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:

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

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:

\[ \iiint_V f(r) \, dr = \iiint_{\text{all space}} D(r) f(r) \, dr \]

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:

\[ D(k) = \iiint_{\text{all space}} D(r) e^{-i k \cdot r} \, dr = \iiint_{V} e^{-i k \cdot r} \, dr \]

This is the only place where the actual shape information is used as integration boundaries.
Example Shape Amplitudes

Sphere: \[ D(k) = \frac{4\pi R^2}{k} j_1(kR) \]

Cylinder: \[ D(k) = \frac{4\pi R}{k_k k_z} \sin(dk_z) J_1(k_{\perp}R) \]

Facetted Objects: \[ D(k) = -\frac{1}{k'^2} \sum_{f=1}^{F} \frac{k \cdot n_f}{k'^2 - (k \cdot n_f)^2} \]
\[ \times \sum_{e=1}^{E_f} L_{fe} k \cdot n_{fe}\text{sinc}\left(\frac{L_{fe}}{2} k \cdot t_{fe}\right) e^{-i k \cdot \xi_{fe}^c} \]

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

- Tetrahedron
- Octahedron
- Rhombic dodecahedron
Magnetic Field and Energy of a dipole

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

\[ B(r) = \nabla \times A(r) \]

Permeability of vacuum \( \mu_0 \)

Magnetic Field

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

Magnetostatic Energy:

\[ E(r) = -\mu \cdot B = \frac{\mu_0}{4\pi} \left[ \frac{\mu_1 \cdot \mu_2}{|r|^3} - 3 \frac{(\mathbf{r} \cdot \mu_1)(\mathbf{r} \cdot \mu_2)}{|r|^5} \right] \]
Tensors in Magnetism

\[ E(r) = \frac{\mu_0}{4\pi} \left[ \frac{\mu_1 \cdot \mu_2}{r^3} - 3 \frac{(r \cdot \mu_1)(r \cdot \mu_2)}{r^5} \right] = \mu_0 \mu_1 : \mathbf{D}(r) : \mu_2 \]

Dipolar Tensor

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

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

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

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

\[ D^{\alpha \beta}(r) = \frac{1}{8\pi^3} \int \int \int dk \ \frac{k^\alpha k^\beta}{k^2} e^{ik \cdot r} \]

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 \( M(\mathbf{r}) \)

**Basic Equation:**

\[
A(\mathbf{r}) = \frac{\mu_0}{4\pi} \int M(\mathbf{r}') \times \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \, d\mathbf{r}'
\]

“convolution”

**Vector potential:**

\[
A(\mathbf{k}) = -i\mu_0 \frac{M(\mathbf{k}) \times \mathbf{k}}{k^2}
\]

vector cross product

**Fourier Transform of \( M(\mathbf{r}) \):**

\[
M(\mathbf{k}) = \int M(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}
\]

Includes shape information

**Magnetic Induction:**

\[
B(\mathbf{k}) = -i\mathbf{k} \times A(\mathbf{k})
\]

Nabla operator in Fourier Space

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

Demagnetization Field
Analytical Expressions

For a uniformly magnetized object:

\[
M(k) = M_0 \hat{m} D(k)
\]

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

Demagnetization Field

\[
H(r) = -\frac{M_0}{8\pi^3} \int d^3k \frac{D(k)}{k^2} k (\hat{m} \cdot k) e^{ik \cdot r}
\]

Demagnetization Tensor (point function)

\[
N^{\alpha\beta}(r) = \frac{1}{8\pi^3} \int d^3k \frac{k^\alpha k^\beta}{k^2} D(k) e^{ik \cdot r}
\]

Demagnetization Tensor (ballistic)

\[
\langle N \rangle^{\alpha\beta}(r) = \frac{1}{8\pi^3 V} \int d^3k \frac{k^\alpha k^\beta}{k^2} |D(k)|^2
\]

Demagnetization Energy

\[
E = \frac{\mu_0 M_0^2}{16\pi^3} \int d^3k \frac{|D(k)|^2}{k^2} (\hat{m} \cdot k)^2
\]
Demagnetization Tensor

\[
N^{\alpha \beta}(\mathbf{r}) = \frac{1}{8\pi^3} \int d^3k \frac{k^\alpha k^\beta}{k^2} D(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} \\
= \mathcal{F}^{-1} \left[ \mathcal{F}[D^{\alpha \beta}(\mathbf{r})] \mathcal{F}[D(\mathbf{r})] \right] \\
= D^{\alpha \beta}(\mathbf{r}) \otimes D(\mathbf{r})
\]

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:**

\[ \text{Tr}[N_{\alpha\beta}] = \frac{1}{8\pi^3} \int d^3k \frac{D(k)}{k^2} \sum_{\alpha=1}^{3} k^\alpha k^\alpha e^{ik \cdot r} = \frac{1}{8\pi^3} \int d^3k D(k) e^{ik \cdot r} = D(r) \]

**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:

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

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

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

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

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:

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

But:

\[ \langle N^{\alpha\beta} \rangle = \frac{1}{8\pi^3 V} \int dk \frac{k^\alpha k^\beta}{k^2} |D(k)|^2 \]  \hspace{1cm} \text{(Ballistic)}

No filter function needed!
A symmetric 3x3 matrix has 3 real eigenvalues and associated eigenvectors.

\[ \mathbf{N}_{ij} \rightarrow \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \]

Inside shape: \( \lambda_{1,2,3} > 0 \) → Ellipsoid

Outside shape: \( \lambda_1,2 > 0; \lambda_3 < 0 \) → Single Sheet Hyperboloid

Has eigenvectors as columns
Example: Demagnetization Tensor
More examples
More examples
Application to Electrostatics

A uniformly polarized particle has a potential:

\[ V(r) = \frac{1}{4\pi\varepsilon_0} \int dr' P(r') \cdot \frac{(r - r')}{|r - r'|^3} \]

and a resulting field (in Fourier space):

\[ E(k) = -ikV(k) = -\frac{P_0}{\varepsilon_0} D(k) \frac{\hat{p} \cdot k}{k^2} k \]

The electric displacement is then given by:

\[ D(r) = P - \frac{P_0}{8\pi^3} \int d^3k D(k) \frac{\hat{p} \cdot k}{k^2} k e^{ik \cdot r} \]

which results in:

\[ D_i = P_i + \varepsilon_0 E_i = P_i - N_{ij} P_j \]
Depolarization Energetics

The self-energy of a uniformly polarized particle:

\[ E_e = -\frac{1}{2} \int_V \mathbf{P} \cdot \mathbf{E} \, d^3r = \frac{P_0^2}{16\pi^3\varepsilon_0} \int d^3k \frac{|D(k)|^2}{k^2} (\hat{\mathbf{p}} \cdot \mathbf{k})^2 \]

SEM images of the faceted BaTiO\textsubscript{3} crystals after reaction with AgNO\textsubscript{3}.

The white contrast specks indicate silver metal deposits. (images G. Rohrer)
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How about interacting shapes?

Magnetostatic energy is generally defined as:

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

Converting to Fourier space for uniformly magnetized particles we find:

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

\[ \tilde{K}_d = \frac{1}{2} \mu_0 M_1 M_2 \]

\[ \rho \equiv \mathbf{R}_1 - \mathbf{R}_2 \] is the relative position of the particles

This expression can be rewritten as:

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

Using the convolution theorem, we find:

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

In this expression, we have introduced a new quantity:

\[ C(r) \equiv D_1(r) \otimes D_2(-r) \]

This is the cross-correlation of the shape functions.

Finally, we rewrite the energy in terms of a new tensor field:

\[ E_m(\rho; \hat{m}_1, \hat{m}_2) = 2\bar{K}_d V_1 V_2 m_1^\alpha N^{\alpha\beta}(\rho)m_2^\beta = \mu_0 \mu_1 : N(\rho) : \mu_2 \]

\[ N^{\alpha\beta}(\rho) = \frac{1}{V_1 V_2} C(\rho) \otimes D^{\alpha\beta}(\rho) \]
The Magnetometric Tensor Field

\[ E_m(\rho; \hat{m}_1, \hat{m}_2) = \mu_0 \mu_1 : N(\rho) : \mu_2 \]

This relation is similar to that for pure dipoles:

\[ E_m(\rho; \hat{m}_1, \hat{m}_2) = \mu_0 \mu_1 : D(\rho) : \mu_2 \]

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

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

\[ C(\rho_x, \rho_y, \rho_z) = (2a - |\rho_x|)(2b - |\rho_y|)(2c - |\rho_z|) \]

Magnetometric tensor element:

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

\[
= \frac{1}{32\pi a^3} \left[ 4H(\rho_x, \rho_y, \rho_z) + H(\rho_x, -1 - \rho_y, -1 + \rho_z) - 2H(\rho_x, \rho_y, -1 + \rho_z) + H(\rho_x, 1 - \rho_y, -1 - \rho_z) - H(\rho_x, -1 - \rho_y, 1 - \rho_z) - 2H(\rho_x, \rho_y, 1 + \rho_z) + H(\rho_x, 1 - \rho_y, 1 - \rho_z) - 2H(\bar{\rho}_x, -1 + \bar{\rho}_y, \bar{\rho}_z) - 2H(\bar{\rho}_x, 1 - \bar{\rho}_y, 1 - \bar{\rho}_z) \right]
\]

\[ H(x, y, z) = K(1 + x, y, z) - 2K(x, y, z) - K(-1 + x, y, z) \]

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

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

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.
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...

\[ N^{\alpha \beta}(\rho) = \frac{1}{V_1 V_2} C(\rho) \otimes D^{\alpha \beta}(\rho) \]

Interaction "kernel"

\[ N^\alpha(\rho) = C_{12} C(\rho) \otimes D^\alpha(\rho) \]
Applications to Gravitation

Gravitational potential satisfies Poisson’s equation:

\[ \nabla^2 \Phi(r) = 4\pi G \rho(r) \]

Solution for uniform mass density and arbitrary shape:

\[ \Phi(r) = -G \int \frac{\rho(r')}{|r - r'|} \, dr' = -G \rho \int \frac{D(r')}{|r - r'|} \, dr' \]

Using the Fourier space approach this leads to:

\[ \Phi(r) = -\frac{G \rho}{2\pi^2} \int dk \, \frac{D(k)}{k^2} e^{ik \cdot r} . \]

and also, for the gravitational field:

\[ g(r) = \frac{iG \rho}{2\pi^2} \int dk \, D(k) \frac{k}{k^2} e^{ik \cdot r} \]

Obviously, the same is valid for electrostatic problems...
What about gravitational interactions?

- Interaction energy between two arbitrary bodies:

\[
E(r, r') = -G \int \int \int_{V_1} \, dr \int \int \int_{V_2} \, dr' \frac{\rho(r)\rho(r')}{|r - r'|}
\]

- For uniform mass density we find:

\[
E(r, r') = -G \rho_1 \rho_2 \int \int \int_{V_1} \, dr D_1(r) \int \int \int_{V_2} \, dr' \frac{D_2(r')}{|r - r'|}
\]

\[
= -\frac{G \rho_1 \rho_2}{8\pi^3} \int \int \int_{V_1} \, dr D_1(r) \int \int \int \, dk \frac{D_2(k)}{k^2} e^{ik\cdot r}
\]

\[
= -\frac{G \rho_1 \rho_2}{8\pi^3} \int \int \int \, dk \frac{D_1^*(k)D_2(k)}{k^2}
\]

\[
E(\rho) = -G \rho_1 \rho_2 C(\rho) \otimes \frac{1}{|\rho|}
\]
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:

\[
\frac{1}{k^2} \quad \text{for electrostatic, gravitational, ...}
\]

\[
\frac{k_\alpha k_\beta}{k^4} \quad \text{for dipolar}
\]

\[
\frac{1}{k^2 - \kappa^2} \quad \text{for a Yukawa-type interaction} \quad \frac{e^{-\kappa r}}{r}
\]

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

\[ \nabla D(\mathbf{r}) = \mathcal{F}^{-1} \left[ \mathcal{F}[\nabla D(\mathbf{r})] \right] \]
\[ = -\mathcal{F}^{-1} \left[ i\mathbf{k} D(\mathbf{k}) \right] ; \]
\[ = -\frac{i}{8\pi^3} \int \int \int d\mathbf{k} \, \mathbf{k} D(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} = \mathbf{\hat{n}}_S(\mathbf{r}) \]

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...

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

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: \( I_{ij} \equiv \rho \int_V (r^2 \delta_{ij} - x_i x_j) \ dV \)

Example: \( I_{zz} = \rho \int (x^2 + y^2) D(\mathbf{r}) \ d\mathbf{r} \)

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

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

Working out the convolution products we find:

\[
I_{zz} = -\rho \left. \left( \frac{\partial^2 D}{\partial k_x^2} + \frac{\partial^2 D}{\partial k_y^2} \right) \right|_{k=0}
\]
The full tensor is given by:

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

\[ H^D_{ij}(0) \equiv \frac{\partial^2 D(k)}{\partial k_i \partial k_j} \bigg|_{k=0} \]

Hessian matrix of D, evaluated in k=0

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

We can do the same thing for the quadrupole tensor:

\[ Q_{ij} = \rho_e \int_V (3x_i x_j - r^2 \delta_{ij}) \, dr \]

\[ Q_{ij} = \rho_e \left[ \delta_{ij} \text{Tr}[H^D_{ij}(0)] - 3H^D_{ij}(0) \right] \]
There is a relation between the MOIT and the quadrupole tensor:

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

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:

\[ s_{n}^{\alpha\beta} \equiv \mathcal{F}^{-1} \left[ \frac{k^{\alpha} k^{\beta}}{|k|^n} \right] = \frac{1}{8\pi^3} \iiint dk \frac{k^{\alpha} k^{\beta}}{|k|^n} e^{ik \cdot r}. \]

Integral converges for \( n = 2, 3, \) and \( 4: \)

\[ s_{n}^{\alpha\beta}(r) = \frac{1}{C_n r^{7-n}} \left[ r^{2} \delta^{\alpha\beta} - (5 - n) r^{\alpha} r^{\beta} \right] \]

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!

\[ I^{\alpha\beta} = \frac{\rho}{\pi^2} \iiint dk \, D_{3}^{*}(k) \frac{k^{\alpha} k^{\beta}}{|k|^4} \quad \text{with} \quad D_{n}(k) = \iiint dr \, r^{n} D(r) e^{-ik \cdot r} \]
Additional General Relations

Similarly for the quadrupole tensor:

\[
\frac{Q_{\alpha\beta}}{\rho_e} = -\frac{1}{2\pi^2} \iiint \, dk \, D_5^*(k) \frac{k^{\alpha} k^{\beta}}{|k|^2}
\]

and an even more general relation:

\[
\iiint \, dk \left( 2 \frac{D_3^*(k)}{|k|^4} - \frac{D_5^*(k)}{|k|^2} \right) k^{\alpha} k^{\beta} = \pi^2 (4\delta^{\alpha\beta} - 8) H_D^{\alpha\beta}(0)
\]

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