Cartesian and spherical tensors for NLO

Today

Origin, meaning, and use of tensors and their properties

Spherical tensors and connection with angular momentum

Spherical tensors for NLO

Next time

Explicit calculations of transformation between Cartesian and spherical tensors

Applications to 3D nonlinear optical systems

Rick Lytel

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Reading list

Fundamentals

"Angular momentum in quantum mechanics," A.R. Edmonds (Princeton University Press 1996)

"Lectures on quantum mechanics," Steven Weinberg (Cambridge University Press 2013)

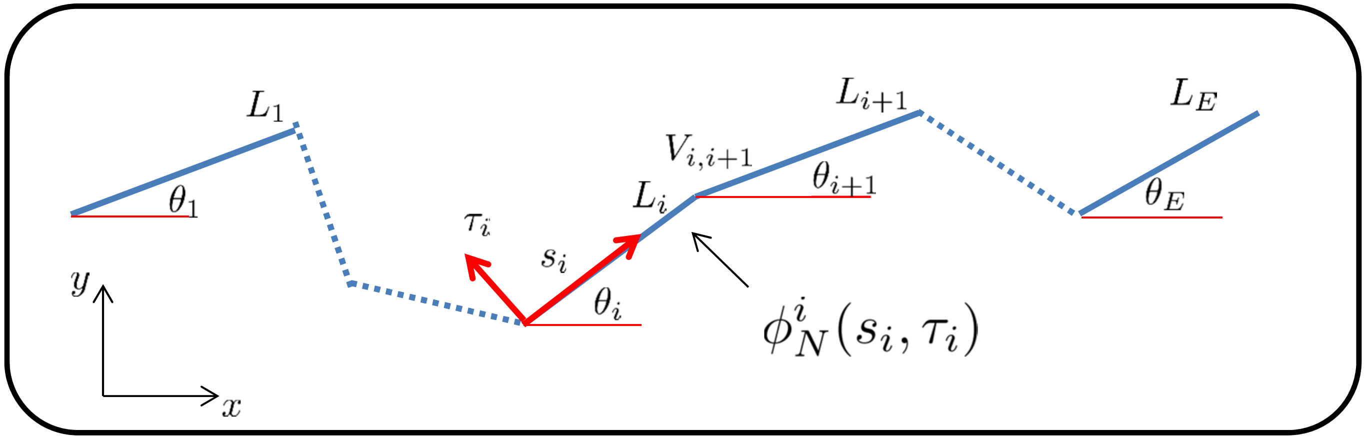
Applications

"The description of the physical properties of condensed matter using irreducible tensors," K. Jerphagnon, D. Chemla, and R. Bonneville, Advances in Physics 27, 609 (1978).

"Transformation between Cartesian and spherical tensors," A.J. Stone, Mol. Phys. 29, 1461 (1975).

" Influence of geometry and topology of quantum graphs on their nonlinear optical properties," Rick Lytel, Shoresh Shafei, Julian H. Smith, and Mark G. Kuzyk, Phys Rev A 87, 043824 (2013).

How to solve a quantum graph



$$H\phi_N^i(s_i, \tau_i) = E_N \phi_N^i(s_i, \tau_i)$$

$$At\ V_{i,i+1},\ \phi_N^i = \phi_N^{i+1},\ \partial\phi_N^i = \partial\phi_N^{i+1}$$

$$Union\ of\ \phi_N^i(s_i, \tau_i) \Rightarrow \psi_N(x, y)$$

$$f_{sec}(E_N; L_i, \theta_i) = 0 \Rightarrow E_N$$

$$H\psi_N(x, y) = E_N \psi_N(x, y)$$

- Eigenstates and eigenvalues
- Complete and orthonormal
- "A solved graph"

Monte Carlo simulation for NLO of quantum graphs

Select & connect vertices, solve for edge functions and energies

$$H\phi_N^i(s_i,\tau_i) = E_N\phi_N^i(s_i,\tau_i)$$

Calculate transition moments in graph's frame

$$r_{NM} = \sum_{i=1}^{E}\int_i ds_i \; r(s_i)\phi_N^{*i}(s_i)\phi_M^i(s_i)$$

Calculate the first hyperpolarizability tensor β_{ijk}

$$\beta_{ijk} = -.5e^3 P_{ijk} \sum_{n,m}{}' \frac{r_{0n}^i \bar{r}_{nm}^j r_{m0}^k}{E_{n0}E_{m0}}$$

Normalize to the fundamental limit

$$\beta_{max} = 3^{1/4}\left(\frac{e\hbar}{\sqrt{m}}\right)^3\left(\frac{N^{3/2}}{E_{10}^{7/2}}\right) \longrightarrow -1 \le \beta_{int} \equiv \frac{\beta}{\beta_{max}} \le 1$$

Which orientation of the graph has the largest β_{xxx} in the lab frame?

How does β_{xxx} change as the graph is rotated?

How does this change depend upon the shape of the graph?

Monte Carlo simulation for NLO of quantum graphs

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Calculate the angle that gives the max value of β_{xxx} in the lab frame, and rotate to that frame

$$\begin{aligned}\beta_{xxx}(\theta) &= \beta_{xxx}\cos^3\theta + 3\beta_{xxy}\cos^2\theta\sin\theta \\ &+ 3\beta_{xyy}\cos\theta\sin^2\theta + \beta_{yyy}\sin^3\theta\end{aligned}$$

Calculate the invariant tensor norm to find the allowable extreme values of the topology

$$|\beta| = \sqrt{\beta_{xxx}^2 + 3\beta_{xxy}^2 + 3\beta_{xyy}^2 + \beta_{yyy}^2}$$

Rotation group (2D example)

Length-preserving, unitary spatial transformations

$$\vec{r} \rightarrow \vec{r}' = R(\theta)\vec{r} \qquad r_i' = R_{ij} r_j \qquad R(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

$R(\theta)R^\dagger(\theta) = 1$ **and** $R(\theta)R^{-1}(\theta) = 1$

Group property

If $R(\theta_1) = \begin{bmatrix} \cos\theta_1 & \sin\theta_1 \\ -\sin\theta_1 & \cos\theta_1 \end{bmatrix}$ **and** $R(\theta_2) = \begin{bmatrix} \cos\theta_2 & \sin\theta_2 \\ -\sin\theta_2 & \cos\theta_2 \end{bmatrix}$

then

$$\begin{aligned} R(\theta_1 + \theta_2) &= \begin{bmatrix} \cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2 & \sin\theta_1\cos\theta_2 + \cos\theta_1\sin\theta_2 \\ -\sin\theta_1\cos\theta_2 - \cos\theta_1\sin\theta_2 & \cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2 \end{bmatrix} \\ &= \begin{bmatrix} \cos(\theta_1+\theta_2) & \sin(\theta_1+\theta_2) \\ -\sin(\theta_1+\theta_2) & \cos(\theta_1+\theta_2) \end{bmatrix} \\ &= R(\theta_1)R(\theta_2) \end{aligned}$$

Cartesian tensor transformations

Definition of an Nth rank Cartesian tensor:

$$T_{i_1 i_2 \ldots i_n} \to T'_{i_1 i_2 \ldots i_n} = R_{i_1 j_1} R_{i_2 j_2} \ldots R_{i_n j_n} T_{j_1 j_2 \ldots j_n}$$

Each index 'rotates' like a vector

But rotation group has the property that:

$$R^\dagger R = 1 \Rightarrow det(R)det(R^\dagger) = det(R)^2 = 1 \Rightarrow det(R) = \pm 1$$

Det(R) = 1 for special orthogonal group of rotations SO(N)
Det(R) = -1 for inversions

$$R^\dagger(\theta) = R^{-1}(\theta) \Rightarrow R_{ij} = R^{-1}_{ji} \Rightarrow R_{ij} R_{ik} = R^{-1}_{ji} R_{ik} = \delta_{jk}$$

So the length of a vector is preserved

$$\vec{r}' \cdot \vec{r}' \equiv r'_i r'_i = R_{ij} r_j R_{ik} r_k = R^{-1}_{ji} R_{ik} r_j r_k = \delta_{jk} r_j r_k = \vec{r} \cdot \vec{r}$$

Contraction and reduction of tensors

Definition of an Nth rank Cartesian tensor:

$$T_{i_1 i_2 \dots i_n} \rightarrow T'_{i_1 i_2 \dots i_n} = R_{i_1 j_1} R_{i_2 j_2} \dots R_{i_n j_n} T_{j_1 j_2 \dots j_n}$$

with $R_{ij} = R_{ji}^{-1}$

Reduction of Nth rank tensor to (N-1)th rank tensor:

$$T_{i_1 i_2 \dots i_n} U_{i_n} \equiv W_{i_1 i_2 \dots i_{n-1}} \quad \Rightarrow$$

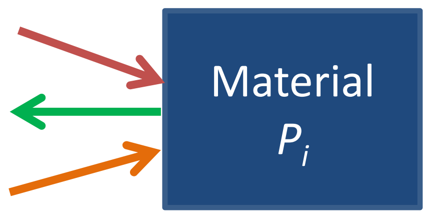
$$W_{i_1 i_2 \dots i_{n-1}} \rightarrow W'_{i_1 i_2 \dots i_{n-1}} = R_{i_1 j_1} R_{i_2 j_2} \dots R_{i_{n-1} j_{n-1}} W_{j_1 j_2 \dots j_{n-1}}$$

Tensor norms are invariant (for any rank):

$$\begin{aligned} T'_{i_1 i_2 \dots i_n} T'_{i_1 i_2 \dots i_n} &= R_{i_1 j_1} R_{i_2 j_2} \dots R_{i_n j_n} T_{j_1 j_2 \dots j_n} R_{i_1 k_1} R_{i_2 k_2} \dots R_{i_n k_n} T_{k_1 k_2 \dots k_n} \\ &= (R_{i_1 j_1} R_{i_1 k_1}) \dots (R_{i_n j_n} R_{i_n k_n}) T_{j_1 j_2 \dots j_n} T_{k_1 k_2 \dots k_n} \\ &= T_{k_1 k_2 \dots k_n} T_{k_1 k_2 \dots k_n} = invariant \end{aligned}$$

Nonlinear optics: Polarizability tensors

Optical fields E(ω)
On, near, off resonance
Multilevel transitions
"Light-by-light control"



Eigenstates $|N\rangle$ and energies E_N
Transition moments $\langle M|r^k|N\rangle$ etc
ΔE_{NM} , $\Delta\Gamma_{NM}$
Nonlinear response to E(ω)

$$P_i = \alpha_{ij}E_j + \beta_{ijk}E_jE_k + \gamma_{ijkl}E_jE_kE_l + \ \ldots$$

α = polarizability tensor

- birefringence
- Snell's law

β = first hyperpolarizability tensor

- 2nd harmonic gen
- EO effect

γ = second hyperpolarizability tensor

- phase conjugation
- optical bistability
- 3rd harmonic gen

Off-resonance tensors: Direct products of vectors

$$\beta_{ijk} = -\frac{e^3}{2}\sum_{n,m}{}' \frac{1}{E_{n0}E_{m0}}\left(r^i_{0n}\bar{r}^j_{nm}r^k_{m0} + r^i_{0n}\bar{r}^k_{nm}r^j_{m0} + r^k_{0n}\bar{r}^i_{nm}r^j_{m0} + h.c\right)$$

3rd rank Cartesian tensor

$$\beta_{max} = 3^{1/4}\left(\frac{e\hbar}{\sqrt{m}}\right)^3\left(\frac{N^{3/2}}{E_{10}^{7/2}}\right) \longrightarrow -1 \leq \beta_{int} \equiv \frac{\beta}{\beta_{max}} \leq 1$$

$$\gamma_{ijkl} = (1/6)P_{ijkl}\left(\sum_{n,m,l}{}' \frac{r^i_{0n}\bar{r}^j_{nm}\bar{r}^k_{ml}r^l_{l0}}{E_{n0}E_{m0}E_{l0}} - \sum_{n,m}{}' \frac{r^i_{0n}r^j_{n0}r^k_{0m}r^l_{m0}}{E^2_{n0}E_{m0}}\right)$$

4th rank Cartesian tensor

$$\gamma_{max} = 4\left(\frac{e^4\hbar^4}{m^2}\right)\left(\frac{N^2}{E^5_{10}}\right) \longrightarrow -1/4 \leq \gamma_{int} \equiv \frac{\gamma}{\gamma_{max}} \leq 1$$

Both tensors transform as products of vectors under the rotation group

Hyperpolarizability tensor norms (2D graphs)

Full contraction produces an invariant sum of eight independent components

$$|\beta|^2 \equiv \beta_{ijk}\beta_{ijk}$$

$$\beta'_{ijk} = R_{il}R_{jm}R_{kn}\beta_{lmn}$$

$$\begin{aligned}
|\beta'|^2 &= (R_{il}R_{jm}R_{kn}\beta_{lmn})\,(R_{ip}R_{jq}R_{kr}\beta_{pqr}) \\
&= (R_{il}R_{ip})(R_{jm}R_{jq})(R_{kn}R_{kr})\beta_{lmn}\beta_{pqr} \\
&= \delta_{lp}\delta_{mq}\delta_{nr}\beta_{lmn}\beta_{pqr} \\
&= \beta_{pqr}\beta_{pqr} \equiv |\beta|^2 = invariant
\end{aligned}$$

$$|\beta|^2 = \beta_{xxx}^2 + \beta_{xxy}^2 + \beta_{xyx}^2 + \beta_{yxx}^2 + \beta_{yyx}^2 + \beta_{yxy}^2 + \beta_{xyy}^2 + \beta_{yyy}^2$$

Full permutation symmetry reduces # independent components to four

$$\beta_{xxy} = \beta_{xyx} = \beta_{yxx} \; and \; \beta_{yyx} = \beta_{yxy} = \beta_{xyy} \Rightarrow |\beta|^2 = \beta_{xxx}^2 + 3\beta_{xxy}^2 + 3\beta_{yyx}^2 + \beta_{yyy}^2$$

$$|\beta| = \sqrt{\beta_{xxx}^2 + 3\beta_{xxy}^2 + 3\beta_{xyy}^2 + \beta_{yyy}^2}$$

Tensor norm (invariant under rotations of graph)

Frame transformation

Cartesian tensor transformation law

$$T_{i_1 i_2 \dots i_n} \rightarrow T'_{i_1 i_2 \dots i_n} = R_{i_1 j_1} R_{i_2 j_2} \dots R_{i_n j_n} T_{j_1 j_2 \dots j_n}$$

$$\begin{aligned}
\beta_{xxx}(\theta) &= R_{xl}(\theta) R_{xm}(\theta) R_{xn}(\theta) \beta_{lmn} \\
&= R_{xx} R_{xx} R_{xx} \beta_{xxx} + R_{xx} R_{xx} R_{xy} \beta_{xxy} + R_{xx} R_{xy} R_{xx} \beta_{xyx} + R_{xy} R_{xx} R_{xx} \beta_{yxx} \\
&+ R_{xx} R_{xy} R_{xy} \beta_{xyy} + R_{xy} R_{xx} R_{xy} \beta_{yxy} + R_{xy} R_{xy} R_{xx} \beta_{yyx} + R_{xy} R_{xy} R_{xy} \beta_{yyy} \\
&= \cos^3\theta \beta_{xxx} + \cos^2\theta \sin\theta (\beta_{xxy} + \beta_{xyx} + \beta_{yxx}) \\
&+ \cos\theta \sin^2\theta (\beta_{xyy} + \beta_{yyx} + \beta_{yxy}) + \sin^3\theta \beta_{yyy}
\end{aligned}$$

Full permutation symmetry reduces # independent components to four

$$\beta_{xxy} = \beta_{xyx} = \beta_{yxx} \ \ and \ \ \beta_{yyx} = \beta_{yxy} = \beta_{xyy}$$

$$\beta_{xxx}(\theta) = \cos^3\theta \beta_{xxx} + 3\cos^2\theta \sin\theta \beta_{xxy} + 3\cos\theta \sin^2\theta \beta_{xyy} + \sin^3\theta \beta_{yyy}$$

Summarizing, for 1st hyperpolarizability…

$$\beta_{ijk} = -\frac{e^3}{2}{\sum_{n,m}}' \frac{1}{E_{n0}E_{m0}} \left(r^i_{0n}\bar{r}^j_{nm}r^k_{m0} + r^i_{0n}\bar{r}^k_{nm}r^j_{m0} + r^k_{0n}\bar{r}^i_{nm}r^j_{m0} + h.c \right)$$

Fully symmetric 3rd rank Cartesian tensor

$$\begin{aligned}\beta_{xxx}(\theta) &= \beta_{xxx}\cos^3\theta + 3\beta_{xxy}\cos^2\theta\sin\theta \\ &+ 3\beta_{xyy}\cos\theta\sin^2\theta + \beta_{yyy}\sin^3\theta\end{aligned}$$

Four independent components relating lab and graph frames

$$|\beta| = \sqrt{\beta^2_{xxx} + 3\beta^2_{xxy} + 3\beta^2_{xyy} + \beta^2_{yyy}}$$

Tensor norm (invariant under rotations of graph)

$$\beta_{max} = 3^{1/4}\left(\frac{e\hbar}{\sqrt{m}}\right)^3\left(\frac{N^{3/2}}{E^{7/2}_{10}}\right) \longrightarrow -1 \le \beta_{int} \equiv \frac{\beta}{\beta_{max}} \le 1$$

Normalization for scale-invariant calculations

Summarizing, for 2nd hyperpolarizability…

$$\gamma_{ijkl} = (1/6)P_{ijkl}\left(\sum_{n,m,l}{}' \frac{r^i_{0n}\bar{r}^j_{nm}\bar{r}^k_{ml}r^l_{l0}}{E_{n0}E_{m0}E_{l0}} - \sum_{n,m}{}' \frac{r^i_{0n}r^j_{n0}r^k_{0m}r^l_{m0}}{E^2_{n0}E_{m0}}\right)$$

Fully symmetric 4th rank Cartesian tensor

$$\begin{aligned}\gamma_{xxxx}(\theta) &= \gamma_{xxxx}\cos^4\theta + 4\gamma_{xxxy}\cos^3\theta\sin\theta \\ &+ 6\gamma_{xxyy}\cos^2\theta\sin^2\theta + 4\gamma_{xyyy}\cos\theta\sin^3\theta \\ &+ \gamma_{yyyy}\sin^4\theta\end{aligned}$$

Five independent components relating lab and graph frames

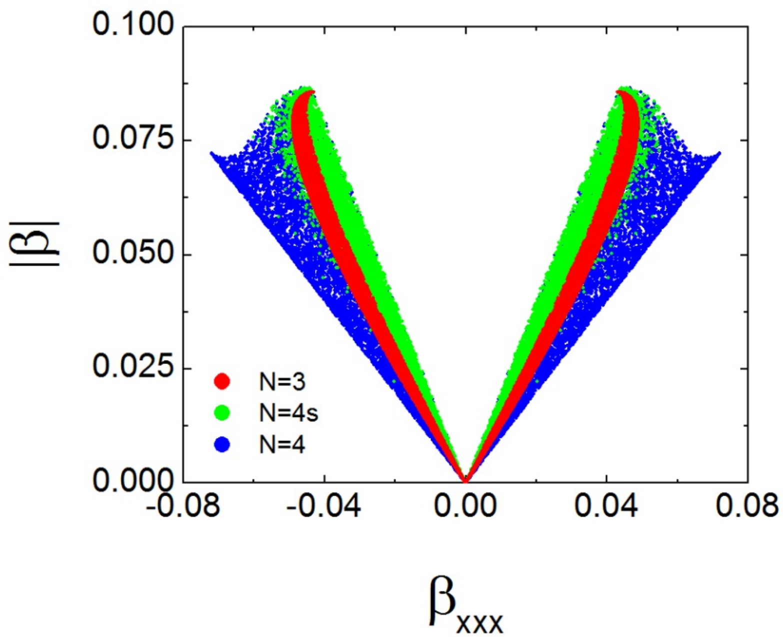
$$|\gamma| = \sqrt{\gamma^2_{xxxx} + 4\gamma^2_{xxxy} + 6\gamma^2_{xxyy} + 4\gamma_{xyyy} + \gamma^2_{yyyy}}$$

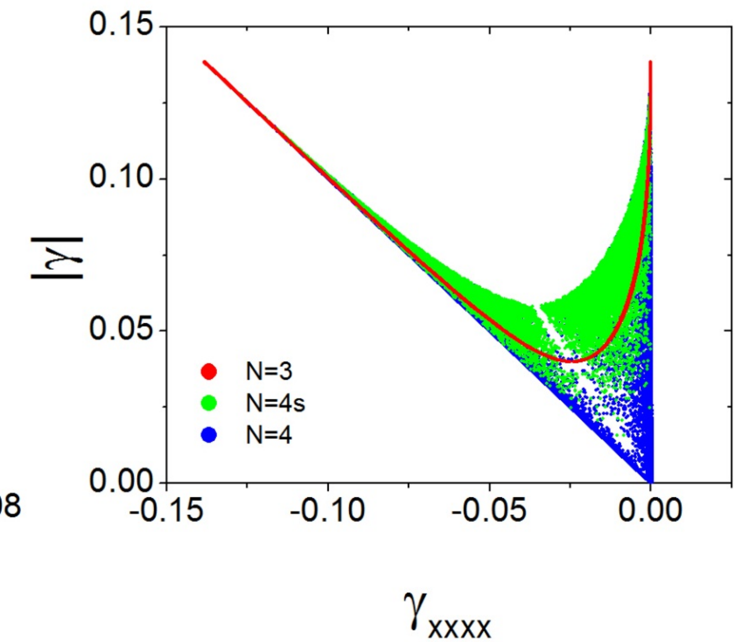
Tensor norm (invariant under rotations of graph)

$$\gamma_{max} = 4\left(\frac{e^4\hbar^4}{m^2}\right)\left(\frac{N^2}{E^5_{10}}\right) \longrightarrow -1/4 \leq \gamma_{int} \equiv \frac{\gamma}{\gamma_{max}} \leq 1$$

Normalization for scale-invariant calculations

Application: Tensor norms for triangle quantum graphs

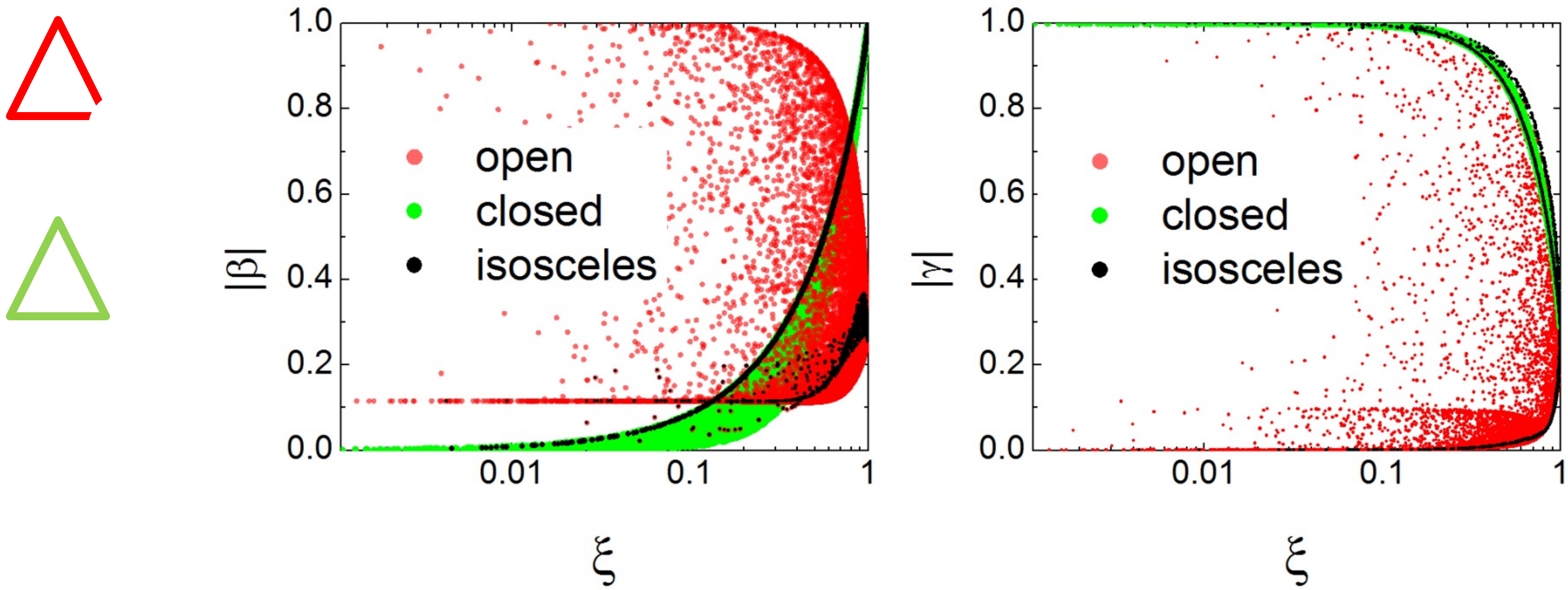




- **3-sided loop is highly constrained and has $\beta_{xxx} << |\beta|$**
- **Additional degrees of freedom open up ranges of hyperpolarizabilities**
- **There is no obvious shape information in these plots**

Extracting shape information from tensor norms

(NOTE: $|\beta|$ and $|\gamma|$ below are both normalized to unity)



- For triangle loops, norms vs area-to-perimeter ratios yield shape info
- Closed-loop triangles have maximum $|\beta|$ when they are ~ equilateral
- Not very satisfying view of the impact of shape on tensor properties

But we still need a general way to relate shape to response

Rotations in quantum mechanics

Angular momentum J generates rotations

$$\Psi \rightarrow \Psi^{'} = U(R)\Psi \qquad U(R) = 1 + \frac{\imath\epsilon \mathbf{J}\cdot\mathbf{n}}{\hbar}$$

$$\Psi \rightarrow U(R_2)U(R_1)\Psi \equiv U(R_2R_1)\Psi \Rightarrow U(R_2)U(R_1) = U(R_2R_1)$$

How do vector *operators* V rotate? V could be x, p, L, etc.

$v_i^{'} = R_{ij}v_j$ **where** $\vec{v} =< \Psi|\mathbf{V}|\Psi >$ **Complex numbers, not operators**

so

$$< \Psi^{'}|\mathbf{V}_i|\Psi^{'} >=< \Psi|U(R^{-1})|\mathbf{V}_i|U(R)|\Psi >= R_{ij} < \Psi|\mathbf{V}_j|\Psi >$$

so

$$U^{-1}(R)\mathbf{V}_iU(R) = \sum_j R_{ij}\mathbf{V}_j$$ **or equivalently,** $$U(R)\mathbf{V}_iU^{-1}(R) = \sum_j R_{ji}\mathbf{V}_j$$

Generalizing, we get for an nth rank Cartesian tensor *operator*

$$U(R)\mathbf{T}_{i_1i_2..i_n}U^{-1}(R) = \sum_{j_1,j_2..j_n} R_{j_1i_1}R_{j_2i_2}..R_{j_ni_n}\mathbf{T}_{j_1j_2..j_n}$$

Commutation relations among rotation generators and operators

Action of rotations on vector operator

$$U^{-1}(R)\mathbf{V}_i U(R) = \sum_j R_{ij}\mathbf{V}_j$$ **where** $$U(R) = 1 + \frac{\imath\epsilon \mathbf{J}\cdot\mathbf{n}}{\hbar}$$

e.g., for a rotation about z-axis: $$R(\epsilon) \approx \begin{bmatrix} 1-\epsilon^2/2 & \epsilon & 0 \\ -\epsilon & 1-\epsilon^2/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

so

$$\left(1 - \frac{\imath\epsilon J_z}{\hbar}\right)\begin{bmatrix} \mathbf{V}_x \\ \mathbf{V}_y \\ \mathbf{V}_z \end{bmatrix}\left(1 + \frac{\imath\epsilon J_z}{\hbar}\right) = \begin{bmatrix} \mathbf{V}_x + \epsilon\mathbf{V}_y \\ \mathbf{V}_y - \epsilon\mathbf{V}_x \\ \mathbf{V}_z \end{bmatrix}$$

so $$[\mathbf{V}_i, \mathbf{J}_j] = \imath\epsilon_{ijk}\mathbf{V}_k$$ **or equivalently,** $$[\mathbf{J}_i, \mathbf{V}_j] = \imath\epsilon_{ijk}\mathbf{V}_k$$

Action of rotations on tensor operator

$$U^{-1}(R)\mathbf{T}_{ij}U(R) = \sum_{kl} R_{ik}R_{jl}\mathbf{T}_{kl}$$

Representations

Definition of an Nth rank Cartesian tensor:

$$T_{i_1 i_2 \ldots i_n} \to T^{'}_{i_1 i_2 \ldots i_n} = R_{i_1 j_1} R_{i_2 j_2} \ldots R_{i_n j_n} T_{j_1 j_2 \ldots j_n}$$

In general, Cartesian tensors are reducible:

$$T_{ij} = U_i V_j$$

$$T_{ij} = \frac{\mathbf{U} \cdot \mathbf{V}}{3} \delta_{ij} + \frac{U_i V_j - U_j V_i}{2} + \left(\frac{U_i V_j + U_j V_i}{2} - \frac{\mathbf{U} \cdot \mathbf{V}}{3} \delta_{ij} \right)$$

scalar under rotations — **antisymmetric under rotations** — **symmetric & traceless under rotations**

$$1 \bigotimes 1 = 0 \bigoplus 1 \bigoplus 2$$

Irreducible subsets transform among themselves

[2(1)+1][2(1)+1] = [2(0)+1] + [2(1)+1] + [2(2)+1]

Looks like the multiplicities for addition of two J=1 angular momentum states!

Addition of angular momenta

Addition of angular momenta

$$|j_1 j_2 j m >= \sum_{m_1=-j_1}^{m_1=+j_1} \sum_{m_2=-j_2}^{m_2=+j_2} < j_1 m_1 j_2 m_2 | j_1 j_2 j m > |j_1 m_1 j_2 m_2 >$$

Clebsch-Gordan coefficients

$$|j_1 - j_2| \leq j \leq |j_1 + j_2| \qquad m = m_1 + m_2$$

Direct product of two kets has a scalar, axial vector, and traceless tensor component

$$j_1 = 1, j_2 = 1 \Rightarrow j = 0, 1, 2$$

$$1 \bigotimes 1 = 0 \bigoplus 1 \bigoplus 2$$

This is identical to the irreducible representation of rotation group for 2nd rank tensor!

Spherical tensors: Irreducible reps of SO(3) that transform like angular momenta

Spherical tensor operator

$$D^{-1}(R)\mathbf{T}_q^{(k)}D(R) = \sum_{q'=-k}^{k} D_{qq'}^{(k)}(R)\mathbf{T}_{q'}^{(k)}$$

$$D_{qq'}^{(k)}(R) =< kq|D(R)|kq' >$$

$$[\mathbf{J}_z, \mathbf{T}_q^{(k)}] = \hbar q \mathbf{T}_q^{(k)}$$

$$D(R) = 1 + \frac{\imath\epsilon\mathbf{J}\cdot\mathbf{n}}{\hbar}$$

$$[\mathbf{J}_\pm, \mathbf{T}_q^{(k)}] = \hbar\sqrt{(k \mp q)(k \pm q + 1)}\mathbf{T}_{q\pm 1}^{(k)}$$

Cartesian tensor operator

$$U^{-1}(R)\mathbf{V}_i U(R) = \sum_j R_{ij}\mathbf{V}_j$$

$$U(R) = 1 + \frac{\imath\epsilon\mathbf{J}\cdot\mathbf{n}}{\hbar}$$

$$[\mathbf{J}_i, \mathbf{V}_j] = \imath\epsilon_{ijk}\mathbf{V}_k$$

Example: Rank k=1 spherical tensors for 1st rank Cartesian tensor (ie, a vector)

Define spherical components T of a vector operator V

$$T_0^{(1)} = V_z \qquad T_{\pm 1}^{(1)} = \mp \frac{V_x \pm \imath V_y}{\sqrt{2}}$$

with $[\mathbf{J}_i, \mathbf{V}_j] = \imath \epsilon_{ijk} \mathbf{V}_k$

Then T is a rank 1 spherical tensor:

$$[\mathbf{J}_z, \mathbf{T}_q^{(1)}] = \hbar q \mathbf{T}_q^{(1)}$$

$$[\mathbf{J}_\pm, \mathbf{T}_q^{(1)}] = \hbar \sqrt{(1 \mp q)(1 \pm q + 1)} \mathbf{T}_{q \pm 1}^{(1)}$$

The explicit expansion is:

$$T_q^{(1)} = \sum_i < i | 1q > V_i$$

$$\begin{array}{cc} & \begin{array}{ccc} |11> & |10> & |1-1> \end{array} \\ \begin{array}{c} <x| \\ <y| \\ <z| \end{array} & \begin{bmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{-\imath}{\sqrt{2}} & 0 & \frac{-\imath}{\sqrt{2}} \\ 0 & 1 & 0 \end{bmatrix} \end{array}$$

Example: Rank k=2 spherical tensors for 2nd rank Cartesian tensor

$$T_{ij} = \frac{\mathbf{U}\cdot\mathbf{V}}{3}\delta_{ij} + \frac{U_iV_j - U_jV_i}{2} + \left(\frac{U_iV_j + U_jV_i}{2} - \frac{\mathbf{U}\cdot\mathbf{V}}{3}\delta_{ij}\right)$$

scalar under rotations

antisymmetric under rotations

symmetric & traceless under rotations

$$1 \bigotimes 1 = 0 \bigoplus 1 \bigoplus 2$$

Define rank 1 spherical components of U and V

$$U_0 = U_z \qquad U_{\pm1} = \mp\frac{U_x \pm \imath U_y}{\sqrt{2}}$$

$$V_0 = V_z \qquad V_{\pm1} = \mp\frac{V_x \pm \imath V_y}{\sqrt{2}}$$

$$[\mathbf{J}_i, \mathbf{U}_j] = \imath\epsilon_{ijk}\mathbf{U}_k \quad [\mathbf{J}_i, \mathbf{V}_j] = \imath\epsilon_{ijk}\mathbf{V}_k$$

$$[\mathbf{J}_z, \mathbf{T}_q^{(k)}] = \hbar q \mathbf{T}_q^{(k)}$$

$$[\mathbf{J}_\pm, \mathbf{T}_q^{(1)}] = \hbar\sqrt{(1\mp q)(1\pm q+1)}\mathbf{T}_{q\pm1}^{(1)}$$

Then the J=0,1, 2 spherical tensors are:

$$T_0^{(0)} = -\frac{\mathbf{U}\cdot\mathbf{V}}{3} = \frac{U_{+1}V_{-1} + U_{-1}V_{+1} - U_0V_0}{3}$$

$$T_q^{(1)} = \frac{(\mathbf{U}\times\mathbf{V})_q}{\imath\sqrt{2}}$$

$$T_{\pm2}^{(2)} = U_{\pm1}V_{\pm1}$$

$$T_{\pm1}^{(2)} = \frac{U_{\pm1}V_0 + U_0V_{\pm1}}{\sqrt{2}}$$

$$T_0^{(2)} = \frac{U_{+1}V_{-1} + 2U_0V_0 + U_{-1}V_{+1}}{\sqrt{6}}$$

Cartesian to spherical tensor conversion

First, convert each Cartesian component to its reducible spherical form for J=1

$$T^J_{m_1 m_2 .. m_n} = < i_1 | 1 m_1 > < i_2 | 1 m_2 > .. < i_n | 1 m_n > T_{i_1 i_2 ... i_n}$$

Then form the irreducible spherical tensors by adding angular momenta

$$T^J_M = \sum_{m_1=-1}^{1} ... \sum_{m_n=-1}^{1} < 1 m_1 1 m_2 .. 1 m_n | JM > T^J_{m_1 m_2 .. m_n}$$

The final form is a direct transformation from Cartesian space to an irreducible angular momentum defined by J

$$T^J_M = \sum_{i_1 i_2 .. i_n} < i_1 i_2 ... i_n | JM > T_{i_1 i_2 ... i_n}$$

Explicit calculation reduces to repeated addition of angular momenta

Spherical tensors for fully symmetric 3rd and 4th rank Cartesian tensors

$$|\beta| = \sqrt{\sum_{J=0}^{3} |\beta^J|^2}$$

$$\beta^J = \sqrt{\sum_{M=-J}^{J} |S_M^J|^2}$$

$$\begin{aligned}
S_{\pm1}^1 &= \sqrt{(3/10)}\,[\pm(\beta_{xxx}+\beta_{xyy}) + \imath(\beta_{yyy}+\beta_{xxy})] \\
S_{\pm1}^3 &= \sqrt{(3/40)}\,[\pm(\beta_{xxx}+\beta_{xyy}) + \imath(\beta_{yyy}+\beta_{xxy})] \\
S_{\pm3}^3 &= \sqrt{(1/8)}\,[\pm(-\beta_{xxx}+3\beta_{xyy}) + \imath(\beta_{yyy}-3\beta_{xxy})]
\end{aligned}$$

$$|\beta| = \sqrt{\beta_{xxx}^2 + 3\beta_{xxy}^2 + 3\beta_{xyy}^2 + \beta_{yyy}^2}$$

$$|\gamma| = \sqrt{\sum_{J=0}^{4} |\gamma^J|^2}$$

$$\gamma^J = \sqrt{\sum_{M=-J}^{J} |T_M^J|^2}$$

$$\begin{aligned}
T_0^0 &= \sqrt{(1/5)}\,[\gamma_{xxxx}+2\gamma_{xxyy}+\gamma_{yyyy}] \\
T_0^2 &= \sqrt{(1/7)}\,[\gamma_{xxxx}+2\gamma_{xxyy}+\gamma_{yyyy}] \\
T_{\pm2}^2 &= \sqrt{(3/14)}\,[(-\gamma_{xxxx}+\gamma_{yyyy}) \mp 2\imath(\gamma_{xxxy}+\gamma_{xyyy})] \\
T_0^4 &= \sqrt{(9/280)}\,[\gamma_{xxxx}+2\gamma_{xxyy}+\gamma_{yyyy}] \\
T_{\pm2}^4 &= \sqrt{(1/28)}\,[(-\gamma_{xxxx}+\gamma_{yyyy}) \mp 2\imath(\gamma_{xxxy}+\gamma_{xyyy})] \\
T_{\pm4}^4 &= \sqrt{(1/4)}\,[(\gamma_{xxxx}-6\gamma_{xxyy}+\gamma_{yyyy}) \pm 4\imath(\gamma_{xxxy}-\gamma_{xyyy})]
\end{aligned}$$

$$|\gamma| = \sqrt{\gamma_{xxxx}^2 + 4\gamma_{xxxy}^2 + 6\gamma_{xxyy}^2 + 4\gamma_{xyyy} + \gamma_{yyyy}^2}$$

Spherical tensors for triangle quantum graphs