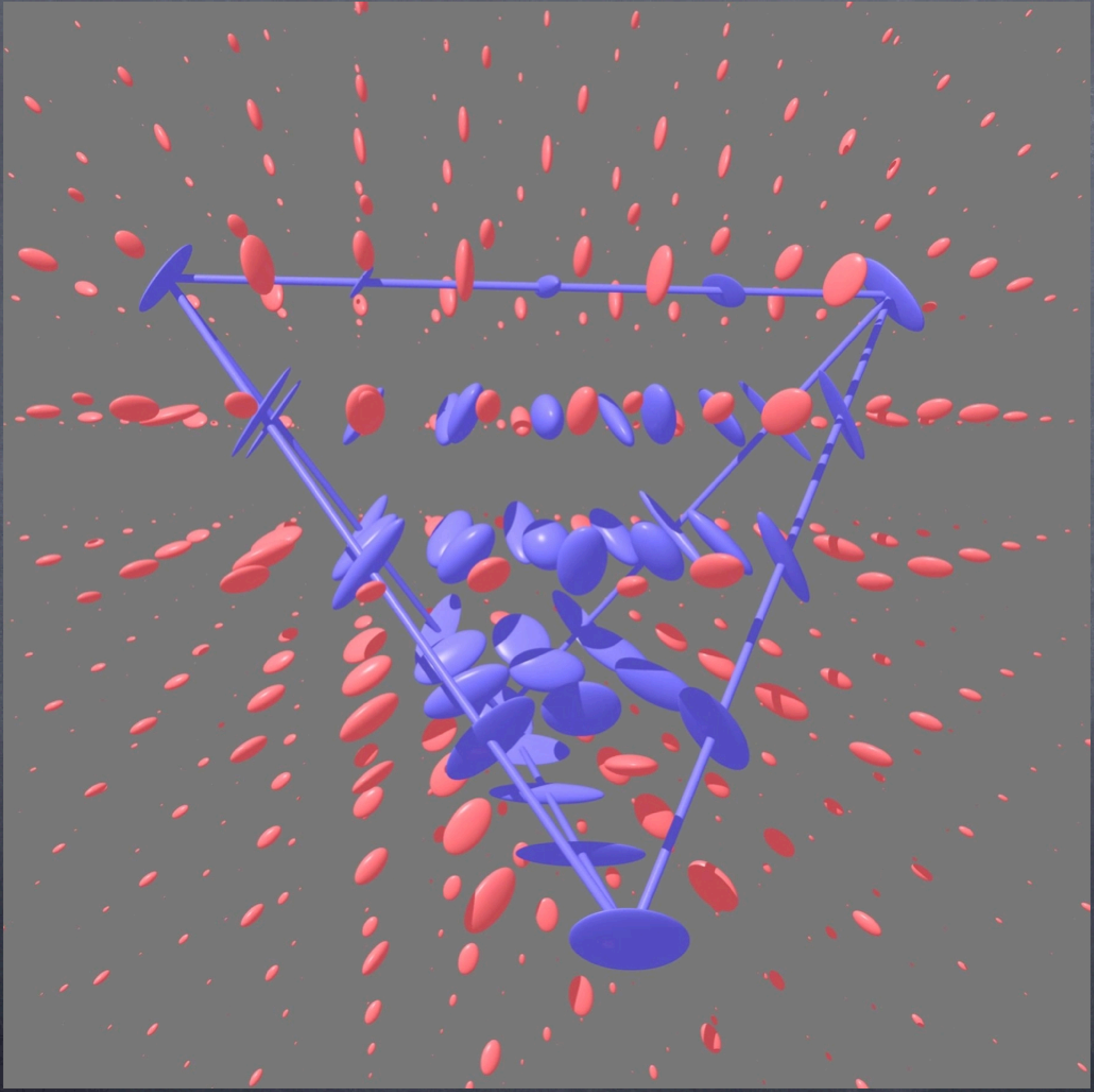
Has eigenvectors as columns

Inside shape: $\lambda_{1,2,3} > 0$ $\Rightarrow$ Ellipsoid

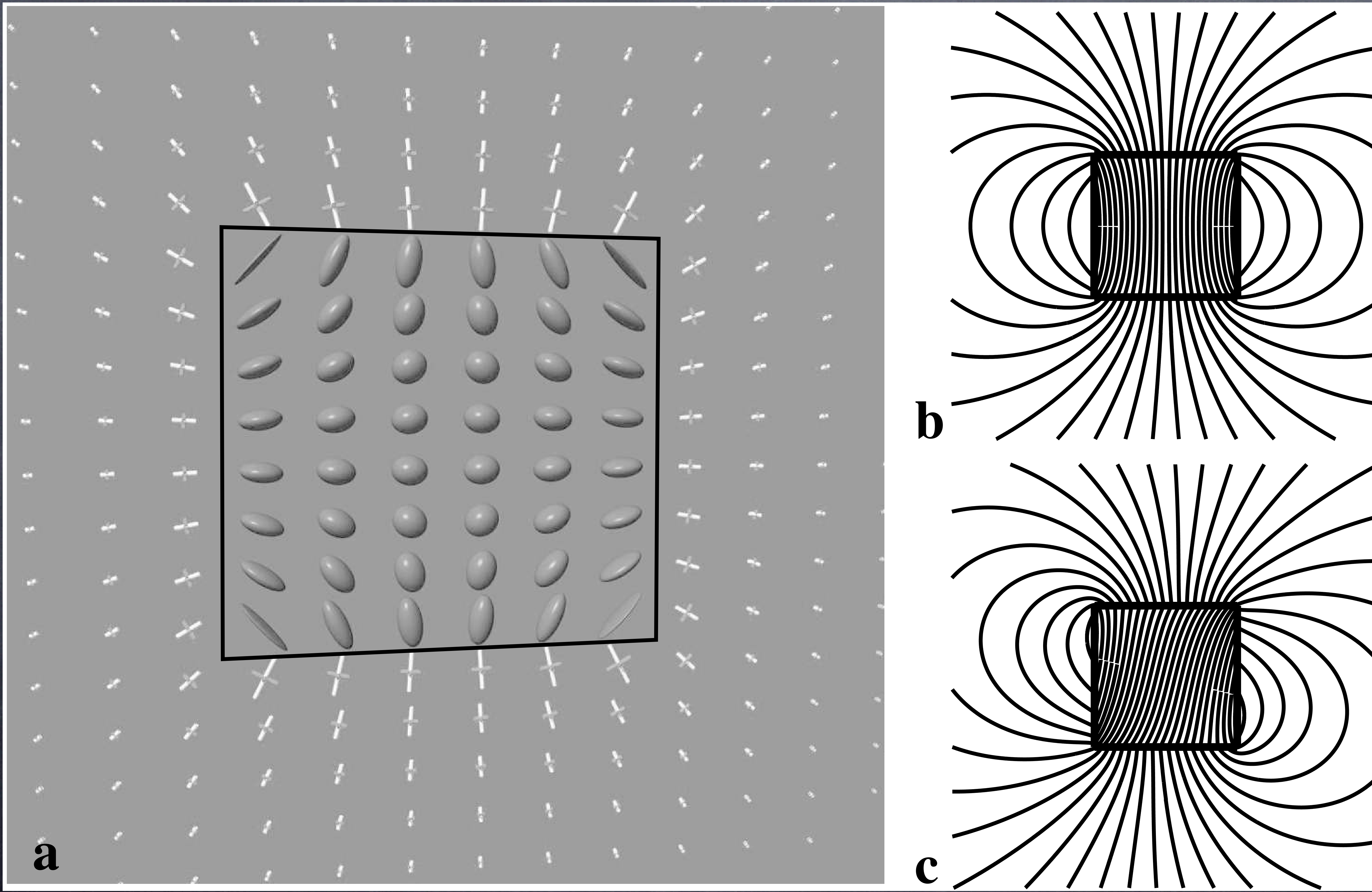
Outside shape: $\lambda_{1,2} > 0; \lambda_3 < 0$ $\Rightarrow$ Single Sheet Hyperboloid

Example: Demagnetization Tensor

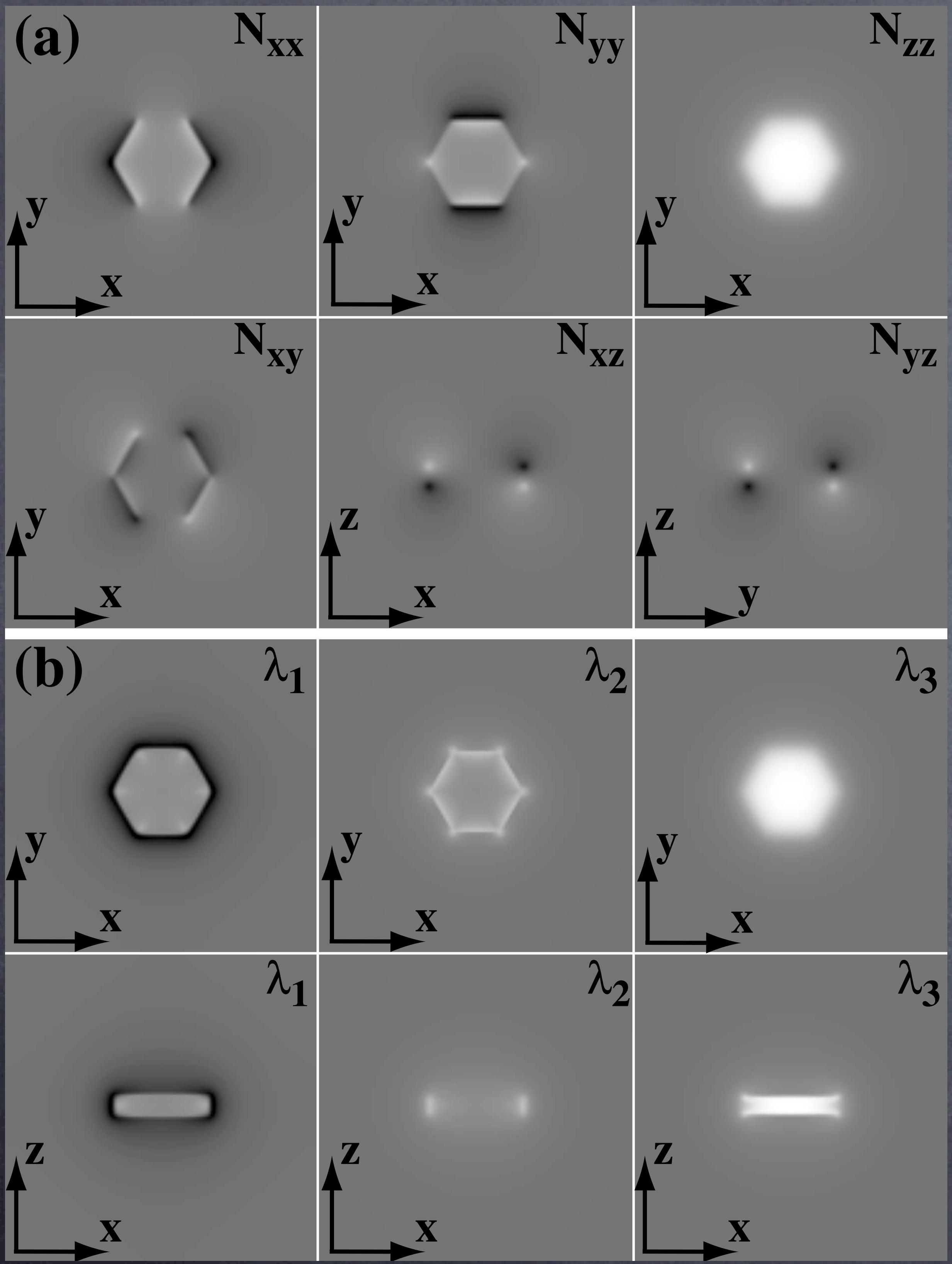


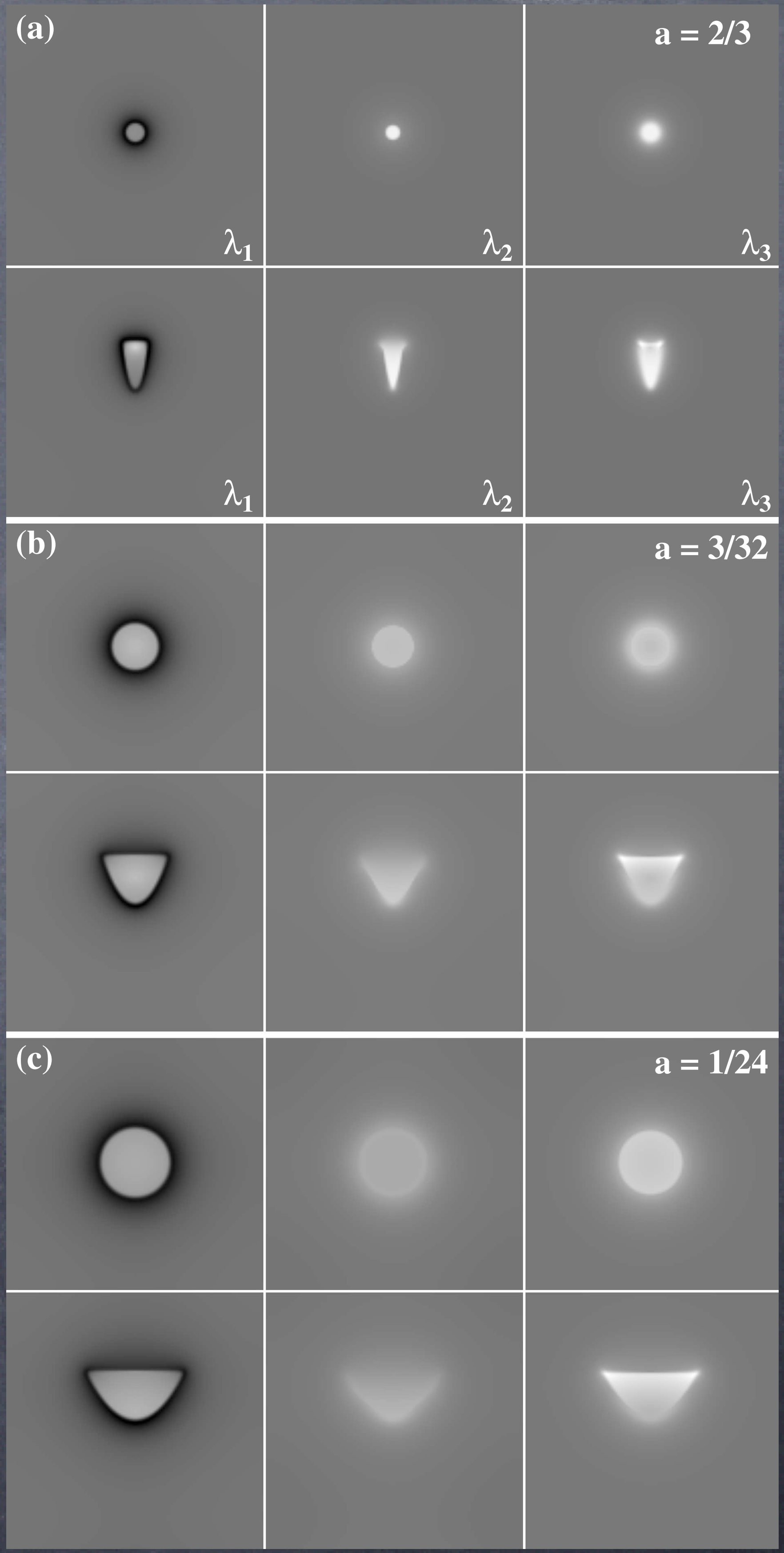


More examples



More examples





Application to Electrostatics

- A uniformly polarized particle has a potential:

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int \mathrm{d}\mathbf{r}'\,\mathbf{P}(\mathbf{r}')\cdot\frac{(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3}$$

- and a resulting field (in Fourier space):

$$\mathbf{E}(\mathbf{k}) = -\mathrm{i}\mathbf{k}V(\mathbf{k}) = -\frac{P_0}{\epsilon_0}D(\mathbf{k})\frac{\hat{\mathbf{p}}\cdot\mathbf{k}}{k^2}\mathbf{k}$$

- The electric displacement is then given by:

$$\mathbf{D}(\mathbf{r}) = \mathbf{P} - \frac{P_0}{8\pi^3}\int \mathrm{d}^3\mathbf{k}\,D(\mathbf{k})\frac{\hat{\mathbf{p}}\cdot\mathbf{k}}{k^2}\mathbf{k}e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$

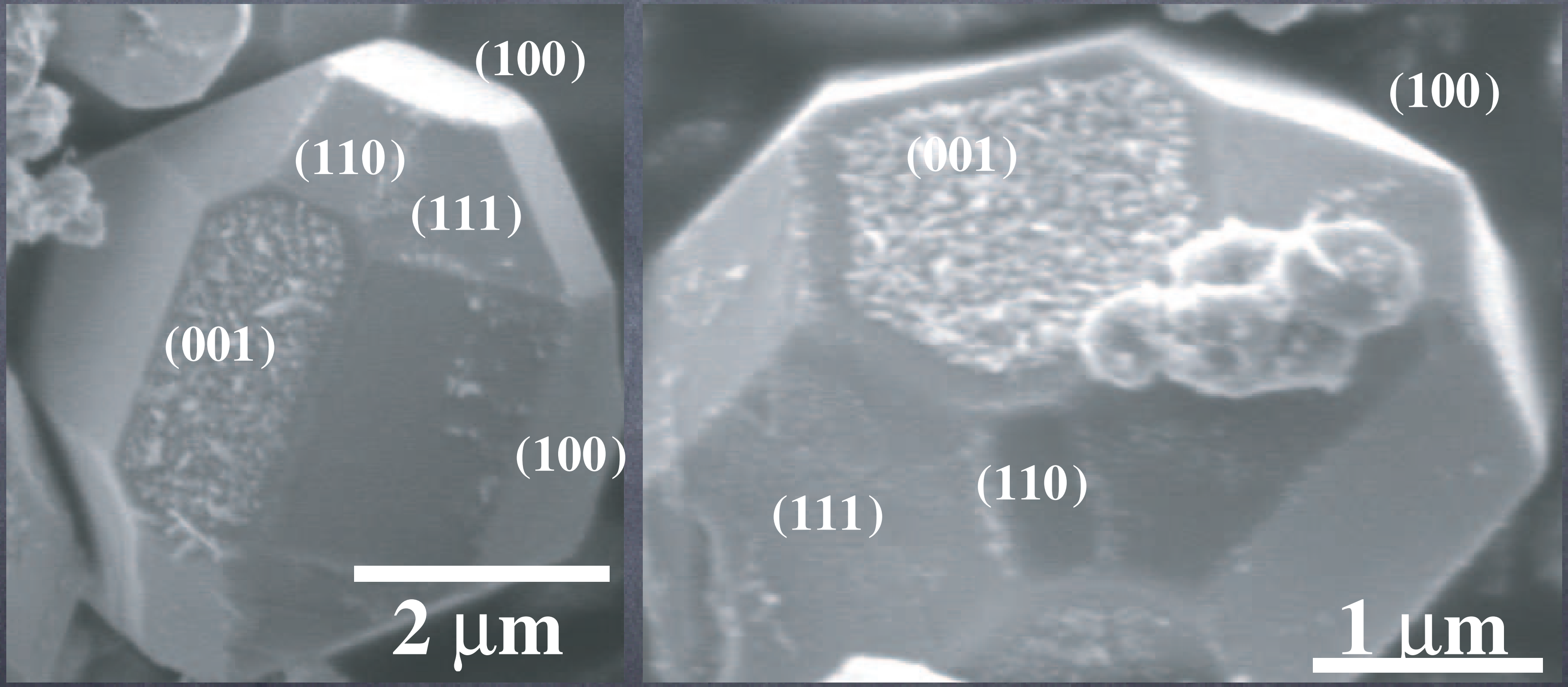
- which results in: $D_i = P_i + \epsilon_0 E_i = P_i - N_{ij}P_j$

SAME TENSOR !!!

Depolarization Energetics

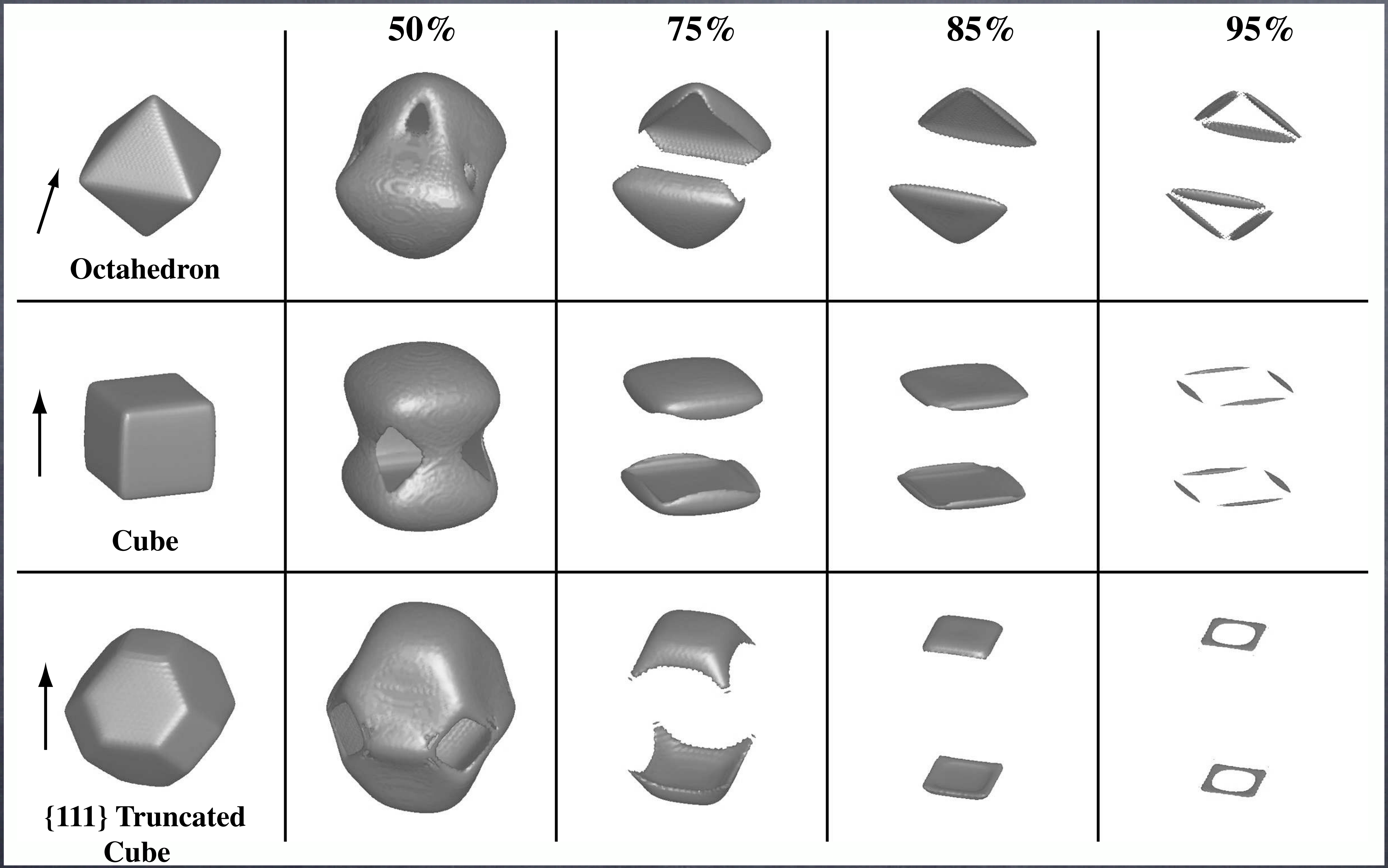
- The self-energy of a uniformly polarized particle:

$$E_e = -\frac{1}{2}\int_V \mathbf{P}\cdot\mathbf{E}\,\mathrm{d}^3\mathbf{r} = \frac{P_0^2}{16\pi^3\epsilon_0}\int \mathrm{d}^3\mathbf{k}\,\frac{|D(\mathbf{k})|^2}{k^2}(\hat{\mathbf{p}}\cdot\mathbf{k})^2$$



SEM images of the faceted $BaTiO_3$ crystals after reaction with $AgNO_3$.

The white contrast specks indicate silver metal deposits. (images G. Rohrer)


50%
75%
85%
95%
Octahedron
Cube
{111} Truncated
Cube

How about interacting shapes?

- Magnetostatic energy is generally defined as:

$$E_m = -\frac{\mu_0}{2}\int_V \mathbf{H}(\mathbf{r})\cdot\mathbf{M}(\mathbf{r})\,\mathrm{d}^3\mathbf{r}$$

- Converting to Fourier space for uniformly magnetized particles we find:

$$E_m = \frac{\mu_0}{16\pi^3}\int \frac{\mathrm{d}^3\mathbf{k}}{k^2}|\mathbf{M}(\mathbf{k})\cdot\mathbf{k}|^2 = \frac{\bar{K}_d}{4\pi^3}\Re\left[\int \mathrm{d}^3\mathbf{k}\, D_1(\mathbf{k})D_2^*(\mathbf{k})(\hat{\mathbf{m}}_1\cdot\hat{\mathbf{k}})(\hat{\mathbf{m}}_2\cdot\hat{\mathbf{k}})e^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}}.\right]$$

$$\bar{K}_d \equiv \frac{1}{2}\mu_0 M_1 M_2$$

- $\boldsymbol{\rho}\equiv\mathbf{R}_1-\mathbf{R}_2$ is the relative position of the particles
- This expression can be rewritten as:

$$E_m = 2\bar{K}_d m_1^\alpha m_2^\beta \Re\left\{\mathcal{F}_{\boldsymbol{\rho}}^{-1}\left[D_1(\mathbf{k})D_2^*(\mathbf{k})\hat{k}^\alpha\hat{k}^\beta\right]\right\}.$$

Interacting shapes

- Using the convolution theorem, we find:

$$E_m(\boldsymbol{\rho}; \hat{\mathbf{m}}_1, \hat{\mathbf{m}}_2) = 2\bar{K}_d\, m_1^\alpha \left[\mathcal{C}(\boldsymbol{\rho}) \otimes \mathcal{D}^{\alpha\beta}(\boldsymbol{\rho})\right] m_2^\beta .$$

- In this expression, we have introduced a new quantity:

$$\mathcal{C}(\mathbf{r}) \equiv D_1(\mathbf{r}) \otimes D_2(-\mathbf{r})$$

- This is the cross-correlation of the shape functions.
- Finally, we rewrite the energy in terms of a new tensor field:

$$E_m(\boldsymbol{\rho}; \hat{\mathbf{m}}_1, \hat{\mathbf{m}}_2) = 2\bar{K}_d V_1 V_2\, m_1^\alpha \mathcal{N}^{\alpha\beta}(\boldsymbol{\rho}) m_2^\beta = \mu_0\, \boldsymbol{\mu}_1 : \mathcal{N}(\boldsymbol{\rho}) : \boldsymbol{\mu}_2$$

$$\mathcal{N}^{\alpha\beta}(\boldsymbol{\rho}) = \frac{1}{V_1 V_2} \mathcal{C}(\boldsymbol{\rho}) \otimes \mathcal{D}^{\alpha\beta}(\boldsymbol{\rho})$$

The Magnetometric Tensor Field

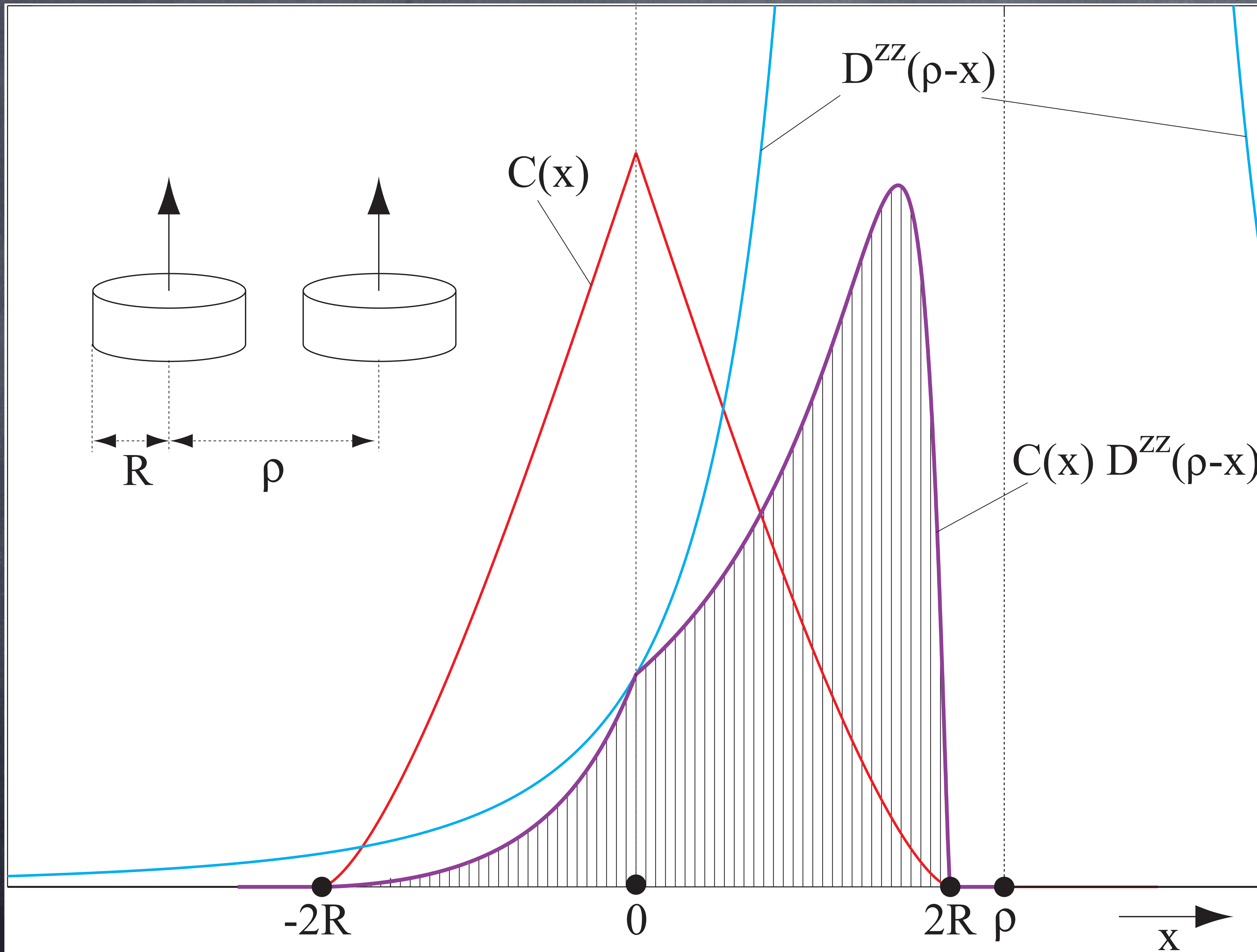
$$E_m(\boldsymbol{\rho}; \hat{\mathrm{m}}_1, \hat{\mathrm{m}}_2) = \mu_0\, \boldsymbol{\mu}_1 \mathbf{:} \mathcal{N}(\boldsymbol{\rho}) \mathbf{:} \boldsymbol{\mu}_2$$

- This relation is similar to that for pure dipoles:

$$E_m(\boldsymbol{\rho}; \hat{\mathrm{m}}_1, \hat{\mathrm{m}}_2) = \mu_0\, \boldsymbol{\mu}_1 \mathbf{:} \mathcal{D}(\boldsymbol{\rho}) \mathbf{:} \boldsymbol{\mu}_2$$

- The magnetometric tensor field contains all the shape-dependent interactions, so that the particles can be represented by their total moments.

Geometrical Interpretation



Example Computations

- Rectangular prism (2a,2b,2c) auto-correlation function:

$$\mathcal{C}(\rho_x, \rho_y, \rho_z) = (2a - |\rho_x|)(2b - |\rho_y|)(2c - |\rho_z|)$$

- Magnetometric tensor element:

$$\mathcal{N}^{zz}(\bar{\rho}) = \frac{1}{32\pi a^3} \int_{-1}^{+1} \mathrm{d}\bar{x} \int_{-1}^{+1} \mathrm{d}\bar{y} \int_{-1}^{+1} \mathrm{d}\bar{z}\, (1-|\bar{x}|)(1-|\bar{y}|)(1-|\bar{z}|)\, \frac{(\bar{\rho}_x - \bar{x})^2 + (\bar{\rho}_y - \bar{y})^2 - 2\bar{\rho}_z - \bar{z})^2}{[(\bar{\rho}_x - \bar{x})^2 + (\bar{\rho}_y - \bar{y})^2 + (\bar{\rho}_z - \bar{z})^2]^{\frac{5}{2}}}$$

$$= \frac{1}{32\pi a^3} [4H(\bar{\rho}_x, \bar{\rho}_y, \bar{\rho}_z) + H(\bar{\rho}_x, -1 + \bar{\rho}_y, -1 + \bar{\rho}_z) - 2H(\bar{\rho}_x, \bar{\rho}_y, -1 + \bar{\rho}_z) +$$

$$H(\bar{\rho}_x, 1+\bar{\rho}_y, -1+\bar{\rho}_z) + H(\bar{\rho}_x, -1+\bar{\rho}_y, 1+\bar{\rho}_z) - 2H(\bar{\rho}_x, \bar{\rho}_y, 1+\bar{\rho}_z) + H(\bar{\rho}_x, 1+\bar{\rho}_y, 1+\bar{\rho}_z)$$

$$- 2H(\bar{\rho}_x, -1 + \bar{\rho}_y, \bar{\rho}_z) - 2H(\bar{\rho}_x, 1 + \bar{\rho}_y, \bar{\rho}_z)]$$

$$H(x, y, z) \equiv K(1 + x, y, z) - 2K(x, y, z) + K(-1 + x, y, z)$$

$$K(x, y, z) \equiv \frac{r}{6}(r^2 - 3z^2) + xyz \arctan\left(\frac{xy}{zr}\right) - xy^2 \ln(x + r) +$$

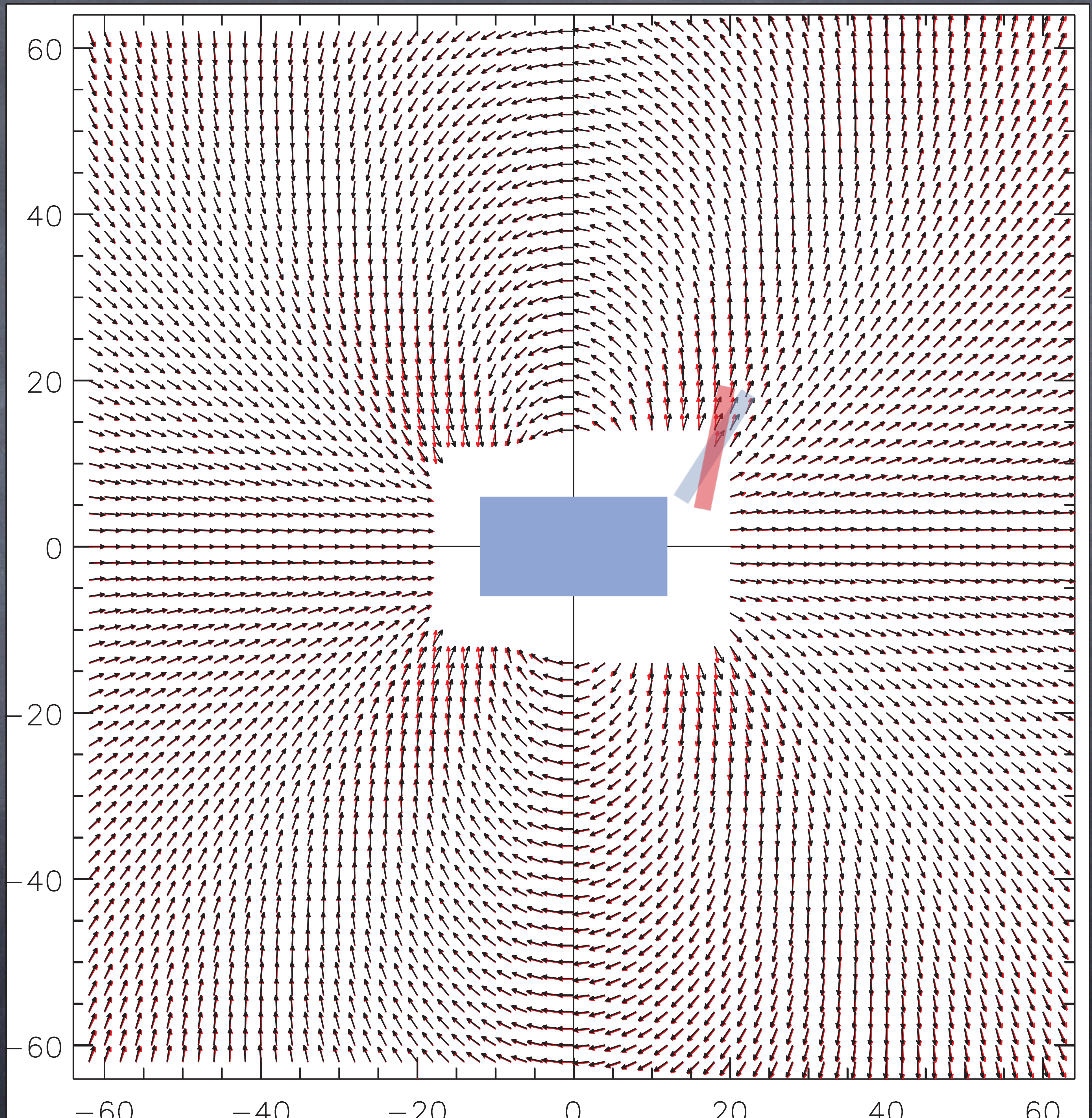
$$\frac{x}{2}(y^2 + z^2)\mathrm{arcsinh}\left(\frac{x}{\sqrt{y^2 + z^2}}\right) + \frac{y}{2}(z^2 - x^2)\mathrm{arcsinh}\left(\frac{y}{\sqrt{x^2 + z^2}}\right)$$

Result is in full agreement with standard expressions used in micromagnetics codes.

Example Computations

- Consider two bar magnets (rectangular prisms). The first magnet has dimensions 24 x 12 x 12 and is uniformly magnetized along the x-axis. The second magnet is smaller (16 x 2 x 2) and is allowed to move in the x-y plane. Its magnetization is along the longest axis. The question to be answered is then: for each location in the x-y plane, what is the orientation of the second magnet for which the interaction energy is minimized?

- 3D computation, using a 256 x 256 x 256 voxel grid, and the analytical expression for the shape amplitude of a rectangular prism.



60
40
20
0
−20
−40
−60
−60
−40
−20
0
20
40
60

Broader Interpretation

- Magnetic particles interact through the dipolar interaction, which is represented by the dipolar tensor.

- Perhaps it is possible to replace the dipolar tensor by another interaction function to describe other physical interactions between particles of arbitrary shape...

$$\mathcal{N}^{\alpha\beta}(\boldsymbol{\rho}) = \frac{1}{V_1 V_2}\mathcal{C}(\boldsymbol{\rho}) \otimes \mathcal{D}^{\alpha\beta}(\boldsymbol{\rho})$$

Interaction "kernel"

$$\mathcal{N}^{\alpha}(\boldsymbol{\rho}) = C_{12}\mathcal{C}(\boldsymbol{\rho}) \otimes \mathcal{D}^{\alpha}(\boldsymbol{\rho})$$

Applications to Gravitation

- Gravitational potential satisfies Poisson's equation:

$$\nabla^2\Phi(\mathbf{r}) = 4\pi G\rho(\mathbf{r})$$

- Solution for uniform mass density and arbitrary shape:

$$\Phi(\mathbf{r}) = -G\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}' = -G\rho\int \frac{D(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}'$$

- Using the Fourier space approach this leads to:

$$\Phi(\mathbf{r}) = -\frac{G\rho}{2\pi^2}\int \mathrm{d}\mathbf{k}\,\frac{D(\mathbf{k})}{k^2}e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}.$$

- and also, for the gravitational field:

$$\mathbf{g}(\mathbf{r}) = \frac{\mathrm{i}G\rho}{2\pi^2}\int \mathrm{d}\mathbf{k}\,D(\mathbf{k})\,\frac{\mathbf{k}}{k^2}e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$

- Obviously, the same is valid for electrostatic problems...

What about gravitational interactions?

- Interaction energy between two arbitrary bodies:

$$E(\mathbf{r},\mathbf{r}') = -G \iiint_{V_1} \mathrm{d}\mathbf{r} \iiint_{V_2} \mathrm{d}\mathbf{r}' \, \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

- For uniform mass density we find:

$$\begin{aligned} E(\mathbf{r},\mathbf{r}') &= -G\rho_1\rho_2 \iiint_{V_1} \mathrm{d}\mathbf{r} D_1(\mathbf{r}) \iiint_{V_2} \mathrm{d}\mathbf{r}' \, \frac{D_2(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ &= -\frac{G\rho_1\rho_2}{8\pi^3} \iiint_{V_1} \mathrm{d}\mathbf{r} D_1(\mathbf{r}) \iiint \mathrm{d}\mathbf{k} \frac{D_2(\mathbf{k})}{k^2} e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \\ &= -\frac{G\rho_1\rho_2}{8\pi^3} \iiint \mathrm{d}\mathbf{k} \frac{D_1^*(\mathbf{k}) D_2(\mathbf{k})}{k^2} \end{aligned}$$

$$E(\boldsymbol{\rho}) = -G\rho_1\rho_2 \mathcal{C}(\boldsymbol{\rho}) \otimes \frac{1}{|\boldsymbol{\rho}|}$$

General interactions

- What we learn from this is that interactions between uniform bodies of arbitrary shape can be written in terms of the shape cross-correlation function and an interaction-dependent kernel, which, in Fourier space, takes on a form of the type:

$$\frac{1}{k^2}$$ for electrostatic, gravitational, ...

$$\frac{k^\alpha k^\beta}{k^2}$$ for dipolar

$$\frac{1}{k^2 - \kappa^2}$$ for a Yukawa-type interaction $\frac{e^{-\kappa r}}{r}$

...

question: Do all factors of this form correspond to physical interactions?

$$\frac{k^\alpha k^\beta k^\gamma}{|\mathbf{k}|^4} \longrightarrow \frac{i\pi^2}{2r^5}\left[r^2\left\{r^\alpha[3\delta^{\alpha\beta}\delta^{\alpha\gamma} + \delta^{\beta\gamma}] + r^\beta[3\delta^{\beta\gamma}\delta^{\beta\alpha} + \delta^{\gamma\alpha}] + r^\gamma[3\delta^{\gamma\alpha}\delta^{\gamma\beta} + \delta^{\alpha\beta}]\right\} - 3r^\alpha r^\beta r^\gamma\right]$$

What about surfaces ?

- Many physical quantities involve integrations over the surface of the object. Could the shape function formalism be used for such problems?
- In other words, is there a "function" related to the shape function that describes the surface?
  - preliminary work shows that the gradient of the shape function results in the unit surface normal...

Surface Normal

$$\begin{aligned}\nabla D(\mathbf{r}) &= \mathcal{F}^{-1}\left[\mathcal{F}[\nabla D(\mathbf{r})]\right] \\ &= -\mathcal{F}^{-1}\left[\mathrm{i}\mathbf{k}D(\mathbf{k})\right]; \\ &= -\frac{\mathrm{i}}{8\pi^3}\iiint \mathrm{d}\mathbf{k}\,\mathbf{k}D(\mathbf{k})e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \qquad = \hat{\mathbf{n}}_S(\mathbf{r})\end{aligned}$$

Explicit computation for a sphere results in the outward unit normal on the surface.

The surface itself can then be described by the norm of this vector, which results in a discontinuous "function" which vanishes everywhere except on the surface where it is unity...

$$S(\mathbf{r}) \equiv \sqrt{(\hat{\mathbf{n}}\cdot\hat{\mathbf{n}})(\mathbf{r})} = |\nabla D(\mathbf{r})|$$

Numerical work shows that this is correct, but the theory needs to be done "properly", using the theory of generalized functions (distribution theory).

Moment of Inertia Tensor

- MOIT is defined as: $I_{ij} \equiv \rho \int_V \left(r^2\delta_{ij} - x_i x_j\right)\, \mathrm{d}V$
- example: $I_{zz} = \rho \int (x^2 + y^2) D(\mathbf{r})\, \mathrm{d}\mathbf{r}$

$$(x^2 + y^2) D(\mathbf{r}) = \mathcal{F}^{-1}\left[\mathcal{F}[x^2 + y^2] \otimes D(\mathbf{k})\right]$$

$$-\delta(k_z)\left[\delta(k_x)\delta''(k_y) + \delta(k_y)\delta(k_x)''\right]$$

Working out the convolution products we find:

$$I_{zz} = -\rho \left(\frac{\partial^2 D}{\partial k_x^2} + \frac{\partial^2 D}{\partial k_y^2} \right)\Bigg|_{\mathbf{k}=\mathbf{0}}$$

MOIT (continued)

- The full tensor is given by:

$$I_{ij} = -\rho \begin{pmatrix} H^D_{yy}(\mathbf{0}) + H^D_{zz}(\mathbf{0}) & H^D_{xy}(\mathbf{0}) & H^D_{xz}(\mathbf{0}) \\ H^D_{xy}(\mathbf{0}) & H^D_{xx}(\mathbf{0}) + H^D_{zz}(\mathbf{0}) & H^D_{yz}(\mathbf{0}) \\ H^D_{xz}(\mathbf{0}) & H^D_{yz}(\mathbf{0}) & H^D_{xx}(\mathbf{0}) + H^D_{yy}(\mathbf{0}) \end{pmatrix}$$

$$H^D_{ij}(\mathbf{0}) \equiv \left.\frac{\partial^2 D(\mathbf{k})}{\partial k_i \partial k_j}\right|_{\mathbf{k}=\mathbf{0}}$$

Hessian matrix of D, evaluated in k=0

$$\boxed{I_{ij} = -\rho\left[\delta_{ij}\mathrm{Tr}[H^D_{ij}(\mathbf{0})] + (1-2\delta_{ij})H^D_{ij}(\mathbf{0})\right]}$$

We can do the same thing for the quadrupole tensor: $Q_{ij} = \rho_e \int_V (3x_i x_j - r^2\delta_{ij})\,\mathrm{d}\mathbf{r}$

$$\boxed{Q_{ij} = \rho_e\left[\delta_{ij}\mathrm{Tr}[H^D_{ij}(\mathbf{0})] - 3H^D_{ij}(\mathbf{0})\right]}$$

MOIT (continued)

- There is a relation between the MOIT and the quadrupole tensor:

$$\frac{Q_{ij}}{\rho_e} + \frac{I_{ij}}{\rho} = (2\delta_{ij} - 4)H_{ij}^{D}(\mathbf{0})$$

- This relation is valid for every shape. This was verified analytically for the sphere and numerically for a number of basic shapes.

Additional General Relations

- Consider the following relation:

$$s_n^{\alpha\beta} \equiv \mathcal{F}^{-1}\left[\frac{k^\alpha k^\beta}{|\mathbf{k}|^n}\right] = \frac{1}{8\pi^3}\iiint \mathrm{d}\mathbf{k}\,\frac{k^\alpha k^\beta}{|\mathbf{k}|^n}e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}.$$

- Integral converges for n=2, 3, and 4:

$$s_n^{\alpha\beta}(\mathbf{r}) = \frac{1}{C_n r^{7-n}}[r^2\delta^{\alpha\beta} - (5-n)r^\alpha r^\beta]$$

- For n=4, we have: $8\pi r^3 s_4^{\alpha\beta} = r^2\delta^{\alpha\beta} - r^\alpha r^\beta$

Integrand for MOIT !

$$I^{\alpha\beta} = \frac{\rho}{\pi^2}\iiint \mathrm{d}\mathbf{k}\,D_3^*(\mathbf{k})\frac{k^\alpha k^\beta}{|\mathbf{k}|^4}$$ with $$D_n(\mathbf{k}) = \iiint \mathrm{d}\mathbf{r}\,r^n D(\mathbf{r})e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$

Additional General Relations

- Similarly for the quadrupole tensor:

$$\frac{Q^{\alpha\beta}}{\rho_e} = -\frac{1}{2\pi^2}\iiint \mathrm{d}\mathbf{k}\, D_5^*(\mathbf{k})\,\frac{k^\alpha k^\beta}{|\mathbf{k}|^2}$$

- and an even more general relation:

$$\iiint \mathrm{d}\mathbf{k}\,\left(2\frac{D_3^*(\mathbf{k})}{|\mathbf{k}|^4} - \frac{D_5^*(\mathbf{k})}{|\mathbf{k}|^2}\right) k^\alpha k^\beta = \pi^2(4\delta^{\alpha\beta} - 8)H_D^{\alpha\beta}(\mathbf{0})$$

- again, valid for all shapes...

Conclusions

- Shape matters and can be correctly included in analytical formalism without approximations!
- The shape amplitude and its derivatives and moments appear to allow for general shape-independent statements or relations to be formulated.
- Fourier space shape formalism is accurate, flexible, and can be used for many other types of interactions...
  - electrostatics, gravitation, moment of inertia tensor, elasticity, ...
- Questions remain about the applicability of this formalism for quantities that depend on surface integrations rather than volume integrations. This research is currently ongoing...

The End